KAJIAN WAKTU DAN TEMPERATUR REAKSI OPTIMAL PADA SIFAT FISIKOKIMIA FMRE (*FUMARIC MODIFIED ROSIN ESTER*)

Skripsi

disusun sebagai salah satu syarat penyelesaian Studi Strata Satu
untuk mencapai gelar Sarjana Sains
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2020

PERNYATAAN KEASLIAN SKRIPSI

Dengan ini, saya

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menyatakan bahwa skripsi saya yang berjudul "Kajian Waktu dan Temperatur Reaksi Optimal pada Sifat Fisikokimia FMRE (*Fumaric Modified Rosin Ester*)" benar-benar karya saya sendiri bukan jiplakan dari karya orang lain atau pengutipan dengan cara-cara yang tidak sesuai dengan etika keilmuan yang berlaku baik sebagian atau seluruhnya. Pendapat atau temuan orang atau pihak lain yang terdapat dalam skripsi ini telah dikutip atau dirujuk berdasarkan kode etik ilmiah. Atas pernyataan ini, saya secara pribadi siap menanggung resiko/sanksi hukum yang dijatuhkan apabila ditemukan adanya pelanggaran terhadap etika keilmuan dalam karya ini.

Semarang, 11 Februari 2020

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PENGESAHAN

Skripsi berjudul Kajian Waktu Dan Temperatur Reaksi Optimal pada Sifat Fisikokimia FMRE (*Fumaric Modified Rosin Ester*) karya Naila Furhatin 4311415065 ini telah dipertahankan dalam Ujian Skripsi FMIPA Universitas Negeri Semarang pada tanggal sidang dan disahkan oleh Panitia Ujian.

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MOTTO DAN PERSEMBAHAN

Motto

"Never trouble about trouble until trouble troubles you"
Banyak orang yang cenderung mempermasalahkan suatu masalah yang belum terjadi, bukannya menghadapi apa yang ada sekarang, justru meramalkan masa depan yang tidak diketahui pasti. Sikap seperti ini sama sekali tidak menguntunkan diri sendiri (Rosemary Kesauly).

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5. Teman-teman seperjuangan Mei, Jannah, Amrul dan teman-teman Kimia 2015.

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Semarang, 11 Februari 2020

Penulis

ABSTRAK

Furhatin, Naila. 2020. Kajian Waktu dan Temperatur Reaksi Optimal pada Sifat Fisikokimia FMRE (*Fumaric Modified Rosin Ester*). Skripsi. Jurusan Kimia Fakultas Matematika dan Ilmu Pengetahuan Alam Universitas Negeri Semarang. Pembimbing utama Dr. Nanik Wijayati, M. Si.

Kata kunci : FMRE, suhu, waktu reaksi, gliserol, asam fumarat, PTSA.

FMRE merupakan produk modifikasi dari gum rosin melalui proses esterifikasi yang bertujuan untuk memperbaiki sifat-sifatnya kearah yang lebih baik dari sifat asalnya. Dalam penelitian ini gum rosin diesterifikasi dengan asam fumarat dan gliserol dengan menggunakan PTSA (*p-toluene sulfonic acid*) sebagai katalis, dilakukan variasi suhu yaitu 140 °C, 160 °C, 180 °C, dan 200 °C serta variasi waktu reaksi 1, 2, 3, dan 4 jam. Hasil analisis GC-MS menunjukkan bahwa hasil esterifikasi FMRE optimum adalah pada suhu 200 °C dengan waktu reaksi 4 jam, total ester yang diperoleh yaitu sebesar 44,03%. Pengujian FT-IR menunjukkan bahwa gugus hidroksil telah berubah menjadi gugus karbonil yang menunjukkan gum rosin telah teresterifikasi. Terdapat serapan gugus karbonil ester pada bilangan gelombang sekitar 1700 cm^{-1} yang merupakan pita khas regangan C=O ester.

ABSTRACT

Furhatin, Naila. 2020. Optimation of Time and Temperature Reactions and their Physicochemical Properties of FMRE (*Fumaric Modified Rosin Ester*). Department of Chemistry Faculty of Mathematics and Natural Sciences, Universitas Negeri Semarang. Supervisor Dr. Nanik Wijayati, M. Si.

Key words: FMRE, temperature, reaction time, glycerol, fumaric acid, PTSA.

FMRE is a modified product of gum rosin through an esterification process aimed at improving its properties in a better direction than its original nature. In this research gum rosin is esterified with fumaric acid and glycerol by using PTSA (*p-Toluene sulphonic acid*) as a catalyst, performed temperature variations i.e. 140 °C, 160 °C, 180 °C and 200 °C and reaction time variations of 1, 2, 3 and 4 hours. The results of the GC-MS analysis showed that the results of the optimal esterification of FMRE is at a temperature of 200 ^{0} C with a reaction time of 4 hours, total ester obtained was equal to 44.03%. The FT-IR test indicates that the hydroxyl group has been transformed into the carbonyl which indicates that gum rosin has been esterified. There is an absorption of the carbonyl ester group at wavenumber 1700 cm^{-1} which is a typical ribbon strain of C = O ester.

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BAB I
PENDAHULUAN

1.1 Latar Belakang

Hutan Indonesia memiliki potensi yang sangat besar, luasnya mencapai 99,6 juta atau 52,3% dari luas wiayah Indonesia. Sumber daya hutan merupakan kekayaan alam yang dapat memberikan manfaat ekonomi, lingkungan, dan sosial bagi kesejahteraan manusia. Hasil hutan bukan kayu dengan jenis dan potensi yang sangat melimpah di hutan dapat memiliki peran yang lebih penting dibandingkan produk-produk kayu (Wiyono *et al*., 2007). Saat ini pemerintah Indonesia mengurangi produk hasil hutan kayu, dengan demikian pemerintah sedang memaksimalkan produk hasil hutan bukan kayu (HHBK) (Daryono, 2015). Pemanfaatan hasil hutan bukan kayu (HHBK) bertujuan selain untuk meningkatkan kesejahteraan masyarakat juga untuk mengoptimalkan sumber daya hutan itu sendiri. Industri hasil hutan bukan kayu (HHBK) tidak memerlukan teknologi yang canggih, namun mampu menghasilkan produk yang memiliki nilai ekonomi tinggi dan juga ramah lingkungan (Waluyo *et al*., 2012).

Getah pinus merupakan salah satu hasil hutan bukan kayu (HHBK) yang bernilai komersial dan potensial untuk dikembangkan saat ini. Getah pinus merupakan hasil penyadapan dari pohon yang tergolong dalam marga *Pinus* khususnya jenis *Pinus merkusii. Pinus merkusii* merupakan sumber penghasil getah pinus yang digunakan untuk menghasilkan minyak terpentin dan gum rosin. Gum rosin dan terpentin merupakan salah satu produk turunan dari getah pinus yang sudah masuk dalam sistem perdagangan internasional. Perdagangan gum rosin dan terpentin Indonesia di pasar internasional menjadi urutan ketiga setelah China dan Brazil (Lempang,2017). Indonesia sebagai produsen gum rosin ke-3 terbesar di dunia dengan volume produksi mencapai 60.000 ton/tahun, harus dapat memanfaatkan gum rosin sebagai bahan baku menjadi produk yang mempunyai nilai tambah agar nilai jual ekspor dari produk gum rosin menjadi lebih meningkat (Khadafi *et al.*, 2014).

Gum rosin merupakan senyawa kompleks yang berasal dari kayu pinus dan terdiri dari asam-asam resin (Jindal *et al*., 2017). Gum rosin secara tradisional dibutuhkan oleh industri batik, sabun dan, kertas, namun saat ini pemanfaatan gum rosin lebih banyak digunakan sebagai pelunak plester, campuran *eyeshadow*, penguat bulu mata, perekat dan, warna dalam industri percetakan (tinta) dan cat (Sukarno, 2018). Ada beberapa jenis rosin berdasarkan sumbernya yaitu gum rosin (gondorukem getah), rosin minyak *(tall-oil rosin)*, dan rosin kayu *(wood rosin)*, ketiga jenis rosin tersebut dikenal sebagai rosin non modifikasi, sedangkan rosin yang sudah mengalami perubahan kimia pada ikatan ganda atau gugus karboksil dari asam resin dalam gum rosin disebut gum rosin modifikasi. Gum rosin non modifikasi mempunyai beberapa kelemahan antara lain terjadi kristalisasi pelarut yang digunakan, terjadi proses oksidasi secara alami, dan dapat menyebabkan reaksi dengan garam-garam logam berat (Kirk dan Othmer, 2007). Menurut Liu *et al*. (2014) aplikasi gum rosin masih terbatas karena kekurangannya, seperti mudah teroksidasi dan degradasi warna di udara.

Oleh karena itu penggunaan gum rosin harus dimodifikasi. Gum rosin dapat dimodifikasi dengan cara memodifikasi ikatan rangkap dan gugus karboksil yang ada pada senyawa asam dalam gum rosin tersebut untuk memperbaiki sifat-sifatnya ke arah yang lebih baik. Susanti *et al*. (2017) menyatakan bahwa penggunaan gum rosin untuk pembuatan vernis harus dilakukan modifikasi karena kualitas gum rosin yang masih rendah. Gum rosin memberikan hasil lapisan yang rapuh atau mudah rusak karena pengaruh lingkungan. Ikatan rangkap dan gugus karboksil dalam gum rosin sangat reaktif yang merupakan kunci kelemahan dari gum rosin. salah satu cara modifikasi terhadap gum rosin adalah dengan proses esterifikasi. Modifikasi gum rosin dilakukan dengan mereaksikan gum rosin dengan bahan-bahan kimia yang sesuai. Sifat-sifat tertentu yang diinginkan dari gum rosin dapat dicapai melalui modifikasi, gum rosin dapat direaksikan dengan maleat anhidrat atau asam fumarat *(fumaric acid)* dengan asam levopimarat dan gliserol yang akan membentuk ester gliserol asam fumarat (Wiyono *et al*., 2007).

Penelitian ini bertujuan untuk meningkatkan kualitas gum rosin dengan memodifikasi gugus karboksilnya menjadi ester. Namun sebelum reaksi esterifikasi

berlangsung gum rosin terlebih dulu direaksikan dengan asam fumarat untuk membentuk *adduct* yang bertujuan untuk melindungi gugus alkena yang ada dalam asam-asam resin sehingga reaksi akan lebih spesifik pada gugus karboksil dalam gum rosin. Senyawa alkohol yang digunakan dalam reaksi esterifikasi ini adalah gliserol. Fungsi dari gliserol sendiri adalah sebagai sumber gugus ester dan pelarut karena titik didih gliserol yang tinggi yaitu 290 °C. Untuk katalis yang digunakan adalah katalis asam *p*-toluenasulfonat yang bersifat non-oksidator dan merupakan senyawa organik kuat. Seperti pernyataan Wang *et al*. (2016) yang menyatakan bahwa asam *p*-toluenasulfonat, baru-baru ini dilaporkan mengkatalisis esterifikasi gum rosin. Katalis ini dikenal untuk meningkatkan laju reaksi dan berasal dari sumber yang tersedia secara luas dan murah selain itu asam *p*-toluenasulfonat stabil dalam hal oksidasi (Wang *et al*., 2016).

Pada penelitian ini dilakukan modifikaasi gum rosin melalui proses esterifikasi dengan melakukan variasi waktu reaksi yaitu 1, 2, 3, dan 4 jam dan variasi suhu reaksi 140 °C, 160 °C, 180 °C, dan 200 °C bertujuan untuk mengetahui pengaruh lamanya waktu dan suhu reaksi terhadap ester yang dihasilkan serta mengetahui waktu dan suhu reaksi optimal pada proses pembentukan ester.

1.2 Rumusan Masalah

Rumusan masalah dalam peelitian ini adalah:

1. Berapa waktu dan temperatur reaksi optimal pada esterifikasi FMRE?
2. Bagaimana kualitas fisikokimia FMREyang dihasilkan?

1.3 Tujuan Penelitian

Tujuan dari penelitian ini adalah:

1. Menganalisis waktu dan temperatur reaksi optimal pada esterifikasi FMRE
2. Menganalisis kualitas fisikokimia FMRE yang dihasilkan.

1.4 Manfaat

Manfaat yang ingin dicapai dalam penelitian ini adalah:

a. Memberikan informasi waktu dan temperatur reaksi optimal pada reaksi esterifikasi FMRE.

b. Menjadi informasi rujukan dalam pengembangan modifikasi gum rosin dengan asam fumarat melalui proses esterifikasi.
c. Memberikan nilai tambah pada produk derivat gum rosin dan memperluas penggunaan gum rosin modifikasi.

BAB II
TINJAUAN PUSTAKA DAN KERANGKA TEORITIS

2.1 Tinjauan Pustaka

Penelitian tentang modifikasi gum rosin ini untuk mengetahui peningkatan kualitas gum rosin setelah dilakukan proses modifikasi dan adanya perlakuan variasi suhu dan waktu reaksi untuk mengetahui pengaruh suhu dan waktu reaksi terhadap produk yang dihasilkan. Berdasarkan hasil referensi yang didapatkan, terdapat beberapa penelitian yang berkaitan dengan penelitian ini diantaranya yaitu:

Penelitian yang dilakukan oleh Khadafi *et al*. (2014), yang melakukan pengolahan gum rosin menjadi bahan pendarihan sebagai aditif pada pembuatan kertas. Penelitian ini bertujuan untuk membuat darih rosin emulsi dari gum rosin serbuk sebagai aditif pada pembuatan kertas. Gum rosin kualitas WW dan X dilakukan reaksi saponifikasi menggunakan soda pada suhu dibawah 100 °C. Modifikasi rosin dilakukan dengan reaksi fortifikasi menjadi rosin terfortifikasi dengan penambahan senyawa anhidrat maleat.

Prasetyo *et al*. (2012) dalam penelitiannya menghasilkan produk turunan gliserol atau konversi gliserol melalui proses esterifikasi menjadi *glycerol ester maleic rosin*. Pembuatan *glycerol ester maleic rosin* dilakukan dengan mereaksikan asam maleat dari gum rosin dengan gliserol melalui proses esterifikasi dan fortifikasi. Ester gliserol gum rosin maleat memiliki titik lunak yang tinggi dan bilangan asam yang rendah. Pembuatan produk turunan gliserol ini dimaksudkan agar produk mempunyai nilai ekonomi yang lebih tinggi. Secara umum penggunaan produk adalah pada cat termoplastik untuk jalan, perekat tahan panas, dan formulasi tinta cetak.

Penelitian yang lain dilakukan oleh Purnavita *et al*. (2017), yang melakukan modifikasi gum rosin dengan asam laktat dan gliserol dalam pembuatan vernis poliester. Penelitian ini bertujuan untuk mempelajari pengaruh rasio mol gum rosin dan asam laktat terhadap jumlah poliester dan mempelajari pengaruh jumlah katalis terhadap jumlah poliester yang dihasilkan. Katalis yang digunakan adalah katalis $SnCl_2$ yang sering digunakan untuk mempercepat reaksi polimerisasi poliester. Rasio gum rosin dan asam laktat yang berbeda memberikan pengaruh terhadap

yield poliester yang dihasilkan. Rasio (%:%) gum rosin dan asam laktat adalah 50:50 mampu menghasilkan *yield* poliester yang cukup tinggi yaitu 72,28%, dibandingan dengan rasio (%:%) adalah 75:25 dan 25:75. Penambahan asam laktat juga dapat menurunkan nilaibilangan asam.

2.2 Kerangka Teoritis

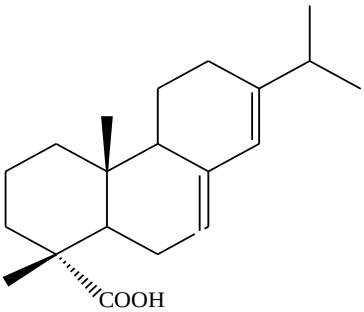
2.2.1 Gum rosin

Gum rosin adalah produk alami yang berasal dari pohon pinus dan terdiri dari campuran kompleks senyawa organik yang saling larut. Menurut Khadafi *et al*. (2014) gum rosin merupakan hasil olahan destilasi uap getah sadapan pohon pinus (*oleoresin*) selain minyak terpentin. Gum rosin berbentuk padatan berwarna kuning kecoklatan, sedangkan minyak terpentin berwujud cairan putih bening. Gum rosin merupakan asam organik *alkyl tricyclic* tak jenuh yang berasal dari derivat alam. Asam abietat dan asam dehidroabietat adalah komponen utama gum rosin, yang banyak digunakan dalam pembuatan solder, kertas, tinta cetak, perekat, dan *plasticizer* (Zhu *et al*., 2014). Fraksi asam resin dari gum rosin adalah campuran kompleks dari isomer asam monokarboksilat diterpenoid dengan rumus molekul empiris $C_{20}H_{30}O_2$ dan terutama mengandung asam abietat. Oleh karena gum rosin berasal dari sumber alami, penggunaan berbagai spesies dan faktor lingkungan (suhu dan konsentrasi tanah, dan lail-lain) dapat mempengaruhi jumlah asam resinnya (Aguilar *et al.*, 2010).

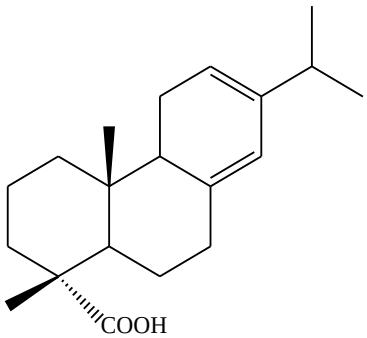
2.2.1.1 Sifat-Sifat Gum rosin

Gum rosin adalah senyawa kompleks yang larut dalam pelarut organik seperti etil alkohol, etil ester, dan benzena, namun tidak larut dalam air. Gum rosin merupakan senyawa kompleks yang terdiri dari 80% - 90% asam-asam resin dan 10% terdiri dari bahan netral. Asam resin adalah campuran kompleks dari beberapa senyawa, terutama jenis abietat dan asam pimarat yang termasuk dalam kelompok senyawa organik yang diterpen (Jindal *et al*., 2017). Menurut Kaith *et al*. (2016) gum rosin terdiri dari asam resin seperti asam resin tipe abietat yang memiliki ikatan rangkap terkonjugasi dan asam resin tipe pimarat dengan ikatan rangkap non-terkonjugasi. Jenis-jenis asam abietat yaitu asam neoabietat, livopimarat, palustrat,

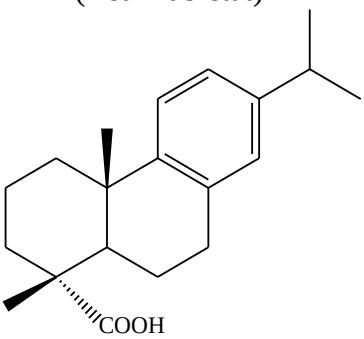
dan asam dehidroabietat, sedangkan yang termasuk dalam jenis-jenis asam tipe pimarat adalah asam pimarat dan isopimarat (Kirk dan Othmer, 2007).



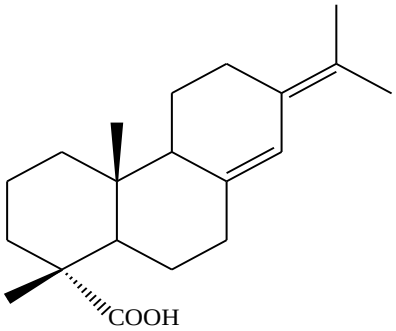
Asam abieta-7, 13-dien-18-oat
(Asam abietat)



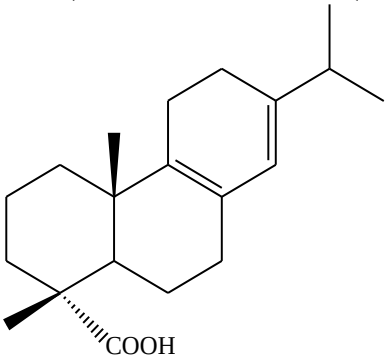
Asam abieta-8(14),12 dien-18-oat
(Asam levopimarat)



Asam abieta-8(14),9(11), 12-trien-18-oic
(Asam dehidroabietat)

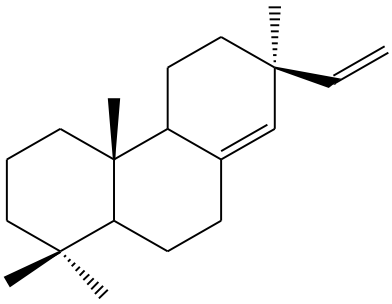


Asam abieta-8(14),13(15)-dien-18-oat
(Asam neoabietat)

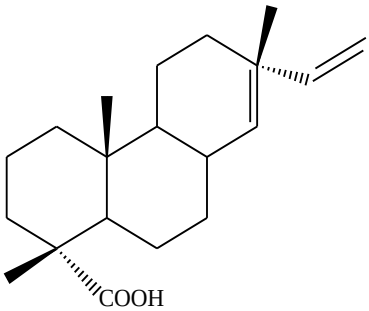


Asam abieta-8,13-dien-18-oat
(Asam Palustrat)

Gambar 2.1. Struktur kimia tipe asam abietat
(Kirk dan Othmer, 2007)



Asam pimara-8(14),15-dien-18-oat
(Asam pimarat)



Asam(13α)-pimara-7,15-dien-18-oat
(Asam isopimarat)

Gambar 2.2. Struktur kimia tipe asam pimarat
(Kirk dan Othmer, 2007)

2.2.1.2 Klasifikasi gum rosin

Menurut Standar Nasional Indonesia 7636: 2011, persyaratan mutu gum rosin dibedakan mejadi tiga kelompok, yaitu syarat mutu, syarat umum dan syarat khusus. Kualitas gum rosin terbagi menjadi empat macam kelas mutu yaitu mutu utama, pertama, kedua, dan ketiga, sedangkan untuk persyaratan klasifikasi khusus gum rosin terdiri dari penilaian warna, titik lunak (*softening point*), kadar abu, kadar kotoran, dan komponen yang menguap, untuk klasifikasi umum gum rosin meliputi bilangan asam, bilangan penyabunan, dan bilangan iod. Klasifikasi mutu gum rosin dapat disajikan pada Tabel 2.1, klasifikasi khusus kualitas gum rosin dapat dilihat pada Tabel 2.2, sedangkan untuk klasifikasi umum kualitas gum rosin dapat dilihat pada Tabel 2.3.

Tabel 2.1 Klasifikasi mutu gum rosin

No	Klasifikasi Mutu	Tanda Mutu	
		Dokumen	Kemasan
1.	Utama (U)	X	X
2.	Pertama (P)	WW	WW
3.	Kedua (D)	WG	WG
4.	Ketiga (T)	N	N

(SNI, 2011)

Tabel 2.2 Klasifikasi khusus kualitas gum rosin

No	Jenis Uji	Satuan	Persyaratan Mutu			
			U	P	D	T
1.	Warna					
	a. Metode Lovibond		X	WW	WG	N
	b. Metode Gardner		≤6	≤7	≤8	≤9
2.	Titik Lunak	ºC	≥78	≥78	≥76	≥74
3.	Kadar Kotoran	%	≤0,02	≤0,05	≤0,07	≤0,10
4.	Kadar Abu	%	≤0,01	≤0,04	≤0,05	≤0,08
5.	Komponen Menguap	%	≤2	≤2	≤2,5	≤3

(SNI, 2011)

Keterangan :
Kualitas
U (Utama) = kualitas utama
P (Pertama) = kualaitas pertama
D (kedua) = kualitas kedua

X (Extra) = kuning jernih
WW (Water White) = kuning
WG (Window Glass) = kuning kecoklatan

Tabel 2.3 Klasifikasi umum kualitas gum rosin

No	Jenis Uji	Persyaratan
1.	Bilangan asam	160-190
2.	Bilangan penyabunan	170-220
3.	Bilangan iod	5-25

(SNI, 2011)

Klasifikasi mutu gum rosin juga dapat dilihat dari warnanya yang dihasilkan. Warna gum rosin tergantung dari sumber dan metode pembuatannya, warna bisa dari kuning pucat sampai merah tua dan bahkan hampir hitam kecerahan. Menurut Sukarno (2018), sifat fisik gum rosin dapat mempengaruhi kualitas produk gum rosin yang dihasilkan dan nilai jualnya. Sifat fisik juga terkait dengan pengolahan teknis dan bahan baku. Sifat fisik suatu produk harus memenuhi persyaratan kualitas dari standar kualitas yang ditetapkan.

2.2.1.3 Kegunaan gum rosin

Gum rosin dapat digunakan dalam dua bentuk yaitu *modified rosin* (rosin modifikasi) dan *unmodified rosin* (rosin non modifikasi). Pada awalnya gum rosin hanya digunakan dalam bentuk non modifikasi. Seiring dengan perkembanngan riset, gum rosin mulai dilakukan modifikasi dan sekarang penggunaan gum rosin modifikasi lebih disukai dipasaran karena keunggulan yang dimiliki. Potensi penggunaan dari senyawa gum rosin diantaranya banyak dimanfaatkan untuk bahan

industri cat, tinta cetak, pembuatan kertas, dan perekat (Liu *et al*., 2014). Gum rosin digunakan sebagai bahan perekat yang berfungsi sebagai *tackifier*, pemacu perekatan (*adhesion promoter*) atau pemacu kekentalan (*viscosity promoters*) untuk memperbaiki sifat-sifat produk akhir (Khadafi *et al*., 2014)

2.2.2 Rosin modifikasi

Saat ini, gum rosin lebih banyak digunakan dalam bentuk gum rosin modifikasi karena sifatnya yang lebih unggul daripada gum rosin biasa. Gugus karboksil dan ikatan rangkap dalam asam dapat menghasilkan banyak jenis garam dan senyawa termodifikasi untuk tujuan yang lebih baik (Jindal *et al*., 2017). Gum rosin dan turunannya dapat dimodifikasi untuk menyiapkan serangkaian bahan polimer dan aditif. Salah satu modifikasi dari gum rosin adalah asam maleopimarat anhidrat monomer semisintetik-organik, yang dibuat dengan asam levopimarat dari gum rosin dengan maleat anhidrat (Zhen *et al*., 2013). Diketahui bahwa turunan rosin memiliki beberapa keunggulan diantaranya seperti asam N-(dimetilaminometil) imida maleopimarat, komposisi yang terdiri dari kolofoni yang dimodifikasi, ester pentaeritritol dari campuran rosin dan asam lemak, *N-(hydroxyethyl) imide* dari *terpene maleic adduct* (TMA) yang menunjukkan aktivitas fungisida dan bakterisida (Kluve *et al*., 2014).

Pada awalnya gum rosin banyak digunakan dalam bentuk non modifikasi, namun sekarang gum rosin lebih banyak diguakan dalam bentuk modifikasi, dikarenakan sifat dari gum rosin modifikasi yang lebih unggul daripada gum rosin non modifikasi, Menurut Liu *et al*. (2019) masalah serius pada gum rosin adalah karena sifatnya yang mudah teroksidasi saat kontak dengan udara. aplikasi gum rosin masih terbatas karena beberapa kekurangan dari gum rosin non modifikasi dalam aplikasinya sering terjadi kristalisasi, terjadi proses oksidasi secara alami terhadap gum rosin dan dapat menyebabkan reaksi dengan garam-garam logam berat terutama pada penggunaan untuk vernis. Pengguaan gum rosin non modifikasi menjadi tidak efisien, sehingga beralih menggunakan gum rosin modifikasi yang dapat digunakan untuk berbagai macam penggunaan seperti dalam bidang farmasi sebagai pelapis film, pembentukan matriks, mikroenkapsulasi, di bidang industri

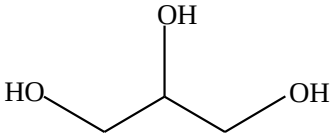
seperti industri perekat, industri kertas, tinta cetak, dan *protective coating* (Raouf *et al*., 2018).

2.2.3 Agen Modifikasi Gum rosin

Untuk membuat gum rosin modifikasi diperlukan bahan-bahan kimia yang dapat mendukung untuk mencapai target yang diinginkan, diantaranya adalah gliserol dan asam fumarat.

2.2.3.1 Gliserol

Gliserol (1, 2, 3-propanetriol) merupakan cairan kental yang memiliki rasa manis (Prasetyo *et al*., 2012). Gliserol ($C_3H_8O_3$) merupakan senyawa golongan alkohol polihidrat dengan tiga buah gugus hidroksil dalam satu molekul, bersifat polar dan kental (*viscous*) (Wahyuni *et al*., 2016). Gliserol tidak berwarna, tidak berbau, rasanya manis, bentuknya liquid, meleleh pada suhu 17,8 °C, mendidih pada suhu 290 °C, dan larut dalam air dan etanol. Sifat gliserol higroskopis, seperti menyerap air dari udara, gliserol terdapat dalam bentuk ester (gliserida) pada semua hewan, lemak nabati, dan minyak. Pengolahan gliserol lebih lanjut dapat meningkatkan nilai ekonominya. Seiring dengan peningkatan produktifitas biodisel produktifitas gliserol juga meningkat. Pada tahun 2010 diperkirakan produksi gliserol sekitar 1,2 juta ton gliserol yang lebih dari separuhnya berasal dari produksi biodisel (Appleby, 2013). Proses esterifikasi gliserol adalah salah satu metode yang banyak digunakan untuk memproduksi produk turunan glisreol. Dalam reaksi esterifikasi dihasilkan bermacam-macam ester yang mempunyai banyak kegunaan dan bernilai lebih tinggi. Produk dari konversi gliserol ini bersifat ramah lingkungan dan terbarukan karena bukan merupakan turunan dari minyak bumi (Prasetyo *et al*., 2012). Sifat karakteristik gliserol lebih lengkapnya dapat dilihat dalam Tabel 2.4. Adapun rumus molekul gliserol dapat ditunjukkan pada Gambar 2.3.



Gambar 2.3 Rumus Molekul Gliserol (Karlberg dan Hagvall, 2018)

Tabel 2.4 Karakteristik gliserol

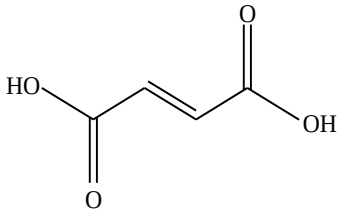
Sifat	Nilai
Tampilan fisik	Cair
Kemurnian	90-95%
Tegangan permukaan	63 Mn/n pada 20 ℃
Berat molekul	92, 09382 g/mol
Densitas	1,261 g/mol
Viskositas	1410 mPa s pada 20 °C
Titik leleh	17,8 ºC (64, 2 ºF)
Titik didih	290 ºC pada 1013 hPa

(Radhiyatullah *et al*., 2015)

2.2.3.2 Asam fumarat

Asam fumarat (FA) atau asam *(E)-butanedioat* adalah senyawa kristal dan merupakan isomer asam dikarboksilat tak jenuh asam maleat. Maleat anhidrida yang bereaksi dengan air akan membentuk asam maleat dengan melalui proses isomerisasi akan menghasilkan asam fumarat (FA). Namun, asam fumarat dapat digunakan secara langsung sebagai reaktan primer yaitu sebagai pengganti anhidrida maleat (Knesebeck *et al*., 2018). Karena strukturnya (ikatan rangkap karbon-karbon dan dua gugus asam karboksilat), FA memiliki banyak aplikasi potensial dalam industri. FA dapat digunakan sebagai bahan awal untuk reaksi polimerisasi dan esterifikasi. Saat ini, FA diproduksi secara kimiawi dari anhidrida maleat melalui oksidasi dalam atmosfer benzena menggunakan V_2O_5 dan MoO_3 sebagai katalis pada suhu tinggi (Liu *et al*., 2015). FA merupakan isomer *trans* dari asam butadioat dengan bentuk kristal berwarna putih yang memiliki titik leleh 300 ºC, dengan pemanasan sampai 300 ºC, FA berubah menjadi anhidrida maleat, kristal FA tidak mudah larut dalam air. Linetrose *et al*. (2015) menyatakan bahwa kedua isomer, asam maleat dan asam fumarat, hanya berbeda dalam posisi gugus karboksil. Isomer *ciss*, asam maleat, adalah asam yang lebih kuat dibandingkan dengan mitra transnya, asam fumarat. FA memiliki rasa seperti buah-buahan. Garam dan ester asam fumarat dikenal sebagai fumarat. FA banyak digunakan dalam industri makanan, farmasi dan kimia, dan menarik perhatian yang semakin meningkat karena dapat dikonversi menjadi obat-obatan terapi dan merupakan bahan awal untuk polimerisasi dan esterifikasi. FA terutama diproduksi secara petrokimia dari anhidrida maleat (Xu, G.,*et al.*, 2012). Asam fumarat termasuk asam lemah yang dapat membentuk ester, dapat mengalami reaksi adisi pada ikatan

rangkapnya, dan juga merupakan dienofil yang baik (Podgorska *et al.*, 2004). Gambar 2.4 merupakan struktur kimia dari FA.



Gambar 2.4 Struktur Asam Fumarat
(Araji *et al.*, 2017)

2.2.4 Katalis

Katalis adalah zat yang mempengaruhi kecepatan reaksi tetapi zat tersebut tidak mengalami perubahan kimia pada akhir reaksi. Katalis tidak berpengaruh dalam energi bebas, juga tidak berpengaruh terhadap tetapan kesetimbangan. Umumnya kenaikan konsentrasi katalis juga menaikkan kecepatan reaksi, jadi katalis ini ikut dalam reaksi tetapi pada akhir reaksi diperoleh kembali (Okvitarini *et al.*, 2013). Berdasarkan fasenya, proses katalis dapat digolongkan menjadi katalis homogen dan heterogen. Katalis homogen ialah katalis yang mempunyai fase sama dengan fase campuran reaksinya, sedangkan katalis heterogen adalah katalis yang berbeda fase dengan campuran reaksinya. Menurut Praputri *et al*. (2018). Jenis katalis homogen yang banyak digunakan adalah katalis asam (HCl, H_2SO_4 dan HNO_3), sedangkan contoh katalis heterogen seperti zeolit, Pd, Ru, Rh, Pt, dan lain-lain. Reaksi katalitik mengikuti persamaan reaksi 1-3.

$$A + C \longrightarrow AC \quad (1)$$

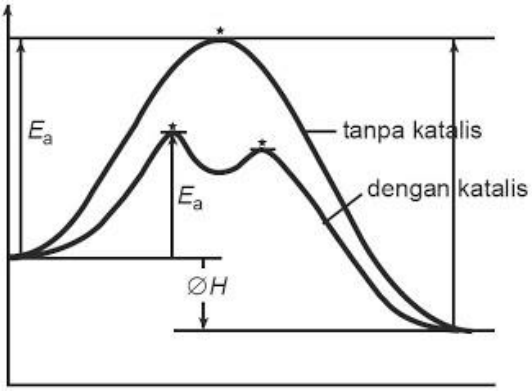
$$B + AC \longrightarrow AB + C \quad (2)$$

Meskipun katalis (C) ikut bereaksi, namun oleh reaksi 2 terbentuk kembali, sehingga untuk reaksi keseluruhannya menjadi seperti reaksi 3:

$$A + B + C \longrightarrow AB + C \quad (3)$$

(Praputri *et al*., 2018)

Fungsi katalis dalam reaksi adalah menurunkan energi aktivasi sehingga jumlah molekul yang dapat melampaui energi aktivasi menjadi lebih besar (Gambar 2.5). Gambar tersebut menunjukkan peranan katalis dalam menentukan energi aktivasi.



Gambar 2.5 Energi potensial reaksi tanpa katalis dan dengan bantuan katalis (Silberberg, 2008)

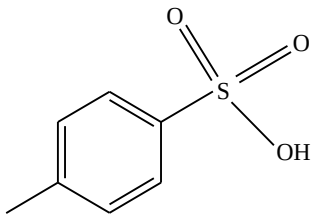
Pada Gambar 2.5 proses reaksi tanpa katalis digambarkan dengan satu kurva yang tinggi sedangkan dengan katalis menjadi dua kurva dengan dua pucak yang rendah sehingga energi aktivasi pada reaksi dengan katalis lebih rendah daripada energi aktivasi pada reaksi tanpa katalis. Berarti secara keseluruhan katalis dapat menurunkan energi kativasi dengan cara mengubah jalannya reaksi atau mekanisme reaksi lebih cepat (Purnami *et al.*, 2015).

2.2.4.1 Katalis asam homogen

Katalis homogen terdiri atas dua jenis yaitu katalis asam dan basa. Katalis homogen mempunyai keunggulan, yaitu tidak mudah teracuni oleh kotoran dan setiap molekul katalis berfungsi aktif sebagai katalis. Kerugian katalis homogen diantaranya sulit dipisahkan dari campurannya dan mudah terurai pada temperatur tinggi. Dibanding katalis homogen, katalis heterogen memiliki kelebihan diantaranya dapat dipisahkan dari campuran reaksi hanya dengan cara penyaringan, sehingga mudah diregenerasi. Katalis heterogen juga mempunyai kekurangan yaitu jika permukaan katalis telah jenuh oleh molekul reaktan, maka reaksi tidak dapat dilanjutkan. Kejenuhan katalis dapat diatasi dengan melakukan regenerasi (Purnami *et al*., 2015).

2.2.4.2 *Para-Toluene Sulphonic Acid* (asam *p*-toluenasulfonat)

Asam *p*-toluenasulfonat (PTSA), atau disingkat TsOH, merupakan senyawa organik yang memiliki rurmus $CH_3C_6H_4SO_3H$, berupa padatan berwarna putih yang larut dalam air, alkohol, dan pelarut organik polar lainnya. PTSA juga sering disebut sebagai $TsOH.H_2O$. Asam *p*-toluenasulfonat merupakan senyawa organik kuat, satu juta lebih kuat dari asam benzoat. Asam *p*-toluenasulfonat merupakan salah saru asam kuat yang berupa zat padat, sehingga mudah ditimbang. Selain itu, berbeda dengan asam mineral kuat lainnya (terutama asam nitrat, asam sulfat, dan asam perklorat), Asam *p*-toluenasulfonat bersifat non-oksidator (Alva, *et al*., 2016).



Gambar 2.6 Struktur Asam *p*-toluenasulfonat
(Alva, *et al.*, 2016)

Pada skala industri, TsOH dihasilkan dari sulfonasi toluena. Asam *p*-toluenasulfonat berhidrasi dengan cepat. Umumnya terdapat pula sebagian kecil asam benzenasulfonat dan asam sulfat yang dihasilkan. Ketidak murnian ini dapat dipisahkan dengan rekristalisasi dari asam klorida, selanjutnya diikuti dengan pengeringan azeotropik TsOH bermanfaat dalam sintesis organik sebagai katalis asam yang larut dalam pelarut organik. Contoh penggunaannya adalah asetilasi aldehida, esterifikasi asam karboksilat, dan *trans*-esterifikasi ester. Asam *p*-toluenasulfonat dapat diubah menjadi *p*-toluenasulfoat anhidrida dengan memanaskannya dengan fosfor pentoksida. Asam *p*-toluenasulfonat, baru-baru ini dilaporkan mengkatalisis esterifikasi gum rosin. Katalis ini dikenal untuk meningkatkan laju reaksi dan berasal dari sumber yang tersedia secara luas dan murah selain itu asam *p*-toluenasulfonat stabil dalam hal oksidasi (Wang *et al*., 2016).

2.2.5 Proses Modifikasi

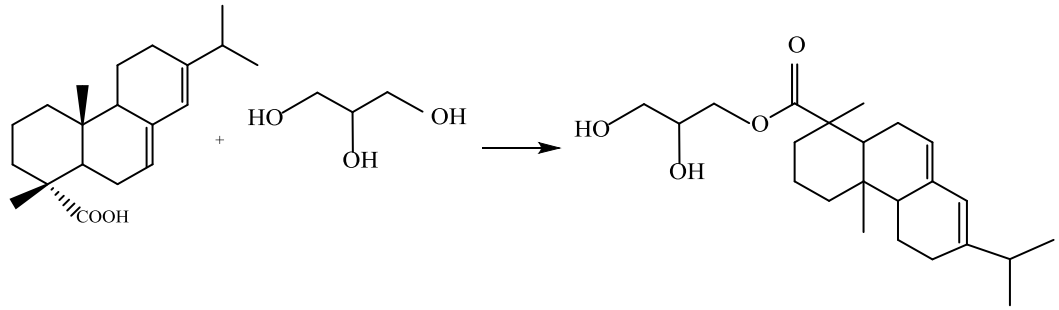
Modifikasi gum rosin dapat dilakukan dengan banyak cara, gugus karboksil dan ikatan rangkap terkonjugasi dalam molekul rosin dengan aktivitas tinggi dapat mudah untuk di lakukan isomerisasi, beberapa cara untuk memodifikasi rosin diantaranya yaitu hidrogenasi, polimerisasi, disproporsionasi, aminolisis, esterifikasi, pembentukan garam, dan reaksi dekarboksilasi (Zhen *et al*., 2013).

2.2.5.1 Proses Esterifikasi

Reaksi esterifikasi adalah reaksi antara asam karboksilat dengan senyawa alkohol yang membentuk ester. Ester asam karboksilat ialah suatu senyawa yang mengandung gugus $–CO_2$ R’ dan R dapat berupa alkil maupun aril. Esterifikasi adalah reaksi bolak-balik sehingga konversi dibatasi oleh konversi kesetimbangannya (Fakhry dan Rahayu, 2016). Proses esterifikasi gliserol adalah salah satu metode yang banyak digunakan untuk memproduksi produk turunan gliserol. Dalam reaksi esterifikasi dihasilkan bermacam-macam ester yang mempunyai banyak kegunaan dan bernilai lebih tinggi. Produk dari konversi gliserol ini bersifat ramah lingkungan dan terbarukan karena bukan merupakan turunan dari minyak bumi (Prasetyo *et al*., 2012).

Menurut Agiular *et al*. (2010), gum rosin yang disuling dipompa ke dalam reaktor, dan diesterifikasi dengan *food grade* gliserol di bawah atmosfer nitrogen. Reaksi gum rosin dan gliserol dilakukan pada suhu 260 - 280 °C dan dibiarkan berjalan sampai spesifikasi produk yang diinginkan terpenuhi. Spesifikasi ini meliputi jumlah asam, warna, dan titik lunak (Ring & Ball Test). Gum rosin ester ini kemudian dimurnikan dengan uap arus balik langsung (260 °C, 2 jam) dan dianalisis untuk jumlah asam, warna, dan titik pelunakan, dan kemudian dihilangkan aromanya. Setelah pendinginan, ester gum rosin mengalami filtrasi melalui filter 10-mikrometer. Produk yang difilter dianalisis untuk angka asam, warna, titik pelunakan, aroma, dan rasa. Reaksi esterifikasi dapat dilakukan dengan atau tanpa menggunakan katalis dalam reaksi. Reaksi esterifikasi akan berjalan lambat jika dilakukan tanpa katalis, oleh karena itu banyak penelitian dilakukan untuk memepelajari kinetika reaksi, baik dengan katalis homogen maupun heterogen (Fakhry dan Rahayu, 2016). Menurut Wang *et al*. (2017) karena

kerangka tiga cincin fenantrena pada molekul gum rosin, yang menghasilkan hambatan spasial dari gugus karboksil, katalis dan suhu tinggi diperlukan selama esterifikasi gum rosin. Reaksi esterifikasi umumnya dilakukan pada bahan yang mengandung asam lemak bebas atau resin (senyawa karboksilat). Ester asam karboksilat ialah suatu senyawa yang mengandung gugus $–CO_2$ R' dan R dapat berupa alkil maupun aril (Prasetyo *et al*., 2012). Gambar 2.7 menunjukkan mekanisme reaksi esterifikasi asam karboksilat dengan alkohol.



Asam abietat Gliserol Gliseril 1-monoabietat

Gambar 2.7 Reaksi esterifikasi asam karboksilat dan alkohol (Karlberg dan Hagvall, 2018)

BAB III
METODOLOGI PENELITIAN

3.1 Tempat dan Waktu Penelitian

Penelitian ini dilakukan di Laboratorium Kimia Fakultas Matematika dan Ilmu Pengetahuan Alam Universitas Negeri Semarang dan Laboratorium Perhutani Pine Chemical Industry Pemalang. Waktu pelaksanaan dilaksankan selama 4 bulan dari bulan Maret sampai bulan Juni 2019.

3.2 Variabel Penelitian

3.2.1 Variabel Bebas

Variabel bebas dalam penelitian ini adalah jenis katalis yang digunakan yaitu katalis asam *p*-toluenasulfonat (PTSA), pengujian sampel yang dilakukan yaitu pada jam pertama, kedua, ketiga dan keempat, suhu reaksi yang digunakan pada reaksi estrerifikasi gum rosin fumarat dengan gliserol yaitu 140 °C, 160 °C, 180 °C, dan 200 °C.

3.2.2 Variabel Terikat

Variabel terikat pada penelitian ini adalah produk dari penelitian ini yaitu *Fumaric Modified Rosin Ester* (FMRE) dari hasil reaksi esterifikasi antara gum rosin fumarat dan gliserol menggunakan katalis asam *p*-toluenasulfonat.

3.2.3 Variabel Terkendali

Variabel terkendali pada penelitian ini adalah perolehan dan perlakuan awal dari bahan baku gum rosin, berat katalis PTSA, dan berat gliserol.

3.3 Alat dan Bahan

3.3.1 Alat

Alat yang digunakandalam penelitian ini adalah labu leher tiga, seperangkat alat refluks, *hotplate*, oven, corong, pipet volume 25 mL, pipet volume 20 mL, buret 50 mL, erlenmeyer, mortar dan alu, *softening point ring and ball apparatus*, termometer raksa, gelas ukur 250 mL, pengaduk kaca, pompa air, beaker glass 250 mL, stirer, klem dan statif, timbangan analitik, corong, pipet tetes, kondensor, wadah pencetak gum rosin, FTIR *Shimadzu Instrument Spectrum One 8400S*, dan GC-MS *Agilent 7890 MS 5975C FL MSD*.

3.3.2 Bahan

Bahan baku yang digunakan dalam penelitian ini adalah gum rosin kualitas WW, bahan kimia yang digunakan untuk pembuatan ester gliserol gum rosin fumarat dan pengujian sifat fisik dan kimia produk antara lain asam fumarat (*fumaric acid*) *Merck*, katalis PTSA (asam *p*-toluenasulfonat) *Merck*, gliserol, etanol teknis, larutan standar kalium hidroksida (KOH) 0,5 N, indikator *phenopthalein* 1% dalam alkohol 95%, toluena, etanol netral, natrium tiosulfat *Merck*, KI 10 %, amilum, larutan kloroform *Merck*, larutan Wijs *Merck* dan aquades.

3.4 Prosedur Kerja

Proses pembuatan FMRE ada tiga metode yang dapat digunakan secara umum antara lain metode pertama yaitu gum rosin, gliserol dan asam fumarat direaksikan bersama, metode kedua yaitu gum rosin direaksikan pertama dengan asam fumarat untuk memproduksi *adduct* kemudian diesterifikasikan dengan gliserol dan metode ketiga yaitu mereaksikan asam fumarat dengan gliserol kemudian diikuti oleh penambahan gum rosin (Prasetyo *et al*., 2012). Pada penelitian ini meode yang dipakai adalah metode kedua yaitu pertama gum rosin direaksikan terlebih dahulu dengan asam fumarat, setelah itu diesterifikasikan dengan gliserol untuk memperoleh produk FMRE yang diinginkan.

3.4.1 Karakterisasi Bahan Baku

Bahan baku pada pembuatan FMRE (*Fumaric Modified Rosin Ester*) yaitu gum rosin dilakukan pengujian sifat fisikokimia dan pengujian menggunakan instrumen GC-MS untuk mengetahui kandungan asam resinnya.

3.4.2 Sintesis FMRE (*Fumaric Modified Rosin Ester*)

Pada proses ini, dalam 100 mL labu alas bulat berleher tiga yang dilengkapi dengan pengaduk magnet, 150 gram gum rosin yang sudah dihaluskan dan asam fumarat dipanaskan sampai suhu 100 °C untuk melelehkan gum rosin, kemudian ditambahkan dengan katalis asam *p*-toluenasulfonat sebanyak 0,3% dan ditambahkan gliserol 10%, campuran diaduk dengan magnetik stirer sampai homogen, dilakukan proses pemanasan dengan menggunakan variasi suhu yaitu pada suhu 140 °C, 160 °C, 180 °C, dan 200 °C. Pengujian sampel dilakukan setiap

satu jam (Tabel 3.1). Proses pemanasan dilakukan selama 4 jam, dilakukan pengambilan sampel pada jam ke pertama, kedua, ketiga dan keempat, setelah itu produk dituang kedalam cetakan yang sudah disiapkan.

Tabel 3.1 Proses Esterifikasi gum rosin fumarat dan gliserol dengan variasi suhu reaksi dan persentase penambahan katalis.

Gum rosin : Asam Fumarat	Gliserol (%)	PTSA (%)	Temperatur (°C)	Waktu (Jam)
1 : 2	10	0,3	140	1
1 : 2	10	0,3	140	2
1 : 2	10	0,3	140	3
1 : 2	10	0,3	140	4
1 : 2	10	0,3	160	1
1 : 2	10	0,3	160	2
1 : 2	10	0,3	160	3
1 : 2	10	0,3	160	4
1 : 2	10	0,3	180	1
1 : 2	10	0,3	180	2
1 : 2	10	0,3	180	3
1 : 2	10	0,3	180	4
1 : 2	10	0,3	200	1
1 : 2	10	0,3	200	2
1 : 2	10	0,3	200	3
1 : 2	10	0,3	200	4

3.5 Pengujian Kualitas

Dilakukan pengujian produk akhir dari FMRE yaitu meliputi *yield*, pengujian sifat fisik dan kimia gum rosin. Pengujian sifat fisik dan kimia gum rosin yang dilakukan meliputi pengujian warna dengan *Coloumeter Lico 620*, pengujian titik lunak, bilangan asam, dan bilangan iod berdasarkan SNI 7636 : 2011.

3.5.1 *Yield* FMRE

Pengujian rendemen produk FMRE yang dihasilkan dari penelitian ini dapat dihitug dengan rumus sebagai berikut:

$$Yield = \frac{\text{Hasil Sintesis}}{\text{Hasil Teoritis}} \times 100\%$$

3.5.2 Pengujian Sifat Fisik

a. Warna

Pengujian warna dilakukan dengan metode Gardner. Sampel diuji sesuai *Instruction Manual Gardner Liquid Color Standard*. Cara kerjanya yaitu dengan melarutkan produk rosin pada etanol dengan perbandingan 1:1, kemudian dilakukan pengecekan dengan alat *Coloumeter Lico 620*.

b. Titik Lunak (*Softening Point*)

Pengujian titik lunak (*Softening Point*) dilakukan berdasarkan SNI 7636 : 2011 menggunakan *softening point ring and ball apparatus.* Sampel uji yag telah dibuat serbuk halus dicairkan pada suhu rendah, kemudian dimasukkan kedalam ring, selanjutnya permukaan ring yang telah diisi sampel uji diratakan dan dibiarkan beberapa waktu hingga mengeras. Letakkan ring yang berisi sampel uji pada ring holder dan letakkan bola baja diatas sampel uji tersebut. Setelah itu *beaker glass* 1000 mL diisi air sampai volume 800 mL, masukkan termometer ke dalam *beaker glass* saat suhu *beaker glass* sudah mencapai 40 °C masukkan ring beserta bola baja ke dalam *beaker glass*. Pemanasan dilakukan sampai gum rosin tersebut melunak dan bola baja menyentuh plat dasar. Titik lunak adalah suhu rata-rata dari hasi pembacaan pada waktu bola baja turun menyentuh plat dasar.

2.5.3 Pengujian Sifat Kimia

a. Bilangan Asam

Pengujian bilangan asam dilakukan berdasarkan SNI 7636 : 2011 dilakukan dengan cara menimbang sampel uji rosin yang telah dibuat serbuk halus sebanyak 4 gram dalam erlenmeyer 250 mL yang sudah diketahui beratnya, kemudian ditambahkan etanol netral sebanyak 100 mL dan ditambah indikator *phenopthalein* sebanyak tiga tetes. Titik akhir titrasi dicapai apabila terjadi perubahan warna menjadi merah muda. Bilangan asam dihitung dengan menggunakan rumus sebagai berikut:

$$\frac{\text{V KOH x N KOH x } 56{,}1}{\text{W}}$$

Keterangan : V : volume larutan kalium hidroksida yang digunakan (mL)

N : adalah normalitas kalium hidroksida (0.1 N)

W : berat contoh uji (g)

56,1 : berat molekul KOH

b.Bilangan Iod

Pengujian bilangan iod dilakukan dengan menimbang sampel gum rosin yang telah dibuat serbuk halus sebanyak 1 gram kemudian ditambah dengan 20 mL larutan kloroform dan 25 mL larutan Wijs dengan menggunakan pipet ukur 25 mL, simpan larutan ditempat yang gelap selama ± 30 menit. Setelah ± 30 menit, ditambahkan larutan KI 10% kemudian diencerkan dengan 100 mL aquades. Titrasi larutan sampel dengan larutan standard natrium thiosulfat 0,1 N sampai 10 mL, kemudian tambahkan 1-2 mL indikator amilum. Lanjutkan titrasi sampai warna biru hilang. Bilangan iod dapat dihitung dengan rumus:

$$\text{IV} = \frac{(V_2 - V_1) \times 12{,}69}{W}$$

Keterangan : V_1 : volume titrasi contoh uji, dinyatakan dalam milimeter.

V_2 : avolume titrasi blanko, dinyatakan dalam milimeter.

N : normalitas $Na_2S_2O_3$.

W : berat contoh uji, dinyatakan dalam gram.

12,69 : bobot setara bilangan iod.

c. Kelarutan dalam toluena

Pengujian kelarutan dalam toluena (1:1) dilakukan dengan cara menimbang 1 gram contoh uji yang telah dibuat serbuk halus dan memasukkan ke dalam gelas piala 50 mL yang sudah diketahui beratnya. Tambahkan toluena sebanyak 1 mL sampai larut.

3.6 Karakterisasi Data

Metode analisis data yang digunakan dalam penelitian ini adalah analisis hasil produk FMRE menggunakan instrumen FTIR dan GC-MS. Instrumen FTIR digunakan untuk mengetahui gugus fungsi suatu senyawa organik, sedangkan GC-MS digunakan untuk menganalisis komposisi asam-asam resin dan ester yang terkandung di dalam sampel FMRE.

BAB IV

HASIL DAN PEMBAHASAN

4.1 Karakterisasi Bahan Baku

Gum rosin merupakan senyawa kompleks yang berasal dari kayu pinus dan terdiri dari asam-asam resin (Jindal *et al*., 2017). Sifat fisiko kimia bahan baku gum rosin yang digunakan akan mempengaruhi proses esterifikasi yang dilakukan. Sifat fisiko kimia bahan baku gum rosin awal dapat dilihat pada Tabel 4.1

Tabel 4.1 Sifat fisikokimia gum rosin

Jenis Uji	Hasil analisis
Warna	6,6
Titik Lunak	78
Bilangan Asam (mg KOH/g)	189,361
Bilangan Iod (mg iod/g)	24,47
Kelrutan dalam toluen	Larut

Sesuai dengan SNI 7636:2011 dapat diketahui bahwa hasil analisis bahan baku yang digunakan memiliki mutu warna yang sudah memenuhi standar gum rosin dengan grade 6,6 sesuai dengan rentang standar gum rosin kualitas WW. Titik lunak bahan baku berada pada suhu 78 °C yang mana sudah sesuai dengan rentang standar gum rosin yaitu sebesar ≥78 °C. Titik lunak menunjukkan salah satu sifat khas gum rosin dan tingkat kemasakannnya. Tingkat kemasakan ini berhubungan dengan kadar terpentin sisa dalam gum rosin, dimana semakin kecil kadar terpentin sisa maka semakin tinggi titik lunak gum rosin. Menurut Khadafi *et al*. (2014) bilangan asam adalah banyaknya kalium hidroksida (KOH) dalam miligram yang diperlukan untuk menetralkan satu gram asam resin yang terkandung dalam senyawa gum rosin. Bilangan asam ditentukan untuk mengetahui jumlah asam lemak bebas yang terkandung dalam gum rosin dan dipergunakan untuk mengetahui tingkat kerusakan bahan yang disebabkan adanya proses hidrolisis. Bilangan asam gum rosin dari hasil analisis sebesar 189,36 mg KOH/g yang sudah memenuhi standar gum rosin yaitu 160-190 mg KOH/g. Bilangan iod menunjukkan jumlah ketidakjenuhan asam lemak bebas dalam bentuk ikatan rangkap yang bereaksi dengan senyawa iod, sehingga semakin banyak ikatan C=C dalam gum rosin maka bilangan iodnya akan semakin tinggi pula. Nilai bilangan iod yang didapatkan yaitu sebesar 24,47 mg

iod/g yang mana sudah sesuai dengan standar bilangan iod gum rosin yaitu 5-25. Sedangkan untuk hasil analisis kelarutan dalam toluena (1:1) menunjukkan gum rosin dapat larut sempurna dalam toluena. Hasil yang didapat menunjukkan bahwa secara keseluruhan bahan baku gum rosin yang digunakan sudah sesuai dengan SNI 7636:2011.

4.2 Sifat Fisikokimia FMRE

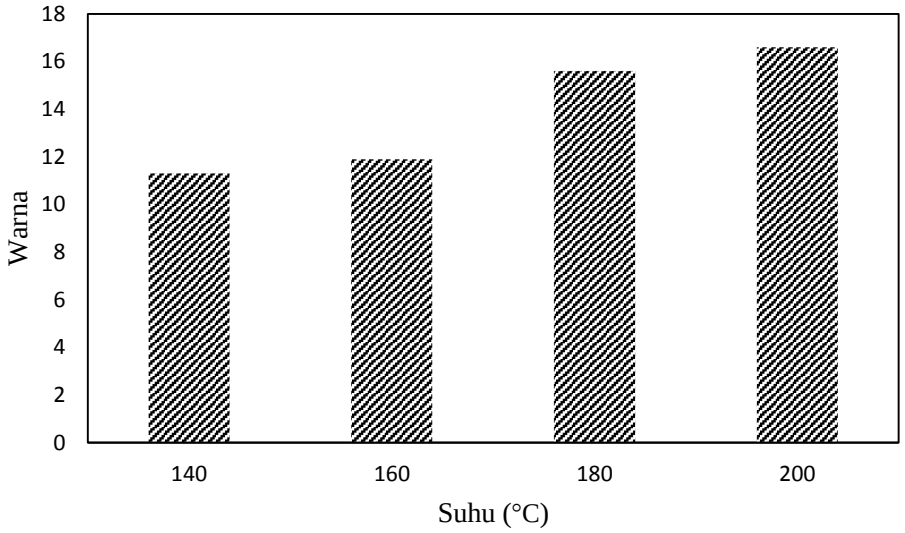
Hasil analisis sifat fisikomia FMRE dapat disajikan pada Tabel 4.2

Tabel 4.2. Hasil analisis fisiko kimia FMRE

Suhu (°C)	Karakterisasi				
	Kelarutan dalam toluena (1:1)	Warna	Titik lunak (°C)	Bilangan asam (mg KOH/g)	Bilangan Iod (mg iod/g)
140	Larut	11,3	81	183,05	28,31
160	Larut	11,9	81	176,75	28,88
180	Larut	15,6	81	176,04	30,67
200	Larut	16,6	83	175,30	31,84

4.2.1 Warna

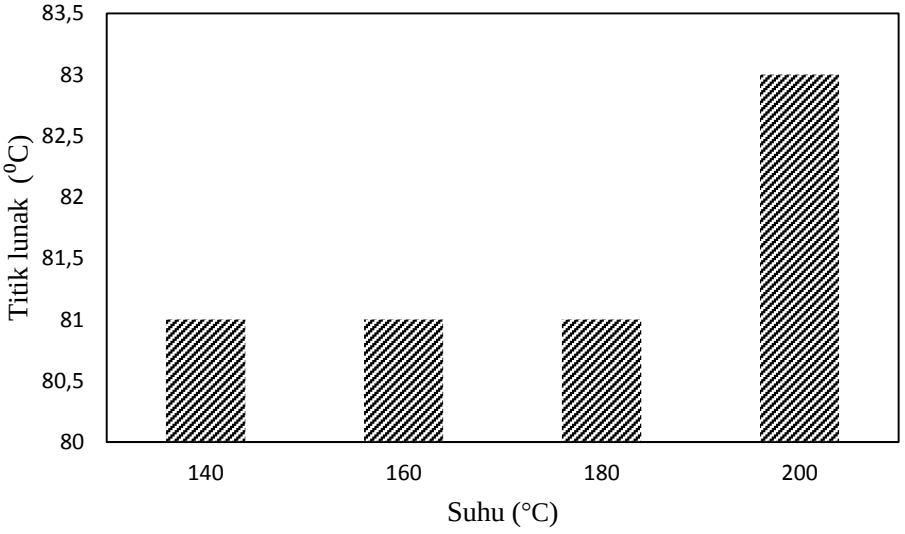
FMRE yang dihasilkan dari penelitian ini memiliki warna yang cukup gelap dari kuning kecoklatan hingga hitam kemerahan. Variasi warna ester gliserol tersebut sangat dipengaruhi oleh bahan baku awal dan metode pengolahannya (Kirk dan Othmer, 2007). Kualitas warna yang dihasilkan dari hasil esterifikasi ini lebih rendah dibandingkan dengan bahan baku awal hal ini dikarenakan gum rosin telah mengalami pemanasan berulangkali dengan waktu yang lama. Dari hasil analisis juga menunjukkan bahwa suhu reaksi sangat mempengaruhi warna dari ester yang terbentuk, terbukti dari data hasil analisis pada Tabel 4.2 yang menunjukkan semakin tinggi suhu reaksi yang digunakan maka warna yang dihasilkan akan semakin tinggi juga yang menunjukkan kualitas warna ester tersebut semakin rendah. Hasil analisis warna terbaik secara keseluruhan ditunjukkan pada suhu 140 °C. Gambar 4.1 dibawah disajikan hasil analisis warna dari ester, yang menunjukkan suhu sangat mempengaruhi kualitas warna dari ester yang terbentuk.



Gambar 4.1. Analisis warna FMRE

4.2.2 Titik Lunak

Titik lunak adalah suhu saat gum rosin mulai melunak, diukur dengan cincin dan bola (s*oftening ring and ball apparatus*) yang dinyatakan dalam derajat Celcius (°C) (SNI 7636:2011). Titik lunak FMRE yang dihasilkan berkisar antara 81-83 °C. Nilai titik lunak secara lengkap dapat dilihat pada Gambar 4.2.



Gambar 4.2 Analisis titik lunak FMRE

Nilai titik lunak FMRE yang dihasilkan lebih tinggi dibandingkan dengan gum rosin awal yaitu 78 °C. Nilai titik lunak pada Gambar 4.2 cenderung konstan.

Kenaikan terjadi pada suhu 200 °C. Besarnya nilai titik lunak ini terjadi karena suhu reaksi yang tinggi dalam waktu yang lama, sehingga tingkat kemasakan yang terjadi tinggi, menunjukkan semakin sedikit kadar terpentin yang tersisa. Penambahan gliserol pada proses esterifikasi ini bereaksi dengan gum rosin, selain itu diduga kadar terpentin yang tersisa sedikit, sehingga nilai titik lunak FMRE yang dihasilkan lebih tinggi dari gum rosin awal. Titik lunak menunjukan sifat khas gum rosin dan tingkat kemasakannya. Wiyono *et al*. (2007) menyatakan bahwa tingkat kemasakan berhubungan erat dengan kadar terpentin yang tersisa dalam gum rosin. Semakin kecil kadar terpentin sisa, semakin tinggi nilai titik lunaknya.

4.2.3 Kelarutan dalam Toluena (1:1)

FMRE yang dihasilkan larut dalam toluena dengan perbandingan 1:1. Hal ini karena toluena adalah hidrokarbon aromatik yang banyak digunakan dalam industri sebagai pelarut. Toluena adalah salah satu jenis pelarut yang bersifat non polar sehingga dapat melarutkan zat yang terdapat dalam rosin ester (Khadafi, *et al*., 2014). Kelarutan adalah kemampuan suatu zat terlarut untuk larut dalam suatu pelarut. Suatu senyawa dapat larut bergantung pada sifat fisik dan kimia zat terlarut dan pelarut, selain itu suhu, tekanan dan kepolaran juga akan mempengaruhi kelarutan. Kirk dan Othmer (2007) menyatakan bahwa gum rosin dapat larut pada hampir semua pelarut organik seperti etil alkohol, etil eter, benzena, dan larut dalam pelarut non polar seperti toluena. Senyawa yang bersifat non polar akan larut dalam pelarut non polar sedangkan senyawa semi polar akan larut dalam pelarut semi polar, serta senyawa yang bersifat polar akan larut kedalam pelarut polar (Sayuti, 2017). Komponen yang terkandung dalam bahan akan dapat larut pada pelarut yang relatif sama kepolarannya. Kriteria kepolaran suatu pelarut dapat ditinjau dari konstanta dielektrik dan momen dipol. Pelarut polar memiliki konstanta dielektrik yang besar, sedangkan non-polar memiliki konstanta dielektrik yang kecil. Semakin besar nilai konstanta dielektriknya, maka semakin polar senyawa tersebut. Tingkat polaritas pelarut dapat dilihat pada Tabel 4.3

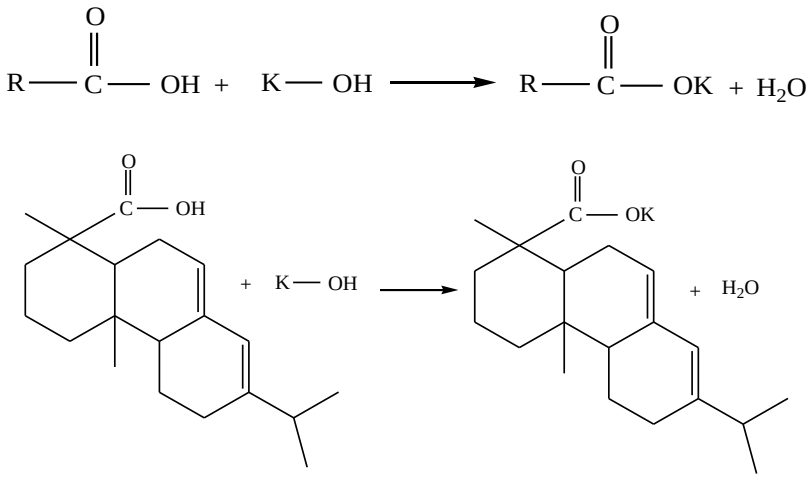
Tabel 4.3 Tingkat polaritas pelarut organik

Pelarut	Polaritas	Konstanta dielektrik
Air	Polar	80,1
Etilen glikol	Polar	37,7
Gliserol	Polar	42,5
Etanol	Polar	25
Methanol	Polar	33,6
Dimetil Sulfoksida	Semi polar	48,9
Dimetil Formamida	Semi polar	38,3
Aseton	Semi polar	20,7
Metil Klorida	Non polar	9,14
Benzena	Non polar	2,27
Toluena	Non polar	2,39
Heksan	Non polar	1,89

(Haidekker *et al*., 2005)

4.2.3 Bilangan Asam

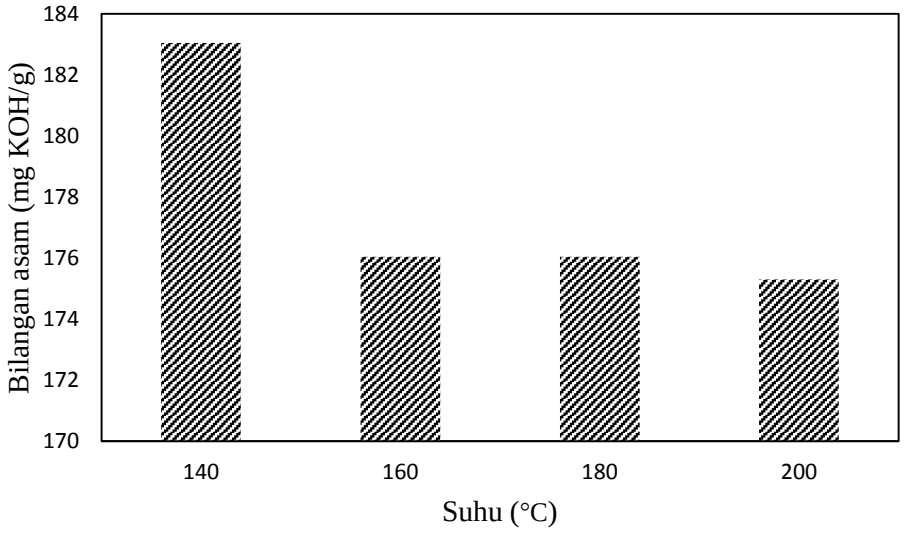
Bilangan asam didefinisikan sebagai banyaknya KOH dalam mg yang diperlukan untuk menetralkan satu gram asam resin yang terkandung dalam senyawa gum rosin (SNI 7636:2011). Reaksi pada bilangan asam disajikan pada Gambar 4.3



Gambar 4.3 Reaksi pada analisis biangan asam

Analisis bilangan asam dilakukan untuk mengetahui sisa asam lemak bebas yang terkandung di dalam produk. Sisa asam lemak tersebut memiliki hubungan dengan kandungan gliserol ester yang terbentuk (Wahyuni *et al*., 2016). Bilangan asam FMRE yang dihasilkan berkisar antara 175-183 °C. Mg KOH/g. Secara umum hasil analisis bilangan asam FMRE pada Gambar 4.4 mengalami penurunan dari

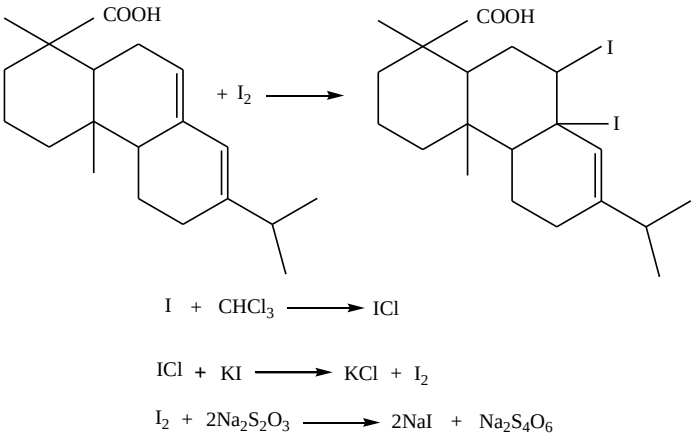
bilangan asam gum rosin awal, selain itu FMRE juga cenderung mengalami penurunan seiring dengan kenaikan suhu reaksi. Penurunan bilangan asam pada proses esterifikasi diduga karena gugus karboksil asam resin pada FMRE bereaksi dengan gliserol membentuk ikatan ester. Semakin lama proses esterifikasi maka semakin banyak asam lemak yang terkonversi. Atom –H sebagai pembawa sifat asam dari gugus karboksil asam resin berikatan dengan –OH dari gliserol. Hal ini menyebabkan jumlah atom –H dalam asam resin berkurang yang berdampak pada penurunan bilangan asam FMRE yang dihasilkan. Selain itu semakin lama reaksi menyebabkan tumbukan antar molekul reaktan semakin sering terjadi sehingga konversi produk menjadi semakin besar (Wahyuni *et al*., 2016). Hasil analisis terhadap bilangan asam FMRE disajikan pada Gambar 4.4.



Gambar 4.4 Bilangan asam FMRE

4.2.5 Bilangan Iod

Bilangan iod menunjukkan derajat ketidakjenuhan minyak dan lemak yang mengekspresikan jumlah yodium yang dapat diadsorpsi (Hasibuan dan Saihaan, 2013). Semakin besar bilangan iod maka derajat ketidakjenuhan semakin tinggi. Asam lemak yang tidak jenuh mampu menyerap sejumlah iod dan membentuk senyawa yang jenuh. Besarnya jumlah iod yang diserap menunjukkan banyaknya ikatan ragkap atau ikatan tidak jenuh. Gambar 4.5 merupakan reaksi pada pengujian bilangan iod

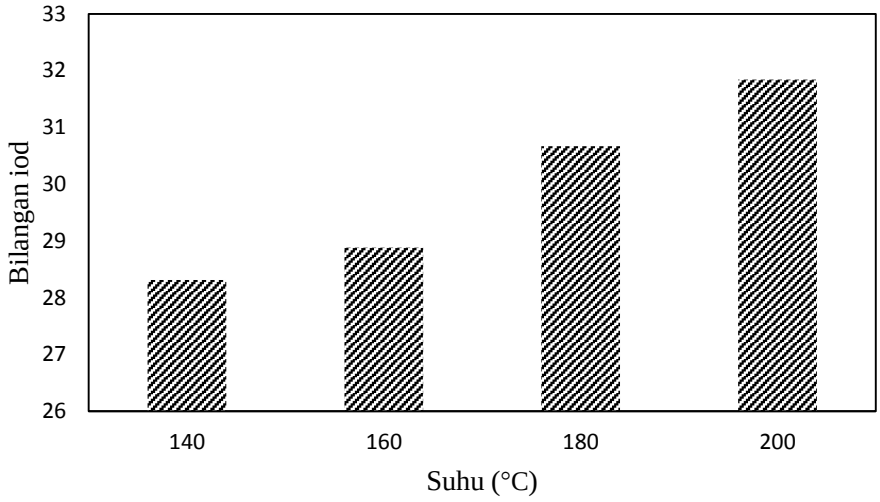


Gambar 4.5 Reaksi pada pengujian bilangan iod

Pengujian bilangan iod bertujuan untuk mengetahui banyaknya ikatan rangkap yang terkandung dalam gum rosin ester. Iodium bereaksi dengan ikatan rangkap dalam sampel gum rosin. Kejenuhan suatu minyak menandai jumlah ikatan rangkap yang terdapat didalamnya, menjadi acuan tingkat kemudahan suatu minyak-lemak teroksidasi, sekaligus mengindikasikan tinggi rendahnya titik cairnya. Semakin jenuh suatu minyak berarti semakin kecil pula jumlah ikatan rangkap pada asam resinnya, semakin sulit minyak untuk teroksidasi dan semakin tinggi titik cairnya. Hal tersebut berlaku sebaliknya. Penambahan kloroform dalam uji iod berfungsi untuk melarutkan minyak atau lemak gum rosin ester yang diuji. Dalam keadaan larut minyak atau lemak akan mudah bereaksi dengan reagen yang diberikan.

Jumlah ikatan rangkap dalam asam resin menentukan seberapa banyak atom I yang dapat bereaksi. Selanjutnya penambahan KI akan memecah kembali ikatan iodin dengan asam resin tersebut sehingga atom I yang sudah berikatan kembali terlepas dan membentuk senyawa I_2, senyawa I_2 inilah yang dijadikan representasi jumlah ikatan rangkap pada minyak atau lemak melalui titrasi dengan $Na_2S_2O_3$.

Bilangan iod FMRE yag dihasilkan dari percobaan ini berkisar antara 28-30 seperti yang terlihat pada Gambar 4.6 semakin tinggi suhu reaksi maka bilangan iod nya akan semakin tinggi pula hal tersebut menunjukkan suhu reaksi berpengaruh terhadap nilai bilangan iod dimana semakin tinggi suhu reaksi maka nilai bilangan iod akan semakin tinggi pula.



Gambar 4.6 Bilangan iod FMRE

4.3 Perbandingan Kualitas FMRE yang Dihasilkan degan Standar Produk China

Standar kualitas yang digunakan sebagai pembanding adalah standar kualitas gum rosin modifikasi dari China karena di Indonesia sendiri belum menerbitkan standar kualitas gum rosin modifikasi. Analisis yang dilakukan diantaranya warna, titik lunak, bilangan asam dan bilangan iod. Perbandingan hasil analisis fisikokimia FMRE dengan gum rosin modifikasi standar China dapat dilihat pada Tabel 4.4

Tabel 4.4 Perbandingan Sifat fisiko kimia FMRE dan gumrosin modifikasi standar China

Sifat fisisko kimia	Variasi Suhu (°C)				Standar China
	140	160	180	200	
	>N	>N	>N	>N	
Warna	11,3	11,9	15,6	16,6	8-9
Kelarutan dalam toluen (1:1)	Larut	Larut	Larut	Larut	Larut
Bilangan asam (mg KOHg)	183,05	176,77	176,04	175,36	5-8
Bilangan iod (%)	30,67	28,31	31,84	28,88	-
Titik Lunak (°C)	81	81	81	81	78-88

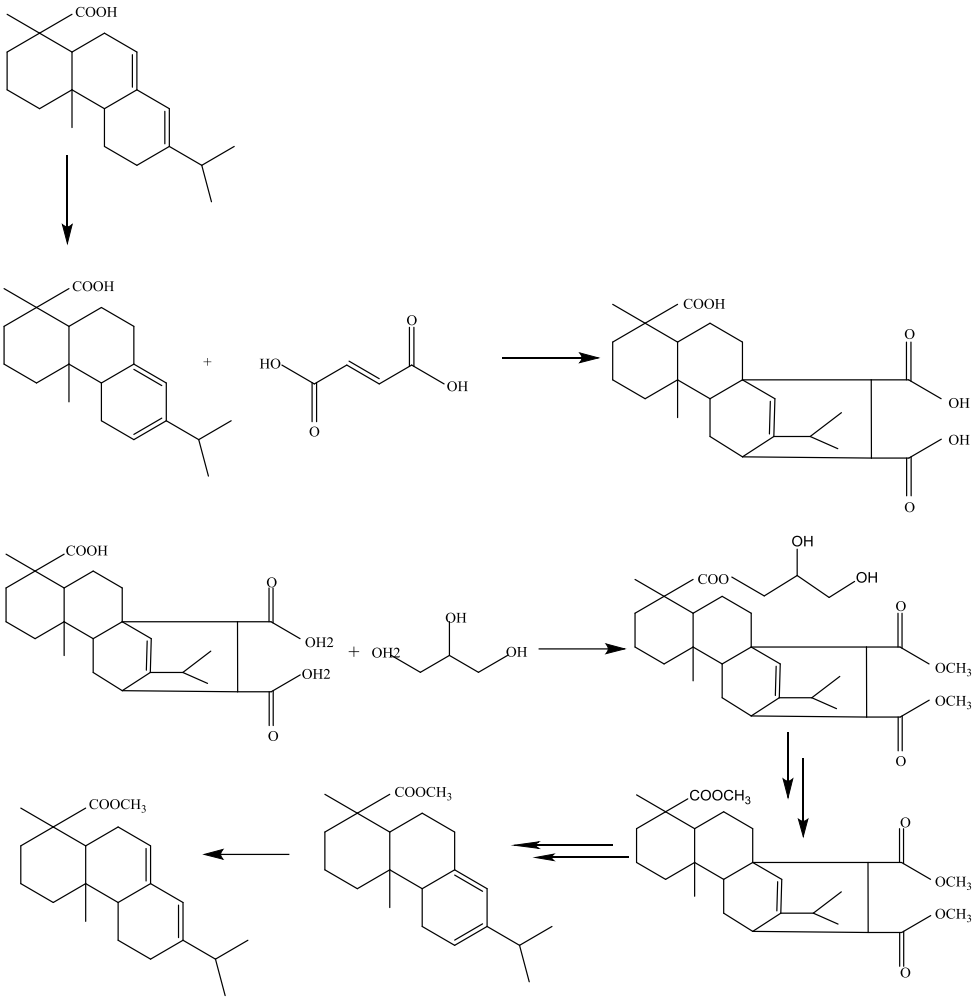
Warna FMRE yang dihasilkan belum memenuhi standar produk China yang menyaratkan rentang *grade* untuk warna adalah 8-9, sedangkan pada hasil analisis menujukkan warna ester yang dihasilkan >9. Proses pemanasan yang berulang pada suhu yang tinggi dan dalam waktu yang lama menyebabkan terjadinya penurunan

kualitas warna pada produk. Kirk dan Othmer (2007) menyatakan bahwa faktor yang sangat berpengaruh terhadap pengotoran warna gum rosin adalah pemanasan yang terlalu lama. FMRE dapat larut dalam toluena, kelarutan dinyatakan dalam jumlah maksimum zat yang larut dalam suatu pelarut. Toluena adalah salah satu jenis pelarut yang bersifat non polar sehingga dapat melarutkan zat yang terdapat dalam rosin ester (Khadafi, *et al*., 2014).

Titik lunak FMRE yang dihasilkan sudah memenuhi pada standar produk China yang menyaratkan nilai titik lunak 78-88 °C. Titik lunak yang tinggi dapat dipengaruhi oleh tingkat kemasakan. Tingkat kemasakan berhubungan erat dengan kadar terpentin yang tersisa dalam gum rosin. Makin kecil kadar terpentin sisa, makin tinggi nilai titik lunaknya (Wiyono *et al*., 2007).

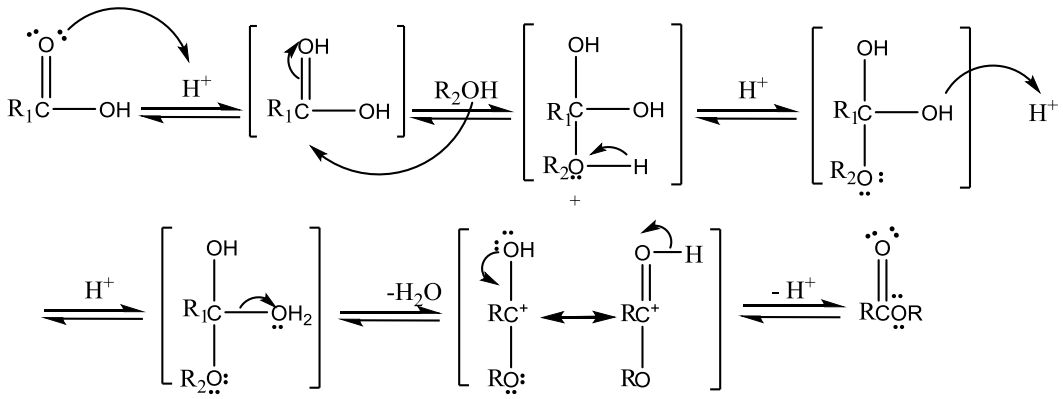
Selain warna dan titik lunak, bilangan asam merupakan salah satu sifat khas kimia gum rosin untuk mengetahui kualitas dari gum rosin tersebut. Salah satu tujuan utama proses esterifikasi gum rosin yaitu menurunkan bilangan asam agar dapat memperluas penggunaannya. Pada hasil analisis FMRE yang dihasilkan terjadi penurunan bilangan asam meskipun tidak secara sigifikan. Penurunan bilangan asam ini disebabkan gugus karboksil asam resin pada FMRE bereaksi dengan gliserol membentuk ikatan ester. Atom H sebagai pembawa sifat asam dari gugus karboksil asam resin berikatan dengan OH dari gliserol. Hal ini menyebabkan jumlah atom H dalam asam resin berkurang yang berdampak pada penurunan bilangan asam ester yang dihasilkan.

Reaksi esterifikasi pada dasarnya adalah penggantian hidrogen pada gugus karbonil dengan hidrokarbon atau alkil. Proses esterifikasi diawali dengan mencampurkan gum rosin dan gliserol dengan ratio mol 2 : 1, kemudian ditambahkan katalis PTSA (*p-toluene sulphonic acid*) dengan konsentrasi 0,3%. Reaksi esterifikasi ini bersifat *reversible* karena dikatalis oleh asam. Katalis asam menyebabkan asam karboksilat mengalami konyugasi (Widyarti dan Hanafi, 2008). Proses esterifikasi dilakukan pada suhu (140 °C, 160 °C, 180 °C, dan 200 °C) dengan lama waktu reaksi (1, 2, 3, dan 4 jam). Reaksi esterifikasi pada asam karboksilat dengan FA dan gliserol disajikan pada Gambar 4.7.



Gambar 4.7 Reaksi esterifikasi asam karboksilat

Pada proses esteriifikasi Gambar 4.7 ini asam-asam resin pada gum rosin yang mempunyai ikatan rangkap *s-trans* akan diubah menjadi asam levopimarat yang mempunyai ikatan rangkap *s-ciss*. Setelah berubah menjadi asam levopimarat kemudian akan bereaksi dengan asam fumarat, baru setelahnya direaksikan dengan alkohol untuk membentuk ester. Reaksi esterifikasi akan menghasilkan karbonil ester (RCOOR'). Produk FMRE yang dihasilkan merupakan campuran antara gliserol monoester, diester, triester, sisa katalis, sisa gliserol, air, dan asam lemak bebas. Sifat fisikokimia FMRE yang dihasilkan dipengaruhi oleh konfigurasi struktural asam lemak seperti struktur molekul, panjang rantai, tingkat kejenuhan, dan cabang rantai (Wahyuni *et al*., 2016). Mekanisme reaksi esterifikasi gum rosin fumarat dan gliserol dengan katalis PTSA disajikan pada Gambar 4.7.

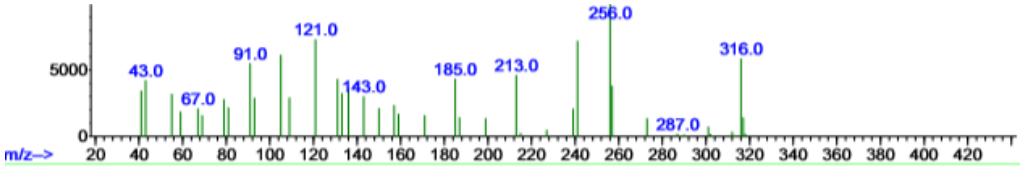


Gambar 4.8. Mekanisme reaksi esterifikasi FMRE

Keterangan : R_1 = Alkil dari asam-asam resin gum rosin

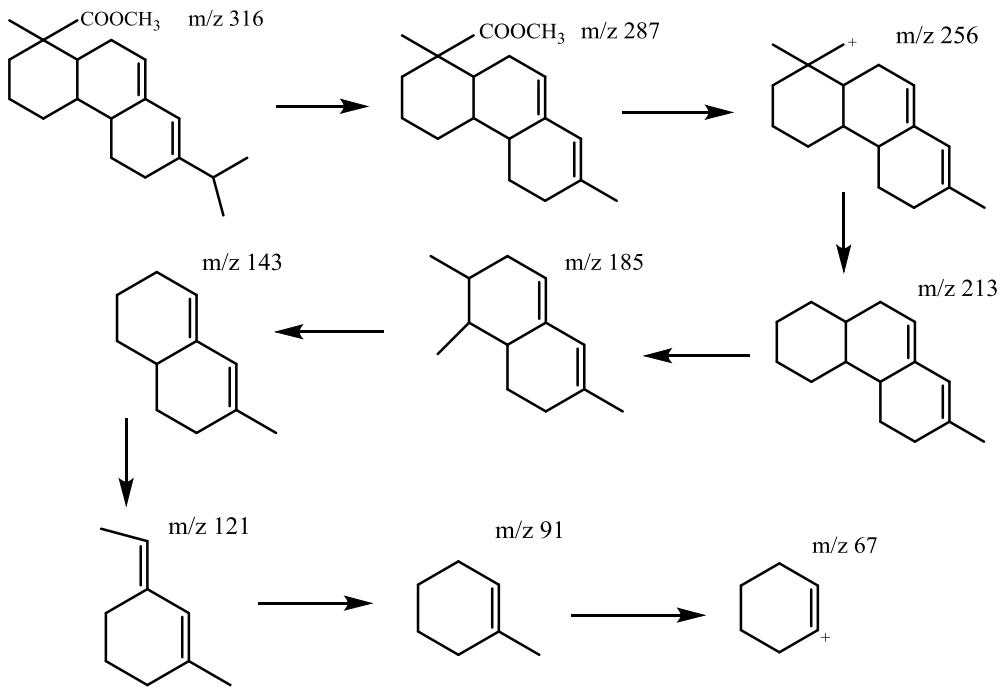
R_2 = Alkohol

Gambar 4.8 menjelaskan bahwa terjadi pembentukan senyawa proton pada asam karboksilat. Pada tahap ini terjadi perpindahan proton dari katalis asam atom oksigen pada gugus karboksil. Kemudian, pada tahapan berikutnya alkohol nukleofilik menyerang karbon positif pada atom karbon karbonil kemudian diserang oleh atom oksigen dari alkohol, yang bersifat nukleofilik sehingga terbentuk ion oksonium. Pada proses ini terjadi pelepasan proton atau deprotonasi dari gugus hidroksil milik alkohol, menghasilkan senyawa kompleks teraktivasi. Protonasi terhadap salah satu gugus hidroksil yang diikuti pelepasan molekul air menghasilkan ester (Prasetyo *et al*, 2012).



Gambar 4.9 Spektum abietat metil ester

Berdasarkan data library GC-MS pada Gambar 4.9 senyawa abietat metil ester mempunyai rumus molekul $C_{21}H_{32}O_2$ dengan berat molekul 316. Spektrum massa yang diperoleh, ion molekul dengan m/z 316 dengan puncak dasar m/z 256. Pola fragmentasi dari spektrum massa di interpretasikan pada reaksi yang disajikan pada Gambar 4.9.



Gambar 4.10 Pola fragmentasi abietat metil ester

Berdasarkan Gambar 4.9 dapat dilihat pola fragmentasi dari abietat metil ester diawali dari terbentuknya ion molekul dengan m/z 316. Puncak dasar dari fragmen atau *base peak* dengan m/z 256.

4.4 Analisis *Gas Chromatograph - Mass Spectrometer* (GC-MS)

Gas Chromatograph adalah analisis yang digunakan untuk mengetahui jumlah komponen yang dikandung oleh sampel gum rosin awal dan FMRE dari setiap perlakuan yang ditentukan dalam penelitian ini. Prinsip analisis kromatografi gas adalah pemisahan komponen berdasarkan perbedaan laju gerak komponen-komponen yang akan di identifikasi. Berat molekul dan polaritas komponen adalah faktor-faktor yang akan mempengaruhi perbedaan laju gerak tersebut. Komponen yang kan menguap pada waktu awal pemisahan komponen adalah komponen dengan berat molekul rendah dan polaritas yang rendah pula. Berdasarkan data hasil analisis GC-MS pada gum rosin dapat dilihat senyawa-senyawa yang terkandung dalam bahan baku gum rosin. Hasil analisis GC-MS gum rosin disajikan pada Tabel 4.5.

Tabel 4.5 Komponen penyusun gum rosin

Waktu retensi	Nama senyawa	Luas area (%)
35,09	Asam 1-fenatrenkarboksilat	0,76
35,16	Asam kaurnenoat	2,38
35,92	Asam abitat	45,85
36,10	Asam pimarat	6,10
36,69	Asam resin	39,46
36,90	Asam palustrat	5,43

Berdasarkan Tabel 4.5 dapat diketahui bahwa komponen senyawa-senyawa yang terdapat didalam gum rosin adalah asam-asam resin diantaranya yaitu asam 1-fenantrenkarboksilat pada waktu retensi 35,09 dengan kisaran luas area 0,76%, asam kaurenoat pada waktu retensi 35,16 dengan kisaran luas area 2,38%, asam abietat pada waktu retensi 35,92 dengan kisaran luas area mencapai 45,85%, asam pimarat pada waktu retensi 36,10 dengan kisaran luas area 6,10%, asam resin pada waktu retensi 36,69 dengan kisaran luas area mencapai 39,46% dan asam palustrat pada waktu retensi 36,90 dengan kisaran luas area 5,43%. dari keseluruhan asam-asam resin didapatkan senyawa asam resin yang memiliki luas area paling besar yaitu asam abietat dengan luas area yang mencapai 45,85%. Hasil analisis ini sesuai dengan pernyataan Wang *et al*. (2016) yang menyatakan bahwa gum rosin merupakan senyawa kompleks yang terdiri dari 70% asam abietat, asam pimarat, dan isomernya. Menurut Kaith *et al*. (2016) gum rosin terdiri dari asam resin seperti asam resin tipe abietat yang memiliki ikatan rangkap terkonjugasi dan asam resin tipe pimarat dengan ikatan rangkap non-terkonjugasi. Asam resin adalah campuran kompleks dari beberapa senyawa, terutama jenis abietat dan asam pimarat yang termasuk dalam kelompok senyawa organik yang diterpen (Jindal *et al*., 2017). Menurut Purnavita *et al*. (2017), gum rosin mengandung 90% asam resin dan 10% komponen selain asam resin, sedangkan kandungan asam karboksilat dalam gum rosin sebagian besar adalah asam abietat.

4.4.1 Sintesis FMRE dengan variasi suhu 140 °C dan waktu reaksi 1 jam

Analisis GC-MS atau Gass *Cromatogaph Mass Spectrometer* merupakan metode pemisahan senyawa organik yang menggunakan dua metode analisis senyawa yaitu kromatografi gas (GC) untuk menganalisis jumlah senyawa secara kuantitatif dan spektrometer massa (MS) untuk menganalsis struktur molekul senyawa analit. Berdasarkan hasil analisis GC-MS maka diperoleh senyawa-senyawa yang terkandung dalam FMRE dengan variasi suhu 140 °C dan waktu reaksi 1 jam seperti pada Table 4.6.

Tabel 4.6 Sintesis FMRE variasi suhu 140 °C; 1 jam

Waktu retensi	Nama senyawa	Luas area (%)
35,75	Dehidroabietat metil ester	1,66
36,09	Asam pimarat	5,80
36,38	Abietat metil ester	2,21
36,59	Asam isopimarat	17,13
36,95	Asam dehidroabietat	8,56
37,20	Asam dehidroepiebietat	0,55
37,31	Asam palustrat	0,55
37,69	Asam abietat	60,49
39,00	Asam pimarat	3,04

Berdasarkan hasil interpretasi analisis GC-MS dengan variasi suhu 140 °C dan waktu 1 jam, dapat diketahui bahwa komponen terbesar dari sampel gum rosin ester pada Tabel 4.6 adalah asam-asam resin, dengan kisaran area mencapai 96,13%. Asam-asam resin tersebut meliputi asam pimarat, asam isopimarat, asam dehidroabietat, asam dehidroepiabietat, asam palustrat, dan asam abietat, dan asam pimarat dengan total presentase luas area tertinggi yaitu asam abietat yaitu 60,49%. Hal ini dikarenakan waktu reaksi yang belum optimal sehingga asam-asam resin dan gliserol masih belum beraksi dengan sempurna. Sedangkan untuk ester yang terbentuk yaitu dehidroabietat metil ester pada retensi 35,75 dengan kisaran area 1,66%, dan abietat metil ester pada retensi 36,38 dengan kisaran area 2,21% sehingga total ester yang didapat pada variasi suhu 140 °C dengan waktu 1 jam yaitu dengan total presentase luas area hanya mencapai 3,87%.

4.4.2 Sintesis FMRE dengan variasi suhu 140 °C dan waktu reaksi 2 jam

Berdasarkan hasil analisis GC-MS maka diperoleh senyawa-senyawa yang terkandung dalam FMRE dengan variasi suhu 140 °C dan waktu reaksi 2 jam seperti pada Table 4.7.

Tabel 4.7 Sintesis FMRE variasi suhu 140 °C ; 2 jam

Waktu retensi	Nama senyawa	Luas area (%)
17,70	3-aminoksi-4-kloro-butirat ester	0,13
34,30	Metil pimara-8, 15-dien-18-oat	0,40
35,16	Antranilat, N-metil-, butil ester	0,27
35,27	3-(3,4,5-trimetoksifenil)-,metil ester	0,13
35,29	Benzenpropanoat, tert-butilmetilsilil ester	0,13
35,47	Asam rosin	7,26
35,75	Dehidroabietat metil ester	2,27
35,91	Asam kaurenoat	0,80
36,31	Asam pimarat	6,69
36,38	Abietat metil ester	2,94
36,58	Asam isopimarat	9,89
36,87	Asam palustrat	0,53
36,94	Asam dehidroabietat	11,63
37,16	Asam dehidroepiabietat	3,21
38,48	Asam abietat	53,35

Senyawa-senyawa yang merupakan komponen utama dari FMRE dapat dilihat pada Tabel 4.7 dari hasil interpretasi analisis GC-MS dengan variasi suhu 140 °C dan waktu 2 jam, dapat diketahui bahwa komponen terbesar dari sampel gum rosin ester pada Tabel 4.7 adalah asam-asam resin, dengan kisaran area mencapai 93,73%. Asam-asam resin tersebut meliputi asam kaurenoat, asam pimarat, asam dehidroabietat, asam abietat, asam palustrat dan asam dehidroepiabietat dengan nilai persentase luas area tertinggi adalah asam abietat yaitu 53,35%. Hal ini dikarenakan waktu reaksi yang belum optimal sehingga asam-asam resin dan gliserol masih belum beraksi dengan sempurna. Sedangkan untuk ester yang terbentuk yaitu 3-aminoksi-4-kloro-, butil ester pada waktu retensi 17,70 dengan kisaran area 0,13%, metil pimara-8, 15-dien-18-oat pada retensi 34,30 dengan kisaran area mencapai 0,40%, antranilat, N-metil-, butil ester pada retensi 35,27 dengan kisaran area 0,27%, 3-(3,4,5-trimetoksifenil)-, metil ester pada retensi 35,27 dengan kisaran area 0,13%, tert-butilmrtilsilil ester pada retensi 35,29 dengan kisaran area 0,13%, dehidroabietat metil ester pada retensi 35,75 dengan kisaran

area mencapai 2,27%, dan abietat metil ester pada retensi 36,38 dengan kisaran area mecapai 2,94% sehingga total ester yang didapat pada variasi suhu 140 °C dengan waktu 2 jam yaitu dengan total presentase luas area hanya mencapai 6,27%.

4.4.3 Sintesis FMRE dengan variasi suhu 140 °C dan waktu reaksi 3 jam

Berdasarkan hasil analisis GC-MS dengan variasi suhu 140 °C dan waktu reaksi 3 jam diperoleh senyawa-senyawa dalam FMRE seperti pada Table 4.8

Tabel 4.8 Sintesis FMRE variasi suhu 140 °C; 3 jam

Waktu retensi	Nama senyawa	Luas area (%)
28,61	Dietil ester malonat	0,16
32,40	Karbamat, 1-naphtalenil-, metil ester	0,16
34,32	Podocarp-8-en-15-oat, 13.alpha.-metil-13-vinil-, metil ester	0,47
34,53	1,4,8-siklodekatrien-1-karboksilat-12-etenil-metil ester	0,98
35,16	Antranilat, n-metil butil ester	0,49
35,40	Asetat-2-asetilamino-fenil ester	0,47
35,66	Asam isopimarat	1,25
35,76	Dehidroabietat metil ester	3,76
35,93	Asam palustrat	1,25
36,01	Asam kaurenoat	1,25
36,38	Abietat metil ester	3,76
36,96	Asam dehidroabietat	17,71
37,27	Asam levopimarat	4,08
38,48	Asam abietat	60,97

Senyawa-senyawa yang merupakan komponen utama dari FMRE dapat dilihat pada Tabel 4.8. Berdasarkan hasil interpretasi analisis GC-MS dengan variasi suhu 140 °C dan waktu 3 jam, dapat diketahui bahwa komponen terbesar dari sampel FMRE adalah asam-asam resin, dengan kisaran area mencapai 89,14%. Asam-asam resin tersebut meliputi asam kaurenoat, asam pimarat, asam dehidroabietat, asam abietat, asam palustrat dan asam levopimarat dengan nilai persentase luas area tertinggi adalah asam abietat yaitu 60,67%. Hal ini dikarenakan suhu reaksi yang belum optimal sehingga asam-asam resin dan gliserol masih belum beraksi dengan sempurna selain itu juga hasil yang terdeteksi pada GC-MS masih belum optimal. Sedangkan untuk ester yang terbentuk yaitu dietil ester malonat pada retensi 28,61 dengan kisaran area mencapai 0,16%, karbamat, 1-naptalenil-, metil ester pada retensi 32,40 dengan kisaran area mencapai 0,16%, podocarp-8-en-15-oat, 13.alpha.-metil-13-vinil-, metil ester pada retensi 33,86

dengan kisaran area mencapai 0,47%, 1,4,8-siklodekatrien-1-karboksilat-12-etenil-, metil ester, pada retensi 34,53 dengan kisaran area mencapai 0,98%, antranilat,n-metil butil ester pada retensi 35,16 dengan kisaran area 0,49%, asetat 2-acetilamino-fenil ester pada retensi 35,54 dengan kisaran area mencapai 0,47%, dehidroabietat metil ester pada retensi 35,76 dengan kisaran area mencapai 3,76% dan abietat metil ester pada retensi 36,38 dengan kisaran area mencapai 3,76%, sehingga total ester yang didapat pada variasi suhu 140 °C dengan waktu 3 jam yaitu dengan total presentase luas area mencapai 10,86%.

4.4.4 Sintesis FMRE dengan variasi suhu 140 °C dan waktu reaksi 4 jam

Berdasarkan data GC-MS yang telah didapatkan, produk hasil sintesis dari gum rosin fumarat dengan gliserol dengan menggunakan asam *p*-toluenasulfonat sebagai katalis pada variasi suhu reaksi 140 °C dan waktu reaksi 4 diperoleh senyawa-senyawa yang terkandung dalam produk akhir FMRE seperti yang tersaji pada Table 4.9.

Tabel 4.9 Sintesis FMRE variasi suhu 140 °C; 4 jam

Waktu Retensi	Nama Senyawa	Luas Area (%)
17,72	3,6,8-nonatrienat, 5-metil-etil ester	0,12
28,61	Dietil ester malonat	0,12
33,86	Metil bisnorabieta	0,85
34,30	Isopimarat metil ester	0,48
35,02	4,5-Bis-dimetoksimetil-oktanadioat, dimetil ester	0,48
35,15	Asam kaurenoat	0,24
35,19	Antranilat, n-metil, butil ester	0,24
35,39	Asam asetat 2-acetilamino-fenil ester	0,48
35,65	Asam pimarat	1,09
35,75	Dehidroabietat metil ester	3,39
35,92	Benza [a] antrasena	4,21
36,01	Asam pimarat	6,65
36,38	Abietat metil ester	2,90
36,47	Asam isopimarat	0,60
36,96	Asam dehidroabietat	6,65
37,24	Asam levopimarat	7,13
38,48	Asam abietat	59,26

Senyawa-senyawa yang merupakan komponen utama dari FMRE dapat dilihat pada Tabel 4.9. Hasil interpretasi analisis GC-MS dengan variasi suhu 140 °C dan waktu 4 jam, dapat diketahui bahwa komponen terbesar dari sampel FMRE adalah asam-asam resin, dengan kisaran area mencapai 92,27%. Asam-asam resin

tersebut meliputi asam kaurenoat, asam pimarat, asam dehidroabietat, asam abietat, asam palustrat, dan asam levopimarat dengan nilai persentase luas area tertinggi adalah asam abietat yaitu 59,26%. Hal ini dikarenakan suhu reaksi yang belum optimal sehingga asam-asam resin dan gliserol masih belum beraksi dengan sempurna selain itu juga hasil yang terdeteksi pada GC-MS masih belum optimal. Sedangkan untuk ester yang terbentuk yaitu 3,6,8-nonatrienat, 5-metil-etil ester pada retensi 17,72 dengan kisaran area mencapai 0,12%, dietil ester malonate pada retensi 28,61 dengan kisaran area mencapai 0,12%, isopimarat metil ester pada retensi 34,30 dengan kisaran area mencapai 0,48%, 4,5-Bis-dimetoksimetil-oktanadioat, dimetil ester pada retensi 35,02 dengan kisaran area mencapai 0,48%, asam asetat 2-acetilamino-fenil ester pada retensi 35,39 dengan kisaran area 0,48%, dehidroabietat metil ester pada retensi 35,75 dengan kisaran area mencapai 3,39%, dan abietat metil ester pada retensi 36,38 dengan kisaran area mecapai 2,90% sehingga total ester yang didapat pada variasi suhu 140 °C dengan waktu reaksi 4 jam yaitu dengan total presentase luas area hanya mencapai 7,73%.

4.4.5 Sintesis FMRE dengan variasi suhu 160 °C dan waktu reaksi 1 jam

Berdasarkan hasil analisis GC-MS maka diperoleh senyawa-senyawa yang terkandung dalam FMRE dengan variasi suhu 160 °C dan waktu reaksi 1 jam seperti pada Table 4.10.

Tabel 4.10 Sintesis FMRE variasi suhu 160 °C; 1 jam

Waktu Retensi	Nama Senyawa	Luas Area (%)
35,75	Dehidroabietat metil ester	6,36
36,09	Asam pimarat	7,73
36,38	Abietat metil ester	2,27
36,58	Asam kaurenoat	5,91
36,75	Asam palustrat	1,36
37,01	Asam dehidroabietat	9,09
37,66	Asam abietat	67,27

Senyawa-senyawa yang merupakan komponen utama dari FMRE dapat dilihat pada Tabel 4.10. Berdasarkan hasil interpretasi analisis GC-MS dengan variasi suhu 160 ^{0}C dan waktu 1 jam, dapat diketahui bahwa komponen terbesar dari sampel FMRE adalah asam-asam resin, dengan kisaran area mencapai 91,37%. Asam-asam resin tersebut meliputi asam kaurenoat, asam pimarat, asam

dehidroabietat, asam abietat, dan asam palustrat dengan nilai persentase luas area tertinggi adalah asam abietat yaitu 67,27%. Hal ini dikarenakan suhu reaksi yang tidak stabil sehingga hasil ester yang dihasilkan lebih rendah dari variasi suhu 140 °C dengan waktu 1 jam. Sedangkan untuk ester yang terbentuk yaitu dehidroabietat metil ester pada retensi 35,75 dengan kisaran area mencapai 6,36%, dan abietat metil ester pada retensi 36.38 dengan kisaran area mecapai 2,27%, sehingga total ester yang didapat pada variasi suhu 160 °C dengan waktu 1 jam yaitu dengan total presentase luas area sebesar 8,63%.

4.4.6 Sintesis FMRE dengan variasi suhu 160 °C dan waktu reaksi 2 jam

Berdasarkan hasil analisis GC-MS maka diperoleh senyawa-senyawa yang terkandung dalam FMRE dengan variasi suhu 160 °C dan waktu reaksi 2 jam seperti pada Table 4.11.

Tabel 4.11 Sintesis FMRE variasi suhu 160 °C; 2 jam

Waktu Retensi	Nama Senyawa	Luas Area (%)
34,30	Isopimarat metil ester	1,09
35,40	Asetat 2-asetilamino-fenil ester	0,54
35,75	Dehidroabietat metil ester	5,80
36,02	Asam pimarat	2,54
36,38	Abietat metil ester	2,72
36,76	Asam palustrat	1,99
36,86	Asam kaurenoat	0,18
37,04	Asam dehidroabietat	12,86
37,73	Asam abietat	69,56

Senyawa-senyawa yang merupakan komponen utama dari FMRE dapat dilihat pada Tabel 4.11. Berdasarkan hasil interpretasi analisis GC-MS dengan variasi suhu 160 °C dan waktu 2 jam, dapat diketahui bahwa komponen terbesar dari sampel FMRE adalah asam-asam resin, dengan kisaran area mencapai 89,85%. Asam-asam resin tersebut meliputi asam kaurenoat, asam pimarat, asam dehidroabietat, asam abietat, dan asam palustrat dengan nilai persentase luas area tertinggi adalah asam abietat yaitu 69,56%. Hal ini dikarenakan suhu reaksi yang tidak stabil sehingga asam-asam resin dan gliserol masih belum beraksi dengan sempurna selain itu juga hasil yang terdeteksi pada GC-MS masih belum optimal. Sedangkan untuk ester yang terbentuk yaitu metil esterpada retensi 34,30 dengan kisaran area mencapai 1,09%, Asetat 2-asetilamino-fenil ester pada retensi 35,40

dengan kisaran area mencapai 0,54%, dehidroabietat metil ester pada retensi 35,75 dengan kisaran area mencapai 5,80%, dan abietat metil ester pada retensi 36,38 dengan kisaran area mencapai 2,72%, sehingga total ester yang didapat pada variasi suhu 160 °C dengan waktu reaksi 2 jam yaitu dengan total presentase luas area mencapai 10,15%.

4.4.7 Sintesis FMRE dengan variasi suhu 160 °C dan waktu reaksi 3 jam

Berdasarkan hasil analisis GC-MS maka diperoleh senyawa-senyawa yang terkandung dalam FMRE dengan variasi suhu 160 °C dan waktu reaksi 3 jam seperti pada Table 4.12.

Tabel 4.12 Sintesis FMRE variasi suhu 160 °C;3 jam

Waktu Retensi	Nama Senyawa	Luas Area (%)
34,31	Metil pimarat	1,16
35,75	Dehidroabietat metil ester	6,71
35,90	Asam pimarat	0,93
36,11	Asam palustrat	4,50
36,38	Abietat metil ester	2,08
37,03	Asam isopimarat	16,20
37,26	Asam abietat	67,82

Senyawa-senyawa yang merupakan komponen utama dari FMRE dapat dilihat pada Tabel 4.12. Berdasarkan hasil interpretasi analisis GC-MS dengan variasi suhu 160 °C dan waktu reaksi 3 jam, dapat diketahui bahwa komponen terbesar dari sampel FMRE adalah asam-asam resin, dengan kisaran area mencapai 90,05%. Asam-asam resin tersebut meliputi asam pimarat, asam abietat, asam palustrat dan asam isopimarat dengan nilai persentase luas area tertinggi adalah asam abietat yaitu 67,82%. Hal ini dikarenakan suhu reaksi yang tidak stabil sehingga asam-asam resin dan gliserol masih belum beraksi dengan sempurna selain itu juga hasil yang terdeteksi pada GC-MS masih belum optimal. Sedangkan untuk ester yang terbentuk yaitu metil pimarat padaretensi 34,31 dengan kisaran area mencapai 1,16%, dehidroabietat metil ester pada retensi 35,75 dengan kisaran area mencapai 6,71%, dan abietat metil ester pada retensi 36,38 dengan kisaran area mecapai 2,08% sehingga total ester yang didapat pada variasi suhu 160 °C dengan waktu reaksi 3 jam yaitu dengan total presentase luas area mencapai 9,95%.

4.4.8 Sintesis FMRE dengan variasi suhu 160 °C dan waktu reaksi 4 jam

Berdasarkan hasil analisis GC-MS maka diperoleh senyawa-senyawa yang terkandung dalam FMRE dengan variasi suhu 160 °C dan waktu reaksi 4 jam seperti pada Table 4.13.

Tabel 4.13 Sintesis FMRE variasi suhu 160 °C ; 4 jam

Waktu retensi	Nama senyawa	Luas area (%)
2,06	Formiat propil ester	0,16
33,79	2,7-dimetiloct-7-en-5-yn-4-yl ester	0,32
33,86	Metil bisnorabieta	1.11
34,31	Isopimarat metil ester	0,80
34,53	Asam kaurenoat	0,96
35,02	Oktadionat, dimetil ester	0,64
35,13	Antranilat, n-metil, butil ester	0,32
35,76	Dehidroabietat metil ester	3,82
35,90	Benza [a] antrasena	1,11
35,93	Asam pimarat	0,96
36,25	Asam palustrat	5,41
36,38	Abietat metil ester	3,03
36,97	Asam dehidroabietat	16,24
37,68	Asam abietat	58,28

Senyawa-senyawa yang merupakan komponen utama dari FMRE dapat dilihat pada Tabel 4.13. Berdasarkan hasil interpretasi analsis GC-MS dengan variasi suhu 160 °C dan waktu 4 jam, dapat diketahui bahwa komponen terbesar dari sampel FMRE adalah asam-asam resin, dengan kisaran area mencapai 86,69%. Asam-asam resin tersebut meliputi asam kaurenoat, asam pimarat, asam abietat, asam palustrat dan asam dehidroabietat dengan nilai persentase luas area tertinggi adalah asam abietat yaitu 58,28%. Hal ini dikarenakan suhu reaksi yang belum optimal dan tidak stabil sehingga jumlah ester yang didapatkan hanya sedikit, asam-asam resin dan gliserol masih belum beraksi dengan sempurna selain itu juga hasil yang terdeteksi pada GC-MS masih belum optimal. Sedangkan untuk ester yang terbentuk yaitu formiat propil ester pada retensi 2,06 dengan kisaran area mencapai 0,16%, 2,7-dimetiloct-7-en-5-yn-4-yl ester pada retensi 33,79 dengan kisaran area mencapai 0,32%, isopimarat metil ester pada retensi 34,31 dengan kisaran area mencapai 0,80%, oktadionat dimetil ester pada retensi 35,02 dengan kisaran area mencapai 0,64%, dehidroabietat metil ester pada retensi 35,76 dengan kisaran area mencapai 3,82%, dan abietat metil ester pada retensi 36,38 dengan kisaran area

mecapai 3,03% sehingga total ester yang didapat pada variasi suhu 160 °C dengan waktu reaksi 4 jam yaitu dengan total presentase luas area mencapai 11,31%.

4.4.9 Sintesis FMRE dengan variasi suhu 180 °C dan waktu reaksi 1 jam

Berdasarkan hasil analisis GC-MS maka diperoleh senyawa-senyawa yang terkandung dalam FMRE dengan variasi suhu 180 °C dan waktu reaksi 1 jam seperti pada Table 4.14.

Tabel 4.14 Sintesis FMRE variasi suhu 180 °C; 1 jam

Waktu Retensi	Nama Senyawa	Luas Area (%)
35,46	Asam pimarat	7,49
35,75	Dehidroabietat metil ester	1,95
36,38	Abietatmetil ester	1,95
36,59	Asam kaurenoat	14,66
36,94	Asam dehidroabietat	7,17
37,69	Asam abietat	66,78

Senyawa-senyawa yang merupakan komponen utama dari FMRE dapat dilihat pada Tabel 4.14. Berdasarkan hasil interpretasi analisis GC-MS dengan variasi suhu 180 °C dan waktu 1 jam, dapat diketahui bahwa komponen terbesar dari sampel FMRE adalah asam-asam resin, dengan kisaran area mencapai 96,1%. Asam-asam resin tersebut meliputi asam kaurenoat, asam pimarat, asam dehidroabietat dan asam abietat dengan nilai persentase luas area tertinggi adalah asam abietat yaitu 66,78%. Hal ini dikarenakan waktu reaksi yang belum optimal dan suhu reaksi yang belum stabil sehingga asam-asam resin dan gliserol masih belum beraksi dengan sempurna selain itu juga hasil yang terdeteksi pada GC-MS masih belum optimal. Sedangkan untuk ester yang terbentuk yaitu dehidroabietat metil ester pada retensi 35,75 dengan kisaran area mencapai 1,95%, dan abietat metil ester pada retensi 36,38 dengan kisaran area mecapai 1,95% sehingga total ester yang didapat pada variasi suhu 180 °C dengan waktu reaksi 1 jam yaitu dengan total presentase luas area hanya 3,9%.

4.4.10 Sintesis FMRE dengan variasi suhu 180 °C dan waktu reaksi 2 jam

Berdasarkan hasil analisis GC-MS maka diperoleh senyawa-senyawa yang terkandung dalam FMRE dengan variasi suhu 180 °C dan waktu reaksi 2 jam seperti pada Table 4.15.

Tabel 4.15 Sintesis FMRE variasi suhu 180 °C ; 2 jam

Waktu retensi	Nama senyawa	Luas area (%)
2,07	Asetat, trifluoro-, desill ester	0,35
33,85	Metil bisnorabieta	0,87
34,30	Metil -13-vinil-, metil ester	0,69
35,75	Dehidroabietat metil ester	4,33
35,90	Asam kaurenoat	1,73
36,27	Asam pimarat	0,87
36,38	Abietat metil ester	2,94
36,74	Asam palustrat	5,02
37,22	Asam dehidroabiatat	15,91
39,30	Asam abietat	58,83

Senyawa-senyawa yang merupakan komponen utama dari FMRE dapat dilihat pada Tabel 4.15. Berdasarkan hasil interpretasi analisis GC-MS pada Tabel 4.13 dengan variasi suhu 180 °C dan waktu 2 jam, dapat diketahui bahwa komponen terbesar dari sampel FMRE adalah asam-asam resin, dengan kisaran area mencapai 90,82%. Asam-asam resin tersebut meliputi asam kaurenoat, asam pimarat, asam dehidroabietat, asam abietat, asam palustrat dan asam isopimarat dengan nilai persentase luas area tertinggi adalah asam abietat yaitu 58,83%. Hal ini dikarenakan suhu reaksi yang belum optimal sehingga asam-asam resin dan gliserol masih belum beraksi dengan sempurna selain itu juga hasil yang terdeteksi pada GC-MS masih belum optimal. Sedangkan untuk ester yang terbentuk yaitu Asetat, trifluoro-, desil ester pada retensi 2,07 dengan kisaran area mencapai 0,35%, metil-13-vinil-metil ester pada retensi 34,30 dengan kisaran area mencapai 0,69%, dehidroabietat metil ester pada retensi 35,75 dengan kisaran area mencapai 4,33%, dan abietat metil ester pada retensi 36,38 dengan kisaran area mecapai 2,94% sehingga total ester yang didapat pada variasi suhu 180 °C dengan waktu reaksi 2 jam yaitu dengan total presentase luas area mencapai 9,18%.

4.4.11 Sintesis FMRE dengan variasi suhu 180 °C dan waktu reaksi 3 jam

Berdasarkan hasil analisis GC-MS maka diperoleh senyawa-senyawa yang terkandung dalam FMRE dengan variasi suhu 180 °C dan waktu reaksi 3 jam seperti pada Table 4.16.

Tabel 4.16 Sintesis FMRE variasi suhu 180 °C ; 3 jam

Waktu retensi	Nama senyawa	Luas area (%)
1,97	Glikolat etil ester	1,31
33,87	Metal bisnorabieta	1,50
35,64	Asam isopimarat	2,25
35,75	Dehidroabietat metil ester	4,87
36,10	Asam palustrat	5,88
36,38	Abietat metil ester	1,12
36,76	Benza [a] antrasena	4,31
37,04	Asam dehidroabietat	20,97
37,24	Asam abietat	63,67

Senyawa-senyawa yang merupakan komponen utama dari FMRE dapat dilihat pada Tabel 4.16. Berdasarkan hasil interpretasi analisis GC-MS dengan variasi suhu 180 °C dan waktu 3 jam, dapat diketahui bahwa komponen terbesar dari sampel FMRE adalah asam-asam resin. Asam-asam resin tersebut meliputi asam abietat, asam palustrat, dan asam dehidroabietat dengan nilai persentase luas area tertinggi adalah asam abietat yaitu 63,67%. Hal ini dikarenakan suhu reaksi yang belum optimal sehingga asam-asam resin dan gliserol masih belum beraksi dengan sempurna selain itu juga hasil yang terdeteksi pada GC-MS masih belum optimal. Sedangkan untuk ester yang terbentuk yaitu glikolat etil ester pada retensi 1,97 dengan kisaran area mencapai 1,31%, dehidroabietat metil ester pada retensi 35,75 dengan kisaran area mencapai 4,87%, dan abietat metil ester pada retensi 36,38 dengan kisaran area mecapai 1,12% sehingga total ester yang didapat pada variasi suhu 180 °C dengan waktu 3 jam yaitu dengan total presentase luas area mencapai 10,68%.

4.4.12 Sintesis FMRE dengan variasi suhu 180 °C dan waktu reaksi 4 jam

Berdasarkan hasil analisis GC-MS maka diperoleh senyawa-senyawa yang terkandung dalam FMRE dengan variasi suhu 180 °C dan waktu reaksi 4 jam seperti pada Table 4.17.

Tabel 4.17 Sintesis FMRE variasi suhu 180 °C ; 4 jam

Waktu retensi	Nama senyawa	Luas area (%)
2,07	Formiat propil ester	0,17
17,72	Propanadioat, (hidroksiamino)-dietil ester	0,17
33,86	Metil bisnorabieta	1,18
34,30	Isodekstropimarat metal ester	0,68
34,90	Beta-dihidroagarofuran	0,17
35,12	Tert-butildimetilsilil ester	0,17
35,30	Antranilat, n-metil, butil ester	0,34
35,39	Asetat 2-asetilamino-fenil ester	0,68
35,66	Asam isopimarat	2,03
35,75	Dehidroabietat metil ester	4,40
35,90	Benza [a] antrasena	2,03
35,99	Asam pimarat	0,85
36,09	Asam palustrat	3,56
36,38	Abietat metil ester	3,21
37,40	Asam abietat	79,53

Senyawa-senyawa yang merupakan komponen utama dari FMRE dapat dilihat pada Tabel 4.17. Berdasarkan hasil interpretasi analisis GC-MS dengan variasi suhu 180°C dan waktu 4 jam, dapat diketahui bahwa komponen terbesar dari sampel FMRE adalah asam-asam resin, dengan kisaran area mencapai 86,63%. Asam-asam resin tersebut meliputi asam asam pimarat, asam abietat, asam palustrat dan asam isopimarat dengan nilai persentase luas area tertinggi adalah asam abietat yaitu 79,53%. Hal ini dikarenakan suhu reaksi yang belum optimal sehingga asam-asam resin dan gliserol masih belum beraksi dengan sempurna selain itu juga hasil yang terdeteksi pada GC-MS masih belum optimal. Sedangkan untuk ester yang terbentuk yaitu formiat propil ester pada retensi 2,07 dengan kisaran area mencapai 0,17%, Propanadioat, (hidroksiamino)-dietil ester, pada retensi 17,72 dengan kisaran area mencapai 0,17%, metil pimarat pada retensi 34,30 dengan kisaran area mencapai 0,68%, Tert-butildimetilsilil ester pada retensi 35,12 dengan kisaran area mencapai 0,17%, Asetat-2-acetilamino-fenil ester pada retensi 35,39 dengan kisaran area mencapai 0,68%, dehidroabietat metil ester pada retensi 35,75 dengan

kisaran area mencapai 4,40%, dan abietat metil ester pada retensi 36,38 dengan kisaran area mecapai 3,21% sehingga total ester yang didapat pada variasi suhu 180 °C dengan waktu reaksi 4 jam yaitu dengan total presentase luas area mencapai 13,37%.

4.4.3 Sintesis FMRE dengan variasi suhu 200 °C dan waktu reaksi 1 jam

Berdasarkan hasil analisis GC-MS maka diperoleh senyawa-senyawa yang terkandung dalam FMRE dengan variasi suhu 200 °C dan waktu reaksi 1 jam seperti pada Table 4.18.

Tabel 4.18 Sintesis FMRE variasi suhu 200 °C; 1 jam

Waktu Retensi	Nama Senyawa	Luas Area (%)
35,75	Dehidroabietat metil ester	3,79
36,38	Abietat metil ester	1,26
36,61	Asam rosin	1,05
36,75	Asam pimarat	5,27
37,04	Asam dehidroabietat	23,18
37,24	Asam abietat	65,32

Senyawa-senyawa yang merupakan komponen utama dari FMRE dapat dilihat pada Tabel 4.18. Berdasarkan hasil interpretasi analisis GC-MS dengan variasi suhu 200 °C dan waktu 1 jam, dapat diketahui bahwa komponen terbesar dari sampel FMRE adalah asam-asam resin. Asam-asam resin tersebut meliputi asam pimarat, asam dehidroabietat, asam abietat, dan asam rosin dengan nilai persentase luas area tertinggi adalah asam abietat yaitu 65,32%. Hal ini dikarenakan waktu reaksi yang belum optimal sehingga asam-asam resin dan gliserol masih belum beraksi dengan sempurna selain itu juga hasil yang terdeteksi pada GC-MS masih belum optimal. Sedangkan untuk ester yang terbentuk yaitu dehidroabietat metil ester pada retensi 35,75 dengan kisaran area mencapai 3,79%, dan abietat metil ester pada retensi 36,38 dengan kisaran area mecapai 1,26% sehingga total ester yang didapat pada variasi suhu 200 °C dengan waktu 1 jam yaitu dengan total presentase luas area hanya mencapai 5,05%.

4.4.14 Sintesis FMRE dengan variasi suhu 200 °C dan waktu reaksi 2 jam

Berdasarkan hasil analisis GC-MS maka diperoleh senyawa-senyawa yang terkandung dalam FMRE dengan variasi suhu 200 °C dan waktu reaksi 2 jam seperti pada Table 4.19.

Tabel 4.19 Sintesis FMRE variasi suhu 200 °C; 2 jam

Waktu retensi	Nama senyawa	Luas area (%)
17,70	3,6,8-nonatrienoat, 5-metil-etil ester	0,17
34,30	Isopimarat metil ester	0,83
35,02	4,5-bis-dimetoksimetil-oktanadioat dimetil ester	0,50
35,11	2-metilpropil ester	0,33
35,38	Asetat 2-acetilamino-fenil ester	0,67
35,75	Dehidroabietat metil ester	4,99
36,18	Asam pimarate	0,67
36,38	Abietat metil ester	3,33
36,50	Asam palustrat	2,00
36,97	Asam dehidroabietat	24,12
38,49	Asam abietat	62,39

Senyawa-senyawa yang merupakan komponen utama dari FMRE dapat dilihat pada Tabel 4.19. Berdasarkan hasil interpretasi analisis GC-MS dengan variasi suhu 200 °C dan waktu 2 jam, dapat diketahui bahwa komponen terbesar dari sampel FMRE adalah asam-asam resin, dengan kisaran area mencapai 89,18%. Asam-asam resin tersebut meliputi asam pimarat, asam palustrat, asam dehidroabietat, dan asam abietat, dengan nilai persentase luas area tertinggi adalah asam abietat yaitu 62,39%. Hal ini dikarenakan waktu reaksi yang belum optimal sehingga asam-asam resin dan gliserol masih belum beraksi dengan sempurna selain itu juga hasil yang terdeteksi pada GC-MS masih belum optimal. Sedangkan untuk ester yang terbentuk yaitu 3,6,8-nonatrienoat, 5-metil-etil ester pada retensi 17,70 dengan kisaran area mencapai 0,17%, isopimarat metil ester pada retensi 34,30 dengan kisaran area mencapai 0,83%, 4,5-bis-dimetoksimetil-oktanadioat dimetil ester pada retensi 35,02 dengan kisaran area mencapai 0,50%, Asetat-2-asetilamino-fenil ester pada retensi 35,38 dengan kisaran area mencapai 0,67%, dehidroabietat metil ester pada retensi 35,75 dengan kisaran area mencapai 4,99%, dan abietat metil ester pada retensi 36,38 dengan kisaran area mecapai 3,33% sehingga total ester yang didapat pada variasi suhu 200 °C dengan waktu reaksi 2

jam yaitu dengan total presentase luas area mencapai 10,82%, hal ini menunjukkan bahwa lamanya waktu reaksi berengaruh nyata terhadap total ester yang di peroleh.

4.4.15 Sintesis FMRE dengan variasi suhu 200 °C dan waktu reaksi 3 jam

Berdasarkan hasil analisis GC-MS maka diperoleh senyawa-senyawa yang terkandung dalam FMRE dengan variasi suhu 200 °C dan waktu reaksi 3 jam seperti pada Table 4.20.

Tabel 4.20 Sintesis FMRE variasi suhu 200 °C; 3 jam

Waktu retensi	Nama senyawa	Luas area (%)
33,85	Metil bisnorabieta	2,95
35,48	5,8-dimetilbeliidinofolin	27,87
35,67	1-sikllopentil-5-hidroksi-2-metil-, etil ester	3,28
35,75	Dehidroabietat metil ester	5,57
36,38	Abietat metil ester	0,98
36,97	Asam dehidroabietat	6,89
37,03	Asam penantrenkarboksilat	16,72
37,23	Asam abietat	35,74

Senyawa-senyawa yang merupakan komponen utama dari FMRE dapat dilihat pada Tabel 4.20 Berdasarkan hasil interpretasi analisis GC-MS dengan variasi suhu 200 °C dan waktu 3 jam, dapat diketahui bahwa komponen terbesar dari sampel FMRE adalah asam-asam resin, dengan kisaran area mencapai 59,35%. Asam-asam resin tersebut meliputi asam dehidroabietat, asam penantrenkarboksilat, dan asam abietat dengan nilai persentase luas area tertinggi adalah asam abietat yaitu 35,74%. Sedangkan untuk ester yang terbentuk yaitu 1-siklopentil-5-hidroksi-2-metil-, etil ester pada retensi 35,67 dengan kisaran area 3,28%, dehidroabietat metil ester pada retensi 35,75 dengan kisaran area mencapai 5,57%, dan abietat metil ester pada retensi 36,38 dengan kisaran area mecapai 0,98% sehingga total ester yang didapat pada variasi suhu 200 °C dengan waktu reaksi 3 jam yaitu dengan total presentase luas area mencapai 40,65%. Total ester pada waktu reaksi 3 jam mengalami peningkatan yang cukup signifikan dari waktu reaksi 2 jam.

4.4.16 Sintesis FMRE dengan variasi suhu 200 °C dan waktu reaksi 4 jam

Berdasarkan hasil analisis GC-MS maka diperoleh senyawa-senyawa yang terkandung dalam FMRE dengan variasi suhu 200 °C dan waktu reaksi 4 jam seperti pada Table 4.21.

Tabel 4.21 Sintesis FMRE variasi suhu 200 °C; 4 jam

Waktu retensi	Nama senyawa	Luas area (%)
33,04	Karbamat, (2-kloroetiliden), dietil ester	0,33
34,30	Isopimarat metil ester	0,66
34,72	4-pentana (dithioic) metil ester	0,33
35,16	Antranilat, n-metil-, butil ester	0,50
35,48	Pine rosin mixture	17,69
35,66	1-siklopentil-5-hidroksi-2-metil-, etil ester	2,31
35,75	Dehidroabietat metil ester	4,30
36,25	Asam Pimarat	2,15
36,37	Kauren-18-karboksilat metil ester	2,64
37,03	4-hidroksi-7-(trifluorometil)-, etil ester	12,72
39,02	Asam abietat	56,35

Hasil total senyawa ester yang didapatkan yaitu 41,48% pada variasi suhu 200 °C dan waktu reaksi 4 jam yang merupakan total ester tertinggi. dapat diketahui bahwa senyawa-senyawa ester yang terbentuk yaitu dehidroabietat metil ester, karbamat, (2-kloroetiliden), dietil ester, 4-pentana (dithioic) metil ester, antranilat, n-metil-, butil ester, 1-siklopentil-5-hidroksi-2-metil-, etil ester, kauren-18-karboksilat-metil ester, dan isopimarat metil ester, sedangkan sisanya adalah asam-asam resin seperti asam abietat dan asam pimarat. dengan total kisaran area asam abietat mencapai 56,35 %. Hal ini mungkin dikarenakan waktu reaksi dan suhu reaksi yang belum optimal sehingga asam-asam resin dan gliserol masih belum beraksi dengan sempurna selain itu juga hasil yang terdeteksi pada GC-MS masih belum optimal dikarenakan suhu reaksi yang kemungkinan masih kurang tinggi dan tidak stabil saat proses esterifikasi berlangsung. Banyak rintangan sterik sehingga proses esterifikasi tidak berlangsung secara keseluruhan seperti yang dijelaskan oleh Arieta *et al*. (2008), bahwa laju esterifikasi asam karboksilat tergantung pada halangan sterik dalam alkohol dan asam karboksilat. Terbentuknya air mengakibatkan terjadinya reaksi kearah produk atau terjadi proses hidrolisis. Namun demikian total ester yang didapat cukup tinggi, sekitar 41,48% dan sudah

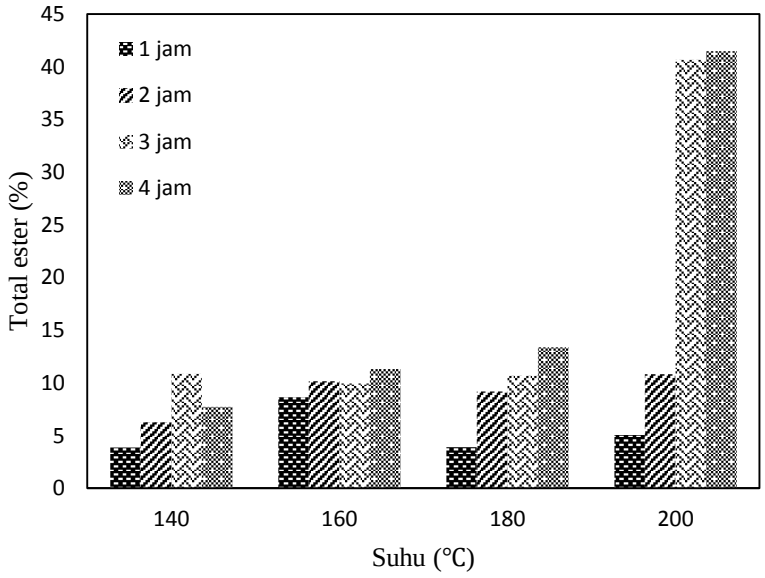
mengalami perubahan sifat fisikokimia sesuai dengan standar China yang menunjukkan gum rosin sudah termodifikasi.

Seperti tersaji dalam Tabel 4.22 dapat dilihat total senyawa ester dari hasil analisis GC-MS variasi suhu 140 °C, 160 °C, 180 °C, dan 200 °C dan waktu 1-4 jam. senyawa target dalam proses esterifikasi ini adalah total senyawa ester yang terkandung dalam FMRE dan seyawa senyawa lainya seperti asam-asam resin, alkohol, dan derivat lainnya.

Tabel 4.22 Total ester hasil analisis GC-MS FMRE

Waktu (jam)	Total ester (%)			
	140 °C	160 °C	180 °C	200 °C
1	3,87	8,63	3,9	5,05
2	6,27	10,15	9,18	10,82
3	10,86	9,95	10,68	40,65
4	7,73	11,31	13,37	41,48

Hasil analisis GC-MS FMRE pada Tabel 4.22 dapat diketahui bahwa total ester tertinggi didapatkan pada variasi suhu 200 °C dengan waktu reaksi 4 jam yaitu sebesar 41,48%. Data hasil analisis GC-MS dapat dilihat pada Gambar 4.9.



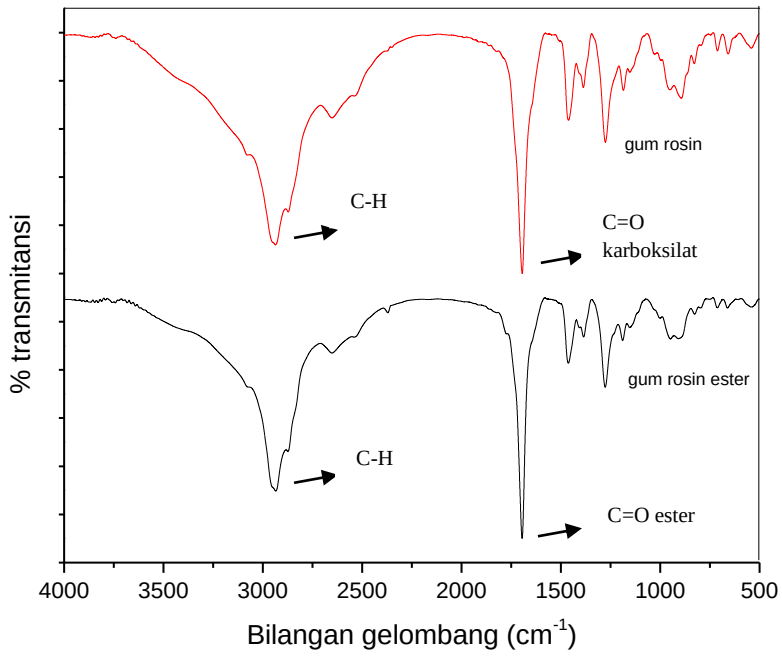
Gambar 4.11 Diagram hasil interpretasi total ester analisis GC-MS FMRE

Hasil interpretasi total ester analisis GC-MS pada Gambar 4.11 dapat diketahui bahwa pembentukan ester terbanyak didapatkan pada suhu 200 °C dengan lama waktu reaksi 4 jam. Semakin tinggi suhu dan waktu reaksi maka jumlah ester

yang terbentuk semakin banyak. Dalam penelitian ini presentase ester terbesar didapatkan pada suhu dan waktu tertinggi hal tersebut menunjukkan bahwa lamamya waktu dan suhu reaksi akan mempengaruhi banyaknya ester yang terbentuk, semakin lama waktu dan suhu reaksi maka ester yang terbentuk akan semakin tinggi.

4.5 Analisis *Fourier Transform Infrared* (FTIR)

FMRE hasil esterifikasi dianalisis dengan FTIR bertujuan untuk melihat perubahan spektrum sebelum dan sesudah. Senyawa-senyawa penyusun dalam FMRE diamati menggunakan *Fourier Transform Infrared* (FTIR) sesuai dengan pernyataan Rahmawati *et al*. (2013) yang menyatakan bahwa analisis FTIR digunakan untuk mengetahui gugus fungsional yang terkandung pada suatu sampel.



Gambar 4.12 Spektra FTIR dari FMRE

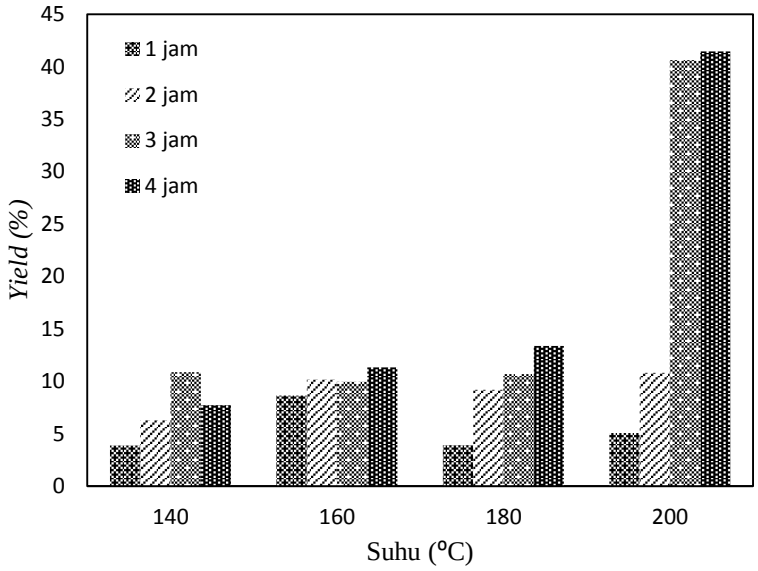
Spektra inframerah yang ditampilkan pada Gambar 4.12 menunjukkan gugus hidroksil (–OH) dari asam karboksilat menyerap kuat pada bilangan gelombang sekitar 3000 cm^{-1}. Dalam hal ini terlihat bahwa pita uluran –OH berasal dari struktur asam karboksilat yang berada dalam keadaan stabil karena adanya ikatan hidrogen yang sangat kuat. Sementara itu hasil esterifikasi FMRE pada

gambar spektra kedua pada Gambar 4.6 serapan gugus hidroksil tersebut melemah dan serapan gugus karbonil menguat pada bilangan gelombang sekitar 1700 cm^{-1}, hal ini menunjukkan bahwa gum rosin telah teresterifikasi. Spektra FTIR pada Gambar 4.6 menginformasikan terdapat beberapa ciri khas dari spektra FTIR dari senyawa ester, yaitu adanya serapan gugus karbonil ester pada bilangan gelombang sekitar 1700 cm^{-1} yang merupakan pita khas regangan C=O ester, sesuai dengan pernyataan Rahmawati *et al*. (2013) yang menyatakan bahwa gugus fungsi C=O dari ester biasanya muncul pada angka gelombang 1690-1760 cm^{-1}. Selain adanya serapan gugus karbonil C=O ester juga terdapat serapan dari C-O. Rentangan C-O menghasilkan dua serapan atau lebih, serapan muncul dalam kisaran bilangan gelombang 1300 cm^{-1} hingga 1000 cm^{-1}. Berdasarkan hasil spektra FTIR FMRE terdapat serapan C-O pada bilangan gelombang 1000 cm^{-1} dan 1250 cm^{-1}. Berdasarkan identifikasi tersebut, maka dapat diketahui bahwa senyawa produk yang terbentuk merupakan senyawa ester.

4.6 *Yield* FMRE

Yield adalah jumlah produk reaksi yang dihasilkan pada suatu reaksi kimia atau presentase produk yang dihasilkan dibanding dengan bahan baku yang terolah sehingga dapat menunjukkan efektifitas dari prosedur (Wahyuni *et al*., 2016). Semakin tinggi nilai *yield* menunjukkan semakin banyak produk ester yang dihasilkan.

Pada proses esterifikasi *yield* tidak mungkin mencapai 100% karena reaksi esterifikasi bersifat bolak-balik (*reversible*) sehingga tidak dapat terkonversi sempurna. Uap air yang terbentuk merupakan salah satu faktor yang dapat mengurangi nilai *yield* produk FMRE karena uap air dapat menghidrolisis produk menjadi gliserol dan asam karboksilat kembali (Wahyuni *et al*., 2016). Hubungan variasi waktu dan suhu reaksi terhadap yield FMRE dapat dilihat pada Gambar 4.13.



Gambar 4.13 Diagram presentase nilai *yield* FMRE

Berdasarkan Gambar 4.13 dapat dilihat bahwa lamanya waktu esterifikasi berpengaruh secara signifikan terhadap nilai *yield*. Penambahan suhu dan lama proses esterifikasi akan meningkatkan nilai *yield* FMRE karena dengan penambahan suhu dan waktu reaksi maka konversi reaktan menjadi gliserol ester akan semakin tinggi. Seperti yang dijelaskan oleh Fatmawati *et al*. (2013) bahwa faktor-faktor yang berpengaruh dalam reaksi esterifikasi diantaranya yaitu waktu reaksi dan suhu reaksi dimana semakin lama waktu reaksi maka kemungkinan kontak antar zat semakin besar sehingga akan menghasilkan konversi yang besar. Begitu pula apabila semakin tinggi suhu yang dioperasikan maka semakin banyak konversi yang dihasilkan. Hal ini sesuai dengan persamaan Archenius. Bila suhu naik maka harga k makin besar sehingga reaksi berjalan cepat dan hasil konversi makin besar. Nilai *yield* tertinggi yaitu 44,06% diperoleh dari produk FMRE pada waktu reaksi 4 jam dan suhu reaksi 200 °C, sedangkan nilai *yield* terendah yaitu sebesar 8,89% pada suhu 160 °C pada waktu reaksi 1 jam. Data tersebut menunjukkan perbedaan secara signifikan.

BAB V

PENUTUP

5.1 Simpulan

Kesimpulan dari hasil penelitian esterifikasi FMRE adalah :

1. Waktu reaksi dan suhu reaksi memberikan pengaruh nyata terhadap produk FMRE dan sifat fisikokimia yang dihasilkan. Berdasarkan data analisis GC-MS dapat disimpulkan bahwa waktu reaksi dan suhu reaksi optimal yang didapat untuk memperoleh produk FMRE adalah pada suhu 200 °C dengan waktu reaksi 4 jam dengan total ester sebanyak 44,03%, hal ini menunjukkan semakin tinggi suhu dan waktu reaksi maka produk yang dihasilkan akan semakin besar.
2. Hasil analisis sifat fisikokimia FMRE menunjukkan adanya peningkatan kualitas dari bilangan asam, titik lunak dan bilangan iod jika dibandingkan dengan uji fisikokimia gum rosin awal, yang menunjukkan gum rosin telah teresterifikasikan.

5.2 Saran

Saran yang dapat diambil dari penelitian ini adalah melakukan proses *bleaching* atau pemucatan pada produk FMRE sehingga didapatkan warna yang lebih baik lagi dan diperlukan penambahan asam seperti Na_2CO_3 untuk menurunkan kadar bilangan asam agar diperoleh produk yang sesuai dengan standar yang sudah ditetapkan.

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LAMPIRAN

Lampiran 1. Perhitungan penggunaan bahan

1. Perhitunga penggunaan gum rosin dan asam fumarat

   Mr gum rosin = 302

   Mr asam fumarat = 117

   1 mol gum rosin $= \frac{\text{gram}}{\text{Mr}}$

   $= \frac{\text{gram}}{302}$

   gram = 302

   1 mol gum rosin = 302 g

   Dalam penelitian ini akan digunakan gum rosin sebanyak 150 g

   150 g gum rosin = 1 mol gum rosin

   1 mol asam fumarat = $\frac{117}{302}$ x 150 = 58,112 g

   Perbandingan ratio mol gum rosin : asam fumarat

   2 : 1

   150 g : 29,06 g

2. Perhitungan katalis PTSA 0,3% .

   Penggunaan 0,3% katalis PTSA adalah 0,3% dari berat gum rosin yaitu 150 g

   $\frac{0.3}{100}$ x 150 g = 0,45 g

3. Perhitungan glisrol 10%.

   Penggunaan 10% gliserol adalah 10% dari berat gum rosin yaitu 150 g

   $\frac{10}{100}$ x 150 g = 15 g.

Lampiran 2. Tabel perhitungan uji fisikokimia

Suhu (^{0}C)	Waktu (jam)	Warna	Titik lunak (^{0}C)	Bilangan asam (mg KOH/g)	Bilangan iod
140	4	11,3	81	W = 4,0202 g V = 26,1 mL	W = 1,0062 g V_1 = 14,7 mL V_2 = 36
160	4	11,9	81	W = 4,0199 g V = 25,2 mL	W = 1,0096 g V_1 = 14,2 mL V_2 = 36 mL
180	4	15,6	81	W = 4,0201 g V = 25,1 mL	W = 1,0072 g V_1 = 12,9 mL V_2 = 36 Ml
200	4	16,6	83	W = 4,0210 g V = 25,0 mL	W = 1,0040 g V_1 = 12,1 mL V_2 = 36 Ml
Gum rosin		6,6	78	W = 4,0202 V = 27 mL	W = 1,0053 V_1 = 12,2 mL V_2 = 36 Ml

Lampiran 3. Perhitungan blanko dan FMRE

1. Blanko
   a. Pengujian bilangan asam

$$AV = \frac{V \text{ x } N \text{ KOH x } 56,11}{\text{m sampel}}$$

$$= \frac{27 \text{ x } 0,5025 \text{ x } 56,11}{4,0202}$$

$$= 189,361$$

   b. Pengujian bilangan iod

$$IV = \frac{(V_2 - V_1) \text{ x } N \text{ } Na_2S_2O_3 \text{ x } 12,69}{\text{m sampel}}$$

$$= \frac{(36 - 157,8) \text{ x } 0,1054 \text{ x } 12,69}{1,0053}$$

$$= 24,214$$

2. FMRE suhu 140 °C waktu reaksi 4 jam
   a. Pengujian bilangan asam

$$AV = \frac{V \text{ x } N \text{ KOH x } 56,11}{\text{m sampel}}$$

$$= \frac{26,1 \text{ x } 0,5025 \text{ ,x } 56,11}{4,0202}$$

$$= 183,05$$

   b. Pengujian bilangan iod

$$IV = \frac{(V_2 - V_1) \text{ x } N \text{ } Na_2S_2O_3 \text{ x } 12,69}{\text{m sampel}}$$

$$= \frac{(36 - 14,7) \text{ x } 0,1054 \text{ x } 12,69}{1,0062}$$

$$= 28,31$$

3. FMRE suhu 160 °Cwaktu reaksi 4 jam

   a. Pengujian bilangan asam

   $$AV = \frac{V \text{ x } N \text{ KOH x } 56,11}{\text{m sampel}}$$

   $$= \frac{25,2 \text{ x } 0,5025 \text{ x } 56,11}{4,0199}$$

   $$= 176,75$$

   b. Pengujian bilangan iod

   $$IV = \frac{(V_2 - V_1) \text{ x N } Na_2S_2O_3 \text{ x } 12,69}{\text{m sampel}}$$

   $$= \frac{(36 - 14,2) \text{ x } 0,1054 \text{ x } 12,69}{1,0096}$$

   $$= 28,88$$

4. FMRE suhu 180 °C waktu reaksi 4 jam

   a. Pengujian bilangan asam

   $$AV = \frac{V \text{ x N KOH x } 56,11}{\text{m sampel}}$$

   $$= \frac{25,1 \text{ x } 0,5025 \text{ x } 56,11}{4,0201}$$

   $$= 176,04$$

   b. Pengujian bilangan iod

   $$IV = \frac{(V_2 - V_1) \text{ x N } Na_2S_2O_3 \text{ x } 12,69}{\text{m sampel}}$$

   $$= \frac{(36 - 12,9) \text{ x } 0,1054 \text{ x } 12,69}{1,0072}$$

   $$= 30,67$$

5. FMRE suhu 200 °C waktu reaksi 4 jam

   a. Pengujian bilangan asam

   $$AV = \frac{V \text{ x N KOH x } 56,11}{\text{m sampel}}$$

$$= \frac{25{,}0 \text{ x } 0{,}5025 \text{ x } 56{,}11}{4{,}0210}$$

$$= 175{,}30$$

b. Pengujian bilangan iod

$$\text{IV} = \frac{(V_2 - V_1) \text{ x N } Na_2S_2O_3 \text{ x } 12{,}69}{\text{m sampel}}$$

$$= \frac{(36 - 12{,}1) \text{ x } 0{,}1054 \text{ x } 12{,}69}{1{,}0040}$$

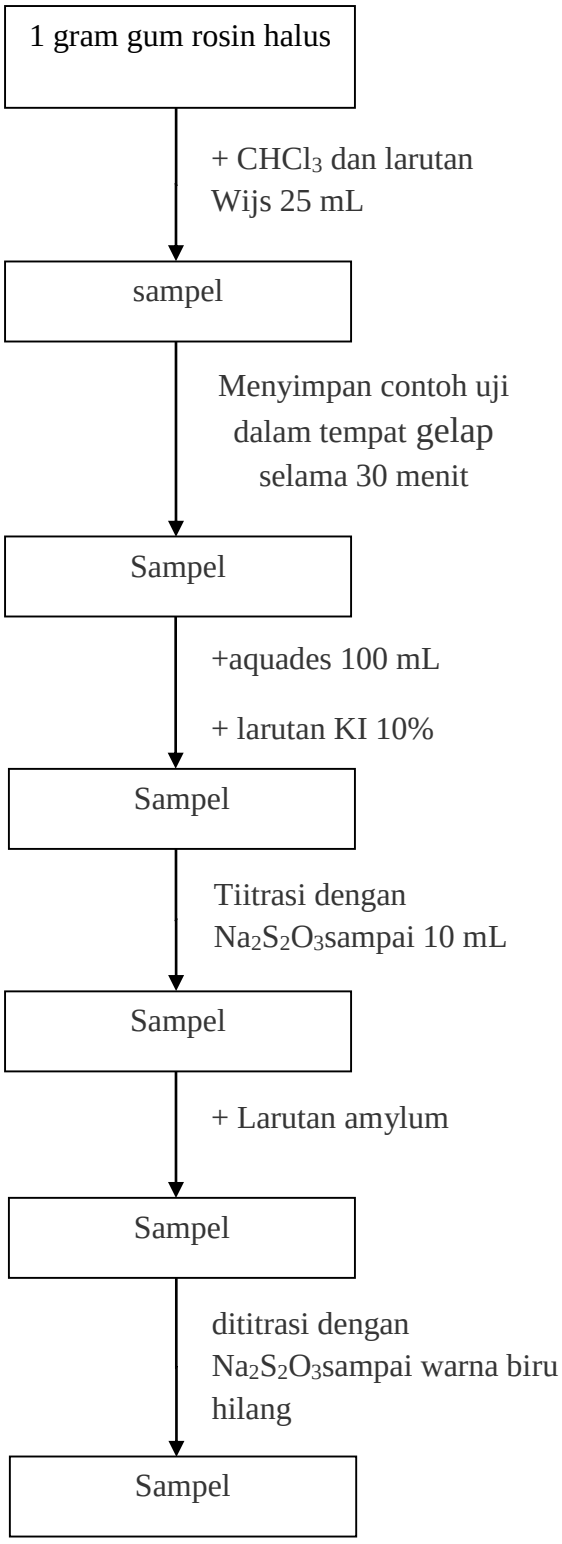
Lampiran 4. Presentase nilai *yield* FMRE

Suhu (^{0}C)	Waktu reaksi (jam)	% luas area asam-asam resin	% area ester	*Yield* (%)
140	1	99.92	3,87	3,87
140	2	99.92	6,27	6,28
140	3	99.92	10,86	10,87
140	4	99.92	7,73	7,74
160	1	99.92	8.63	8,64
160	2	99.92	10,15	10,16
160	3	99.92	9,95	9,96
160	4	99.92	11,31	11,32
180	1	99.92	3,9	3,9
180	2	99.92	9,18	9,19
180	3	99.92	10,68	10,69
180	4	99.92	13,37	13,38
200	1	99.92	5,05	5,06
200	2	99.92	10,82	10,83
200	3	99.92	40,65	40,66
200	4	99.92	41,48	41,49

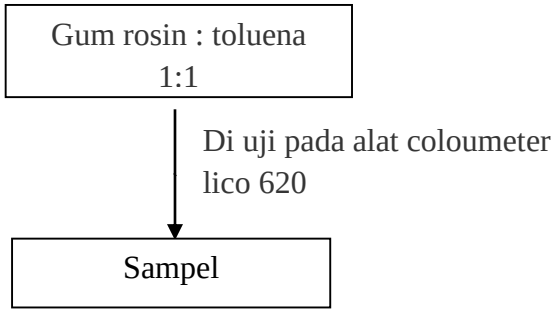
$$Yield = \frac{\text{Hasil Sintesis}}{\text{Hasil Teoritis}} \times 100\%$$

Lampiran 5. Diagram uji fisikokimia dan esterifikasi FMRE

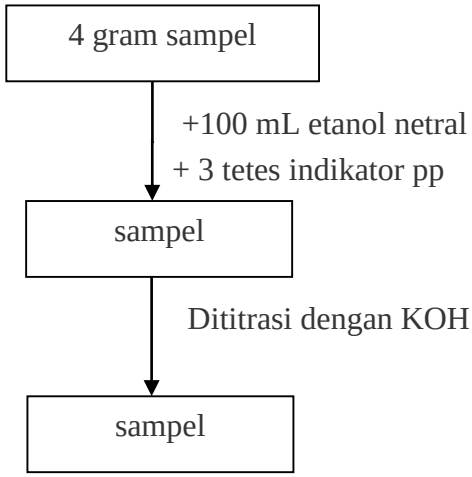
Diagram uji bilangan Iod



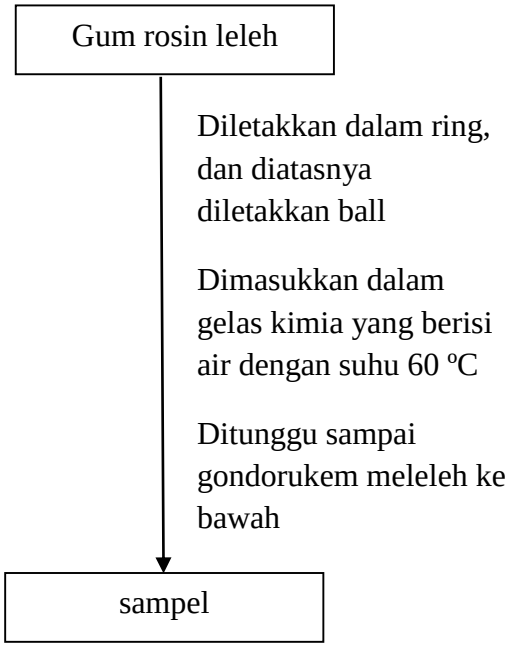
Uji Warna



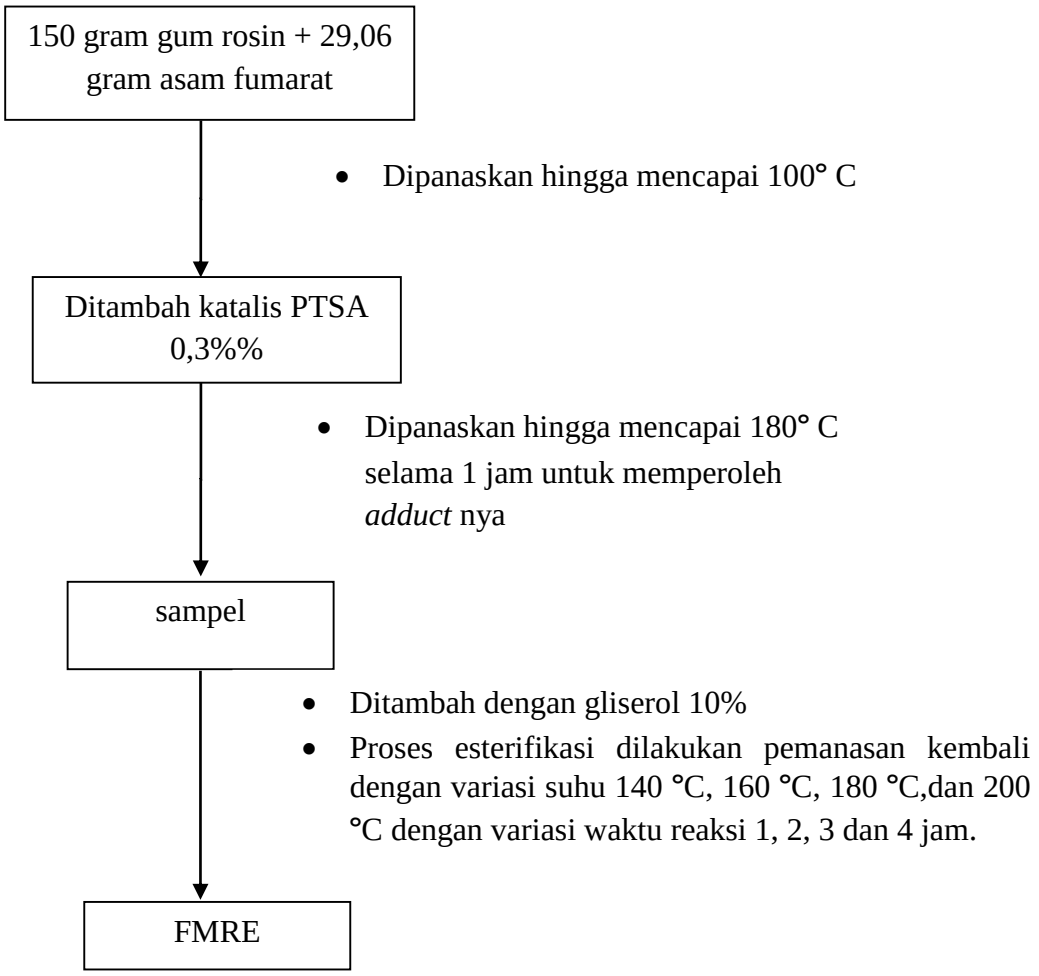
Uji Bilangan Asam



Uji Titik Lunak



Percobaan variasi suhu 140°C, 160°C, 180 °C dan 200°C dan variasi waktu reaksi 1, 2, 3 dan 4 jam



Lampiran 6. Analisa FT-IR

PerkinElmer Spectrum Version 10.4.00
Wednesday, November 27, 2019 1:28 PM

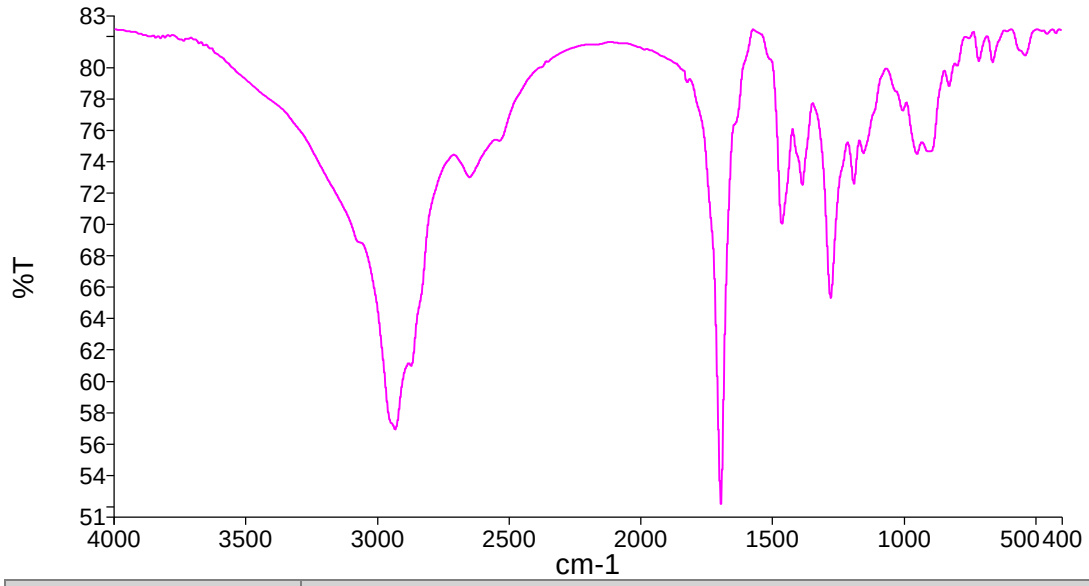
Report Details

Report Location	C:\pel_data\reports\Samples View 2_naila 1_1_1.rtf
Report Creator	Labkim
Report Date	Wednesday, November 27, 2019 1:28 PM

Sample Details

Sample Name	naila 1_1_1
Sample Description	200 10%
Analyst	Labkim
Creation Date	11/27/2019 1:27:58 PM
X-Axis Units	cm-1
Y-Axis Units	%T

Spectrum



Name	Description
naila 1_1_1	200 10%

PerkinElmer Spectrum Version 10.4.00
Monday, January 13, 2020 3:38 PM

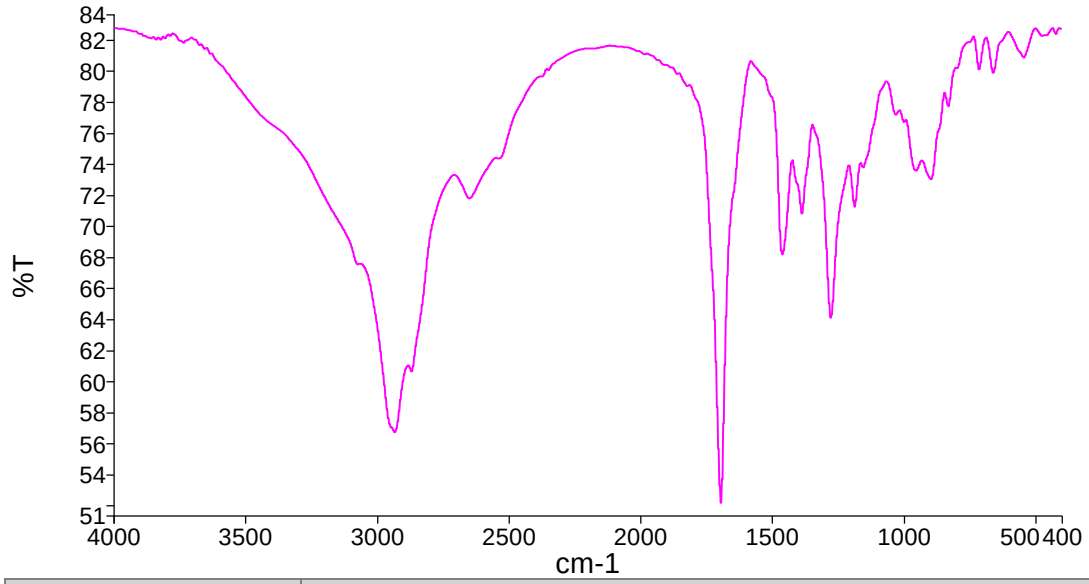
Report Details

Report Location	C:\pel_data\reports\Samples View 2_naila_1_1.rtf
Report Creator	Labkim
Report Date	Monday, January 13, 2020 3:38 PM

Sample Details

Sample Name	naila_1_1
Sample Description	Gumrosin
Analyst	Labkim
Creation Date	1/13/2020 3:38:35 PM
X-Axis Units	cm-1
Y-Axis Units	%T

Spectrum



Name	Description
naila_1_1	Gumrosin

PerkinElmer Spectrum Version 10.4.00
Monday, January 13, 2020 3:39 PM

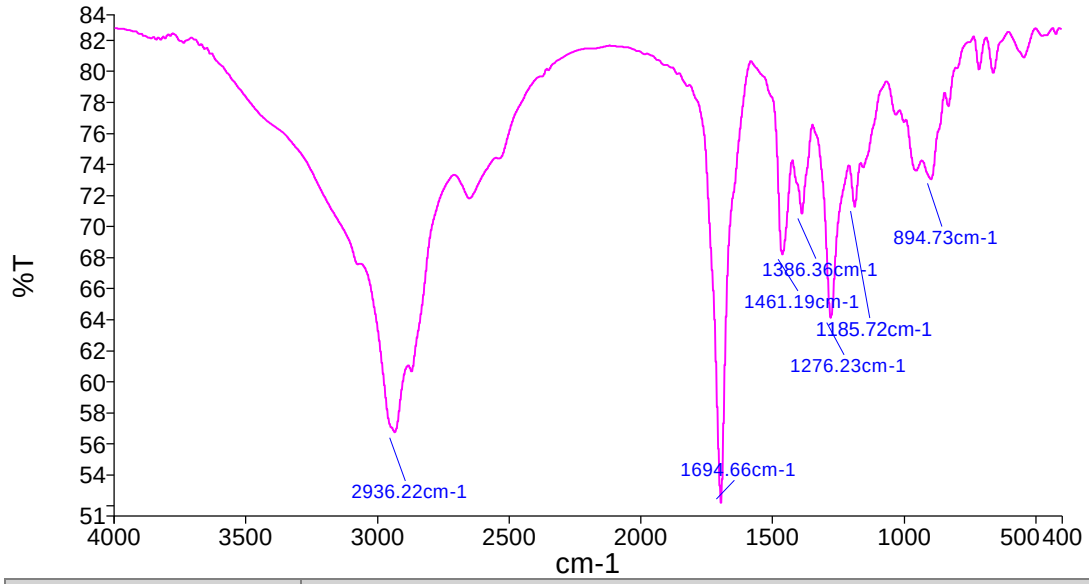
Report Details

Report Location	C:\pel_data\reports\Samples View 2_naila_1_1_1.rtf
Report Creator	Labkim
Report Date	Monday, January 13, 2020 3:39 PM

Sample Details

Sample Name	naila_1_1
Sample Description	Gumrosin
Analyst	Labkim
Creation Date	1/13/2020 3:38:35 PM
X-Axis Units	cm-1
Y-Axis Units	%T

Spectrum



Name	Description
naila_1_1	Gumrosin

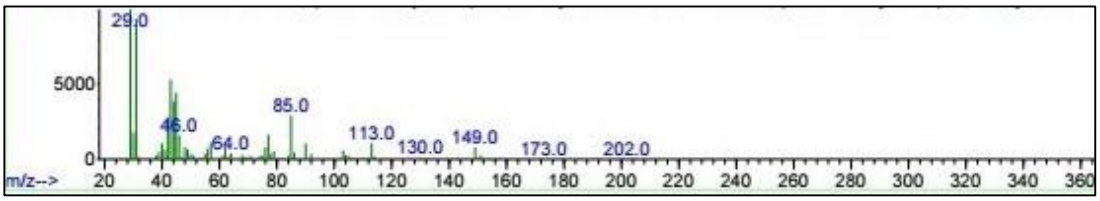
Peak Area/Height Results

Peak	X (cm-1)	Y (%T)	Area (%T)	Start	End	Base1
1	2936.22	56.72	-13932.67	4000	2118.68	4000
2	1694.66	52.14	-2637.12	2118.68	1580.65	2118.68
3	1461.19	68.23	-716.83	1580.65	1423.06	1580.65
4	1386.36	70.87	-77.93	1423.06	1346.08	1423.06
5	1276.23	64.14	-745.65	1346.08	1207.71	1346.08
6	1185.72	71.34	200.25	1207.71	1064.89	1207.71
7	894.73	73.11	152.39	1064.89	400	1064.89

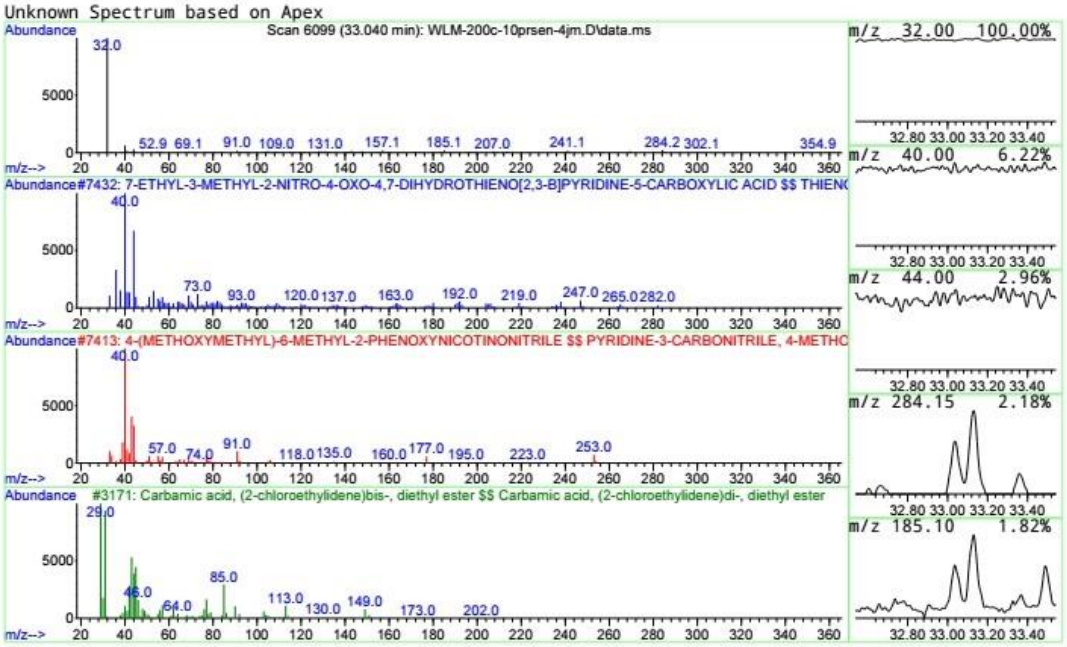
Lampiran 7. Analisis GCMS

Spektrum hasil analisa GCMS FMRE pada suhu 200 ^{0}Cdan waktu reaksi 4 jam

Spektrum pada RT = 33, 040 menit



Carbamic acid, (2-chloroethylidene), dietyl ester

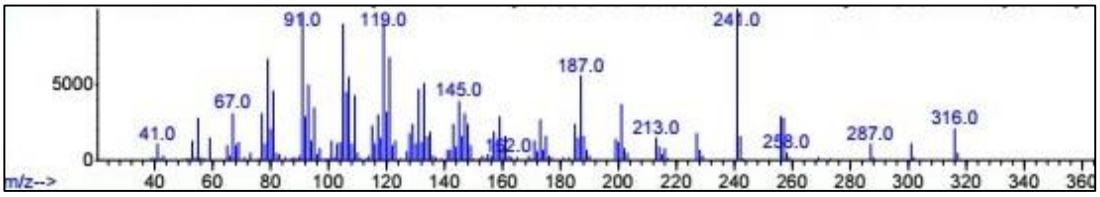



```
Data File: F:\DATA MS\daa\WLM-200c-10prsen-4jm.D
Sample   :

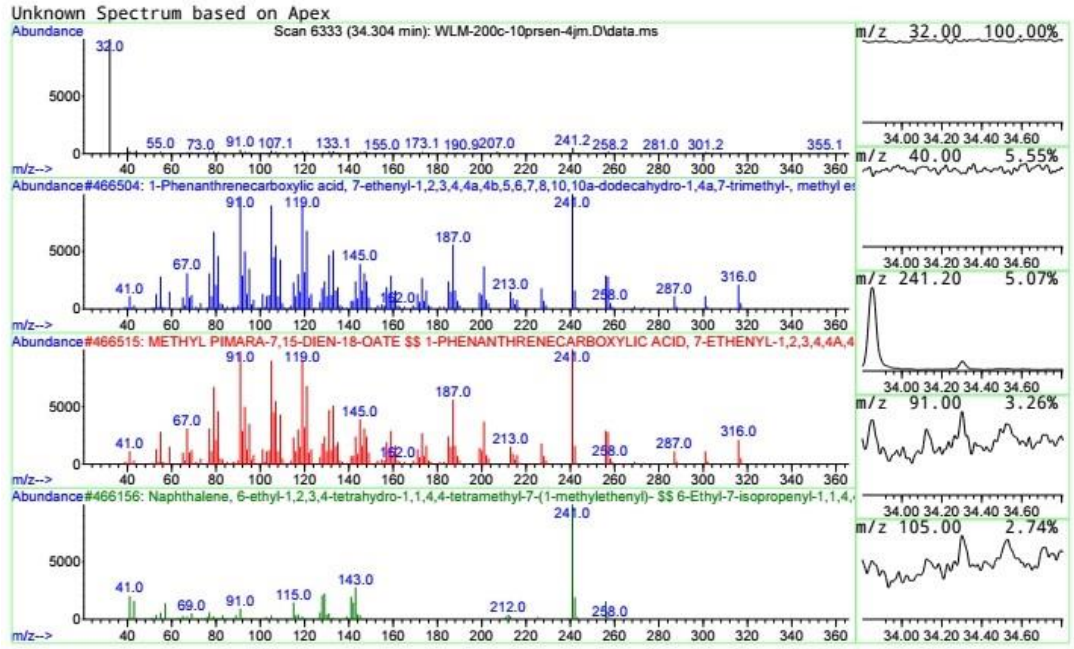
Peak Number:  30    at     33.040 min  Area:    403729  Area % 0.02

 The 3 best hits from each library.          Ref\#    CAS\#      Qual
-------------------------------------------------------------------
    D:\DATABASE\DEMO.L
     1 7-ETHYL-3-METHYL-2-NITRO-4-OXO-4...       7432 999007-43-3   10
     2 4-(METHOXYMETHYL)-6-METHYL-2-PHE...       7413 332057-36-0   10
     3 Carbamic acid, (2-chloroethylide...       3171 005336-13-0    9
```

Spektrum pada RT = 34, 304 menit



Isopimaric acid methyl ester

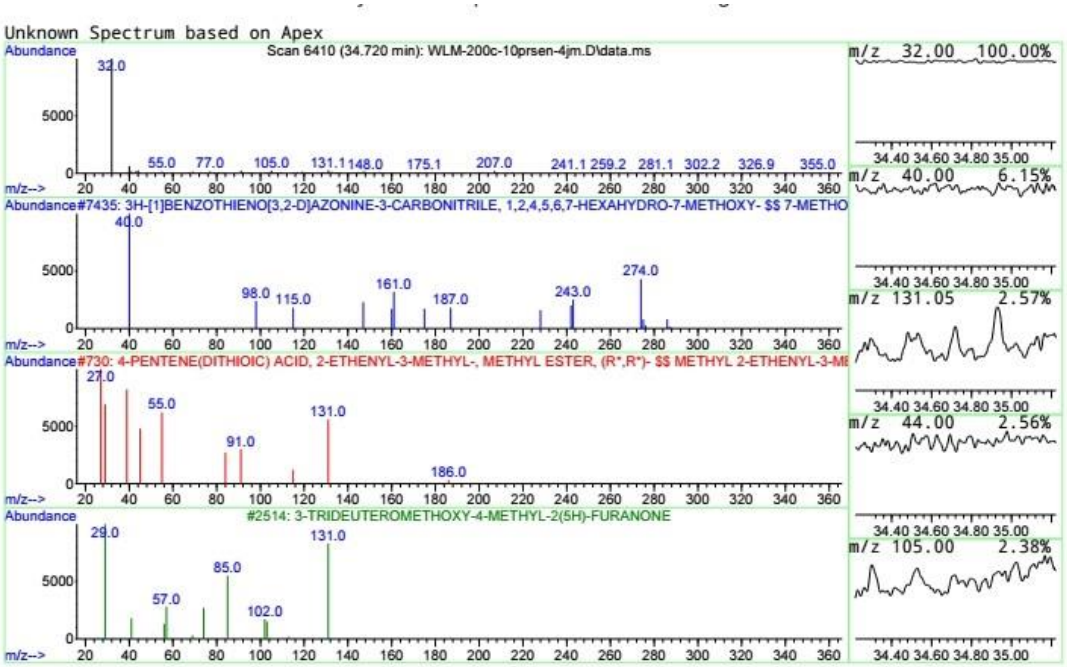



```
Data File: F:\DATA MS\daa\WLM-200c-10prsen-4jm.D
Sample   :

Peak Number:  38    at     34.304 min  Area:    939413  Area % 0.04

 The 3 best hits from each library.          Ref\#    CAS\#      Qual
-------------------------------------------------------------------
    D:\DATABASE\DEMO.L
     1 1-Phenanthrenecarboxylic acid, 7...     466504 001686-62-0   58
     2 METHYL PIMARA-7,15-DIEN-18-OATE ...     466515 001686-62-0   58
     3 Naphthalene, 6-ethyl-1,2,3,4-tet...     466156 301643-35-6   53
```

Spectrum pada RT = 34, 720 menit

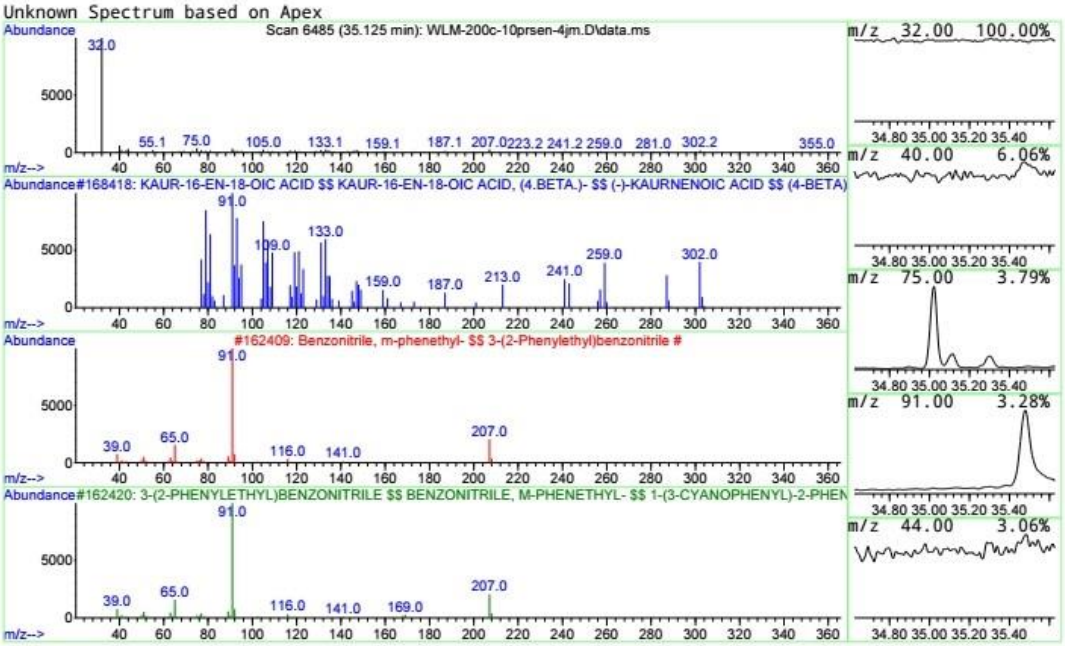


Data File: F:\DATA MS\daa\WLM-200c-10prsen-4jm.D
Sample :

Peak Number: 40 at 34.720 min Area: 413670 Area % 0.02

The 3 best hits from each library.	Ref\#	CAS\#	Qual
D:\DATABASE\DEMO.L			
1 3H-[1]BENZOTHIENO[3,2-D]AZONINE-...	7435	099659-20-8	9
2 4-PENTENE(DITHIOIC) ACID, 2-ETHE...	730	107094-82-6	5
3 3-TRIDEUTEROMETHOXY-4-METHYL-2(5...	2514	000000-00-0	4

Spectrum pada RT = 35, 125 menit

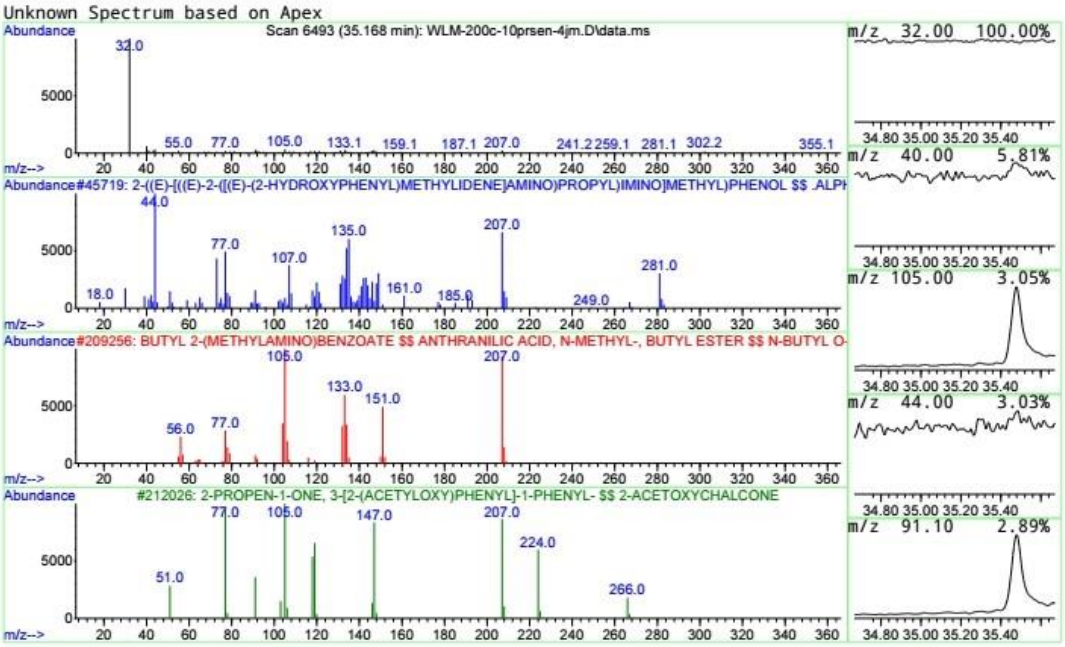


Data File: F:\DATA MS\daa\WLM-200c-10prsen-4jm.D
Sample :

Peak Number: 45 at 35.125 min Area: 619539 Area % 0.03

The 3 best hits from each library.	Ref\#	CAS\#	Qual
D:\DATABASE\DEMO.L			
1 KAUR-16-EN-18-OIC ACID $$ KAUR-1...	168418	020316-84-1	42
2 Benzonitrile, m-phenethyl- $$ 3-...	162409	034176-91-5	10
3 3-(2-PHENYLETHYL)BENZONITRILE $$...	162420	034176-91-5	10

Spectrum pada RT = 35,168 menit

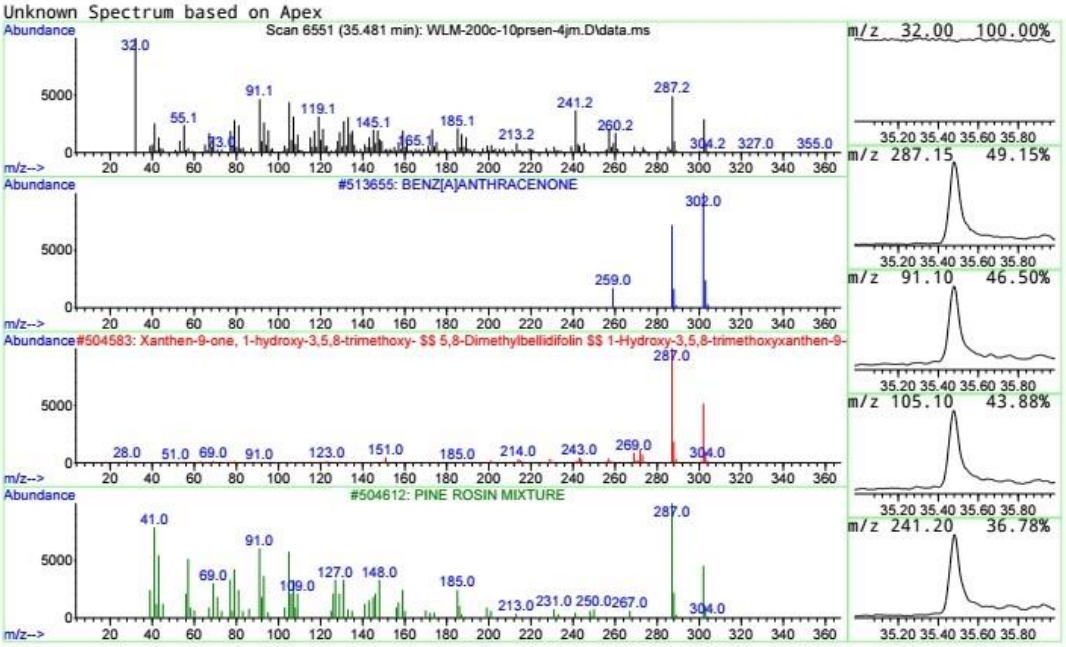



```
Data File: F:\DATA MS\daa\WLM-200c-10prsen-4jm.D
Sample   :

Peak Number:  46    at     35.168 min  Area:    626366  Area % 0.03

 The 3 best hits from each library.          Ref\#    CAS\#      Qual
-------------------------------------------------------------------
    D:\DATABASE\DEMO.L
     1 2-((E)-[((E)-2-([(E)-(2-HYDROXYP...      45719 000094-91-7   25
     2 BUTYL 2-(METHYLAMINO)BENZOATE $$...     209256 015236-34-7   14
     3 2-PROPEN-1-ONE, 3-[2-(ACETYLOXY)...     212026 033777-37-6   12
```

Spectrum pada RT = 35, 481 menit

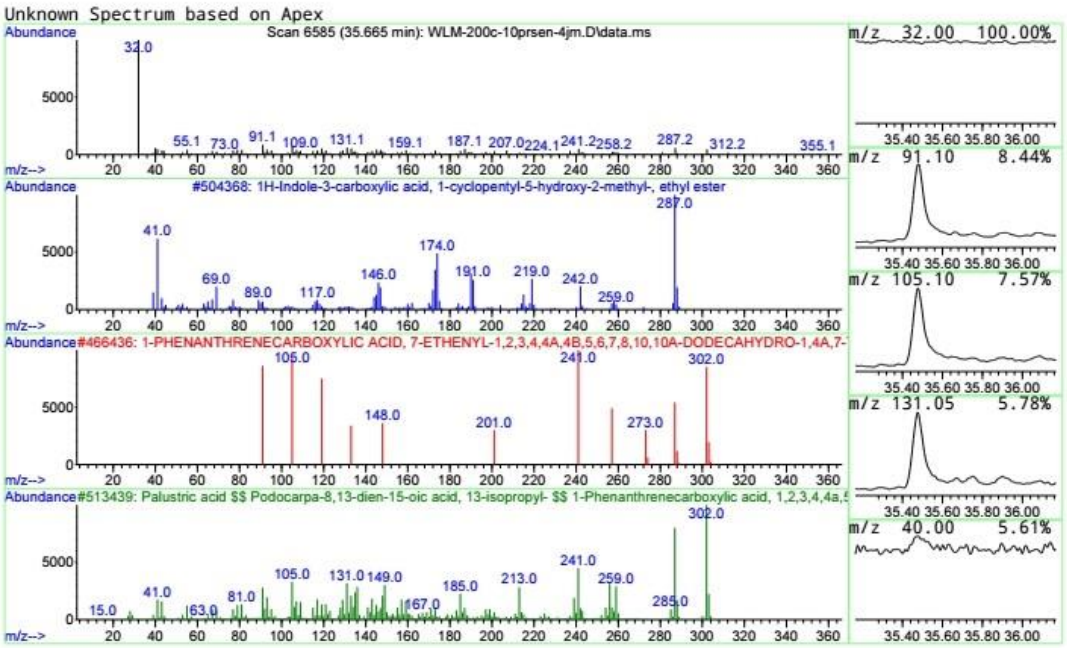


Data File: F:\DATA MS\daa\WLM-200c-10prsen-4jm.D
Sample :

Peak Number: 49 at 35.481 min Area: 22888013 Area % 1.07

The 3 best hits from each library.	Ref\#	CAS\#	Qual
D:\DATABASE\DEMO.L			
1 BENZ[A]ANTHRACENONE	513655	099707-96-7	83
2 Xanthen-9-one, 1-hydroxy-3,5,8-t...	504583	049599-09-9	48
3 PINE ROSIN MIXTURE	504612	000000-00-0	38

Spectrum pada RT = 35, 665 menit

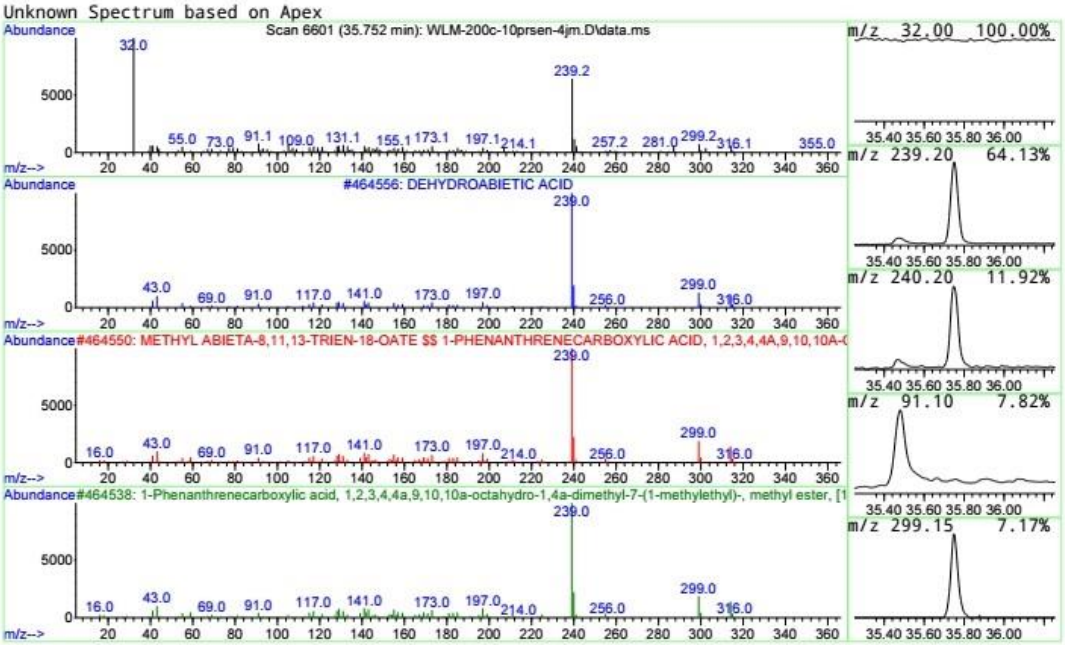


Data File: F:\DATA MS\daa\WLM-200c-10prsen-4jm.D
Sample :

Peak Number: 50 at 35.665 min Area: 3094709 Area % 0.14

The 3 best hits from each library.	Ref\#	CAS\#	Qual
D:\DATABASE\DEMO.L			
1 1H-Indole-3-carboxylic acid, 1-c...	504368	999504-38-0	43
2 1-PHENANTHRENECARBOXYLIC ACID, 7...	466436	005835-26-7	35
3 Palustric acid $$ Podocarpa-8,13...	513439	001945-53-5	35

Spectrum pada RT = 35, 752 menit

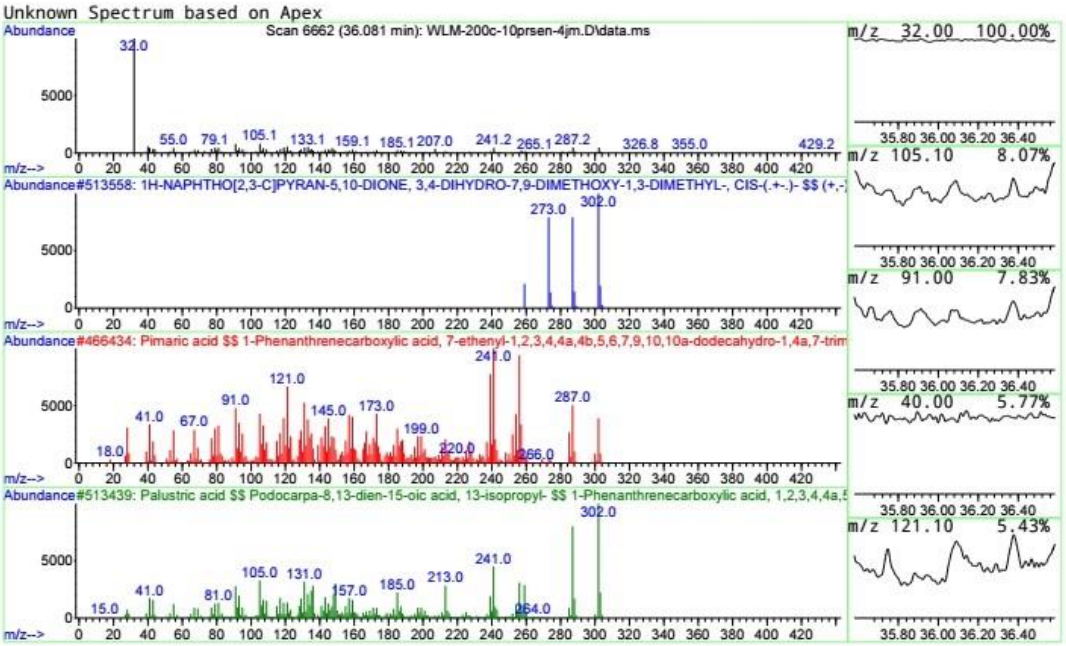



```
Data File: F:\DATA MS\daa\WLM-200c-10prsen-4jm.D
Sample   :

Peak Number:  51    at     35.752 min  Area:   5514847  Area % 0.26

 The 3 best hits from each library.          Ref\#    CAS\#      Qual
-------------------------------------------------------------------------
    D:\DATABASE\DEMO.L
     1 DEHYDROABIETIC ACID                    464556 000000-00-0   97
     2 METHYL ABIETA-8,11,13-TRIEN-18-O...    464550 001235-74-1   96
     3 1-Phenanthrenecarboxylic acid, 1...    464538 001235-74-1   96
```

Spectrum pada RT = 36, 081 menit

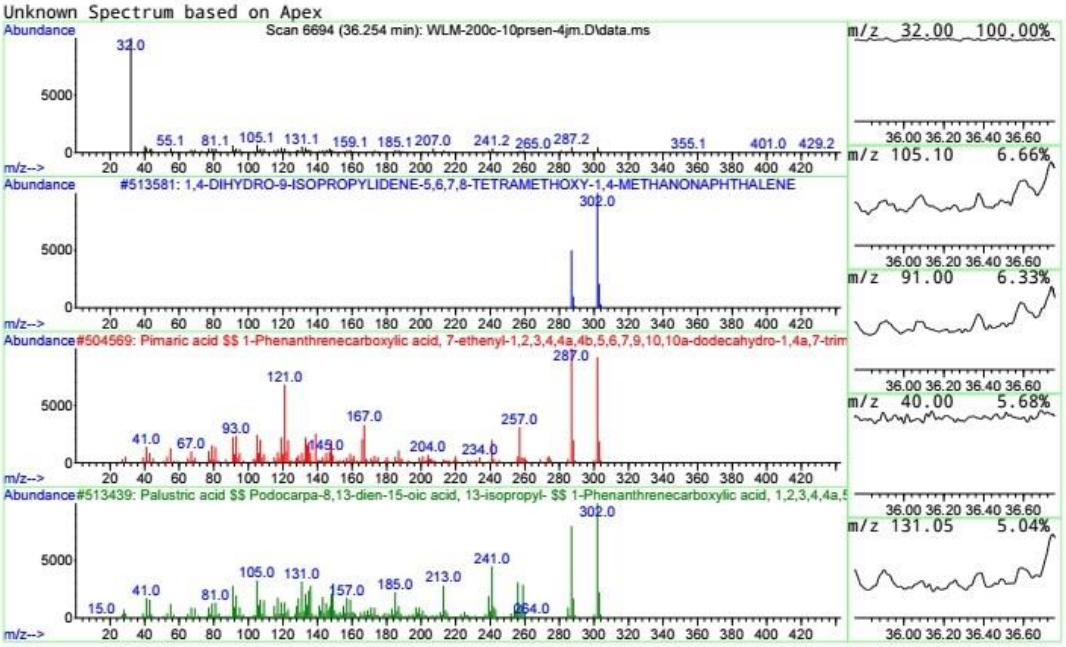


Data File: F:\DATA MS\daa\WLM-200c-10prsen-4jm.D
Sample :

Peak Number: 53 at 36.081 min Area: 5373039 Area % 0.25

The 3 best hits from each library.	Ref\#	CAS\#	Qual
D:\DATABASE\DEMO.L			
1 1H-NAPHTHO[2,3-C]PYRAN-5,10-DION...	513558	084018-43-9	91
2 Pimaric acid $$ 1-Phenanthreneca...	466434	000127-27-5	60
3 Palustric acid $$ Podocarpa-8,13...	513439	001945-53-5	49

Spektrum pada RT = 36, 254 menit

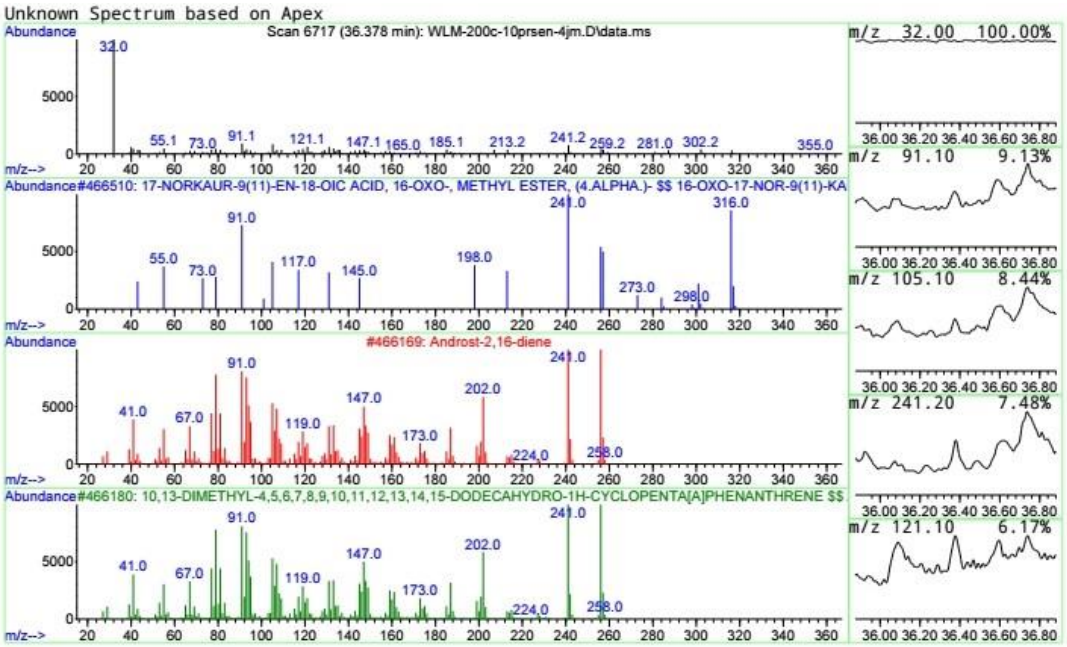


Data File: F:\DATA MS\daa\WLM-200c-10prsen-4jm.D
Sample :

Peak Number: 54 at 36.254 min Area: 2798160 Area % 0.13

The 3 best hits from each library.	Ref\#	CAS\#	Qual
D:\DATABASE\DEMO.L			
1 1,4-DIHYDRO-9-ISOPROPYLIDENE-5,6...	513581	000000-00-0	90
2 Pimaric acid $$ 1-Phenanthreneca...	504569	000127-27-5	55
3 Palustric acid $$ Podocarpa-8,13...	513439	001945-53-5	46

Spectrum pada RT = 36, 378 menit

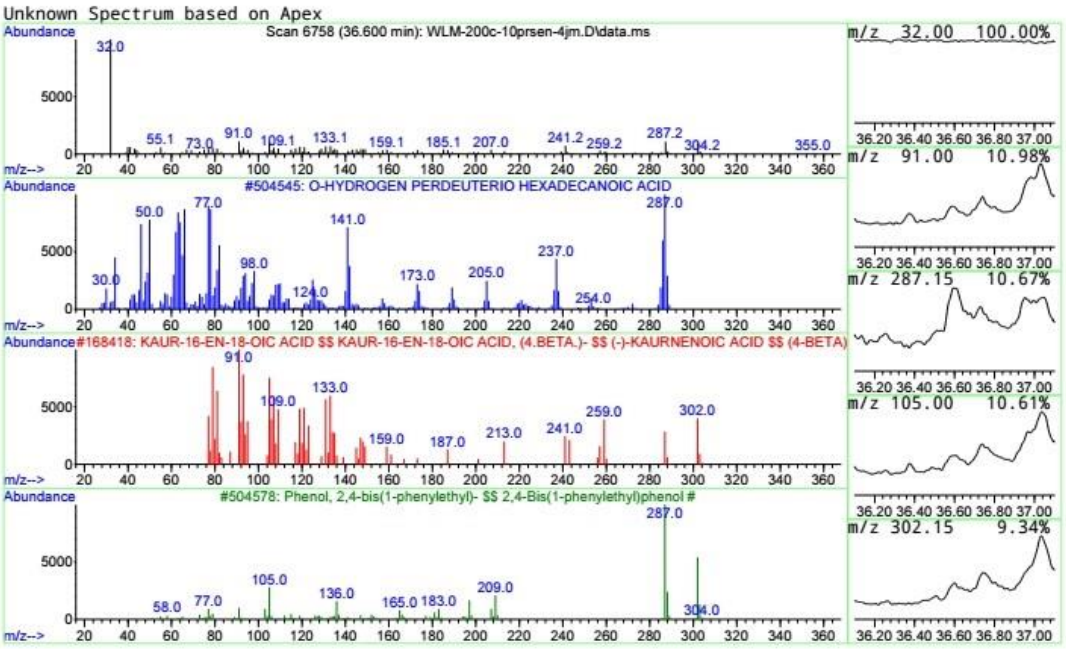


Data File: F:\DATA MS\daa\WLM-200c-10prsen-4jm.D
Sample :

Peak Number: 55 at 36.378 min Area: 3430231 Area % 0.16

The 3 best hits from each library.	Ref\#	CAS\#	Qual
D:\DATABASE\DEMO.L			
1 17-NORKAUR-9(11)-EN-18-OIC ACID,...	466510	063558-42-9	50
2 Androst-2,16-diene	466169	999466-17-7	48
3 10,13-DIMETHYL-4,5,6,7,8,9,10,11...	466180	999466-18-8	48

Soectrum pada RT = 36,60 menit

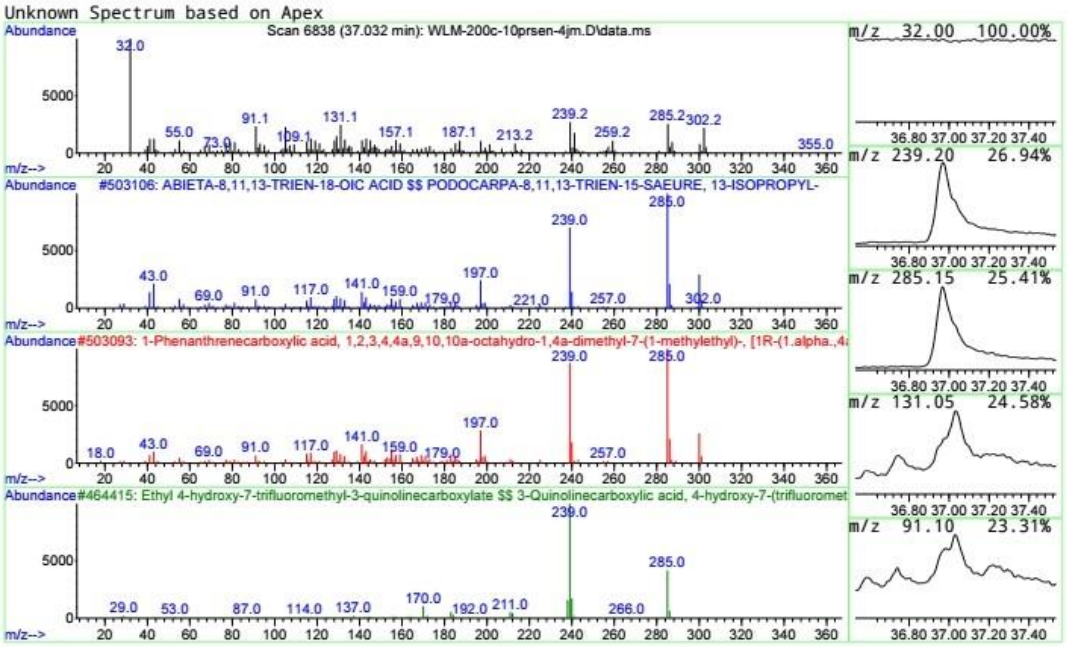


Data File: F:\DATA MS\daa\WLM-200c-10prsen-4jm.D
Sample :

Peak Number: 57 at 36.600 min Area: 6192380 Area % 0.29

The 3 best hits from each library.	Ref\#	CAS\#	Qual
D:\DATABASE\DEMO.L			
1 O-HYDROGEN PERDEUTERIO HEXADECAN...	504545	039756-30-4	90
2 KAUR-16-EN-18-OIC ACID $$ KAUR-1...	168418	020316-84-1	90
3 Phenol, 2,4-bis(1-phenylethyl)- ...	504578	002769-94-0	89

Spectrum pada RT = 37, 032 menit

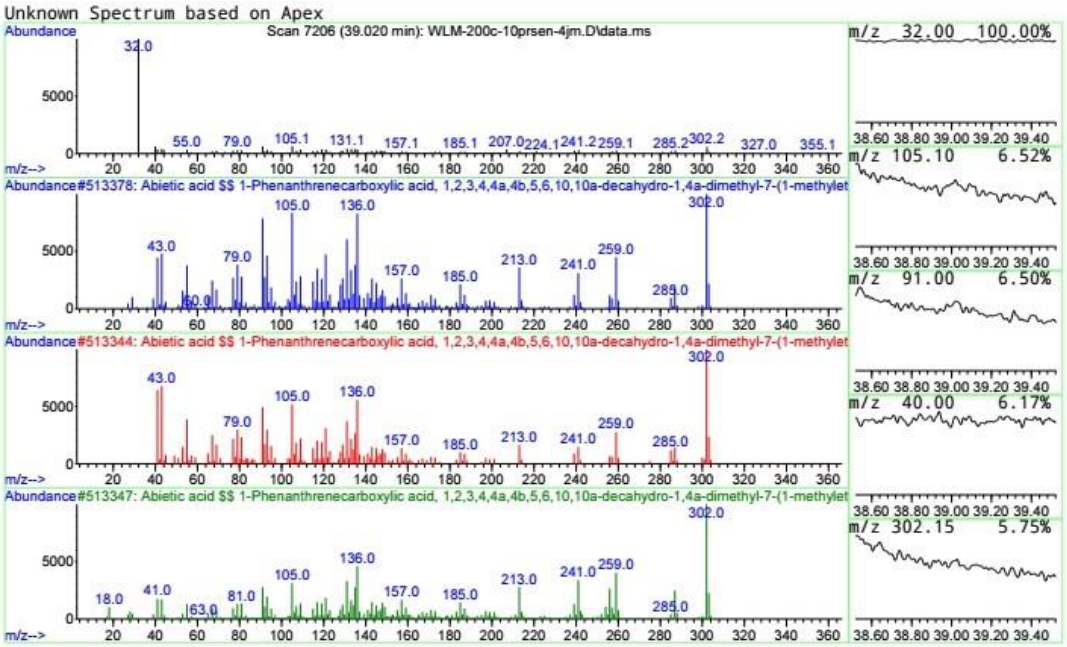


Data File: F:\DATA MS\daa\WLM-200c-10prsen-4jm.D
Sample :

Peak Number: 60 at 37.032 min Area: 16564925 Area % 0.77

The 3 best hits from each library.	Ref\#	CAS\#	Qual
D:\DATABASE\DEMO.L			
1 ABIETA-8,11,13-TRIEN-18-OIC ACID...	503106	999503-11-8	94
2 1-Phenanthrenecarboxylic acid, 1...	503093	001740-19-8	83
3 Ethyl 4-hydroxy-7-trifluoromethy...	464415	000391-02-6	72

Spectra pada RT = 39, 020 menit



Data File: F:\DATA MS\daa\WLM-200c-10prsen-4jm.D
Sample :

Peak Number: 64 at 39.020 min Area: 1220560 Area % 0.06

The 3 best hits from each library.	Ref\#	CAS\#	Qual
D:\DATABASE\DEMO.L			
1 Abietic acid $$ 1-Phenanthreneca...	513378	000514-10-3	84
2 Abietic acid $$ 1-Phenanthreneca...	513344	000514-10-3	80
3 Abietic acid $$ 1-Phenanthreneca...	513347	000514-10-3	70

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-140c-ljm.D
Acq On : 10 Oct 2019 13:01
Operator :
Sample :
Misc :
ALS Vial : 4 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	1.962	2.74	D:\DATABASE\DEMO.L			
			METHANOL $$ HYDROXYMETHANE $$ ALCO HOL, METHYL $$ ALCOOL METHYLIQUE	5075	000067-56-1	2
			Methyl Alcohol $$ Methanol $$ Carb inol $$ Methyl hydroxide	5072	000067-56-1	2
			METHANOL $$ HYDROXYMETHANE $$ ALCO HOL, METHYL $$ BIELESKI'S SOLUTION	5080	000067-56-1	2
2	2.135	0.11	D:\DATABASE\DEMO.L			
			Pentane, 2,4-dimethyl- $$ 2,4-Dime thylpentane	18753	000108-08-7	91
			Pentane, 2,4-dimethyl- $$ 2,4-Dime thylpentane	18799	000108-08-7	90
			Pentane, 2,4-dimethyl- $$ 2,4-Dime thylpentane	18750	000108-08-7	87
3	2.205	11.14	D:\DATABASE\DEMO.L			
			HEXANE, 3-METHYL- $$ 3-METHYLHEXAN E $$ 2-ETHYLPENTANE $$ HEXANE, 3-M ETHYL	18994	000589-34-4	83
			Hexane, 3-methyl- $$ 2-Ethylpentan e $$ 3-Methylhexane	18811	000589-34-4	80
			HEXANE, 3-METHYL- $$ 3-METHYLHEXAN E $$ 2-ETHYLPENTANE $$ HEXANE, 3-M ETHYL	18824	000589-34-4	64
4	2.243	4.43	D:\DATABASE\DEMO.L			
			1,3-DIMETHYLCYCLOPENTANE $$ CYCLOP ENTANE, 1,3-DIMETHYL-, CIS- $$ 1,3 -DIMETHYLCYCLOPENTANE (CIS) $$ 1,3 -DIMETHYLCYCLOPENTANE CIS	62286	002532-58-3	91
			Cyclopentane, 1,3-dimethyl- $$ 1,3 -Dimethylcyclopentane	101343	002453-00-1	91
			Cyclopentane, 1,3-dimethyl-, cis- $$ cis-1,3-Dimethylcyclopentane $$ 1,3-Dimethylcyclopentane cis $$ 1 ,3-Dimethylcyclopentane #	62231	002532-58-3	91
5	2.335	6.98	D:\DATABASE\DEMO.L			
			CYCLOHEXANE, METHYL- $$ METHYLCYCL OHEXANE $$ 1-METHYLCYCLOHEXANE $$ CYCLOHEXANE, METHYL	141469	000108-87-2	96
			CYCLOHEXANE, METHYL- $$ METHYLCYCL OHEXANE $$ 1-METHYLCYCLOHEXANE $$ CYCLOHEXANE, METHYL	141470	000108-87-2	95
			CYCLOHEXANE, METHYL- $$ METHYLCYCL OHEXANE $$ 1-METHYLCYCLOHEXANE $$ CYCLOHEXANE, METHYL	141467	000108-87-2	94
6	2.421	69.76	D:\DATABASE\DEMO.L			
			BENZENE, METHYL- $$ METHYLBENZENE $$ TOLUENE $$ ANTISAL 1A	158622	000108-88-3	91
			Toluene $$ Benzene, methyl $$ Meth acide $$ Methylbenzene	158580	000108-88-3	91
			Toluene $$ Benzene, methyl $$ Meth acide $$ Methylbenzene	158579	000108-88-3	90
7	2.745	0.95	D:\DATABASE\DEMO.L			
			CYCLOHEXANE, ETHYL- $$ ETHYLCYCLOH	141562	001678-91-7	76

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-140c-1jm.D
Acq On : 10 Oct 2019 13:01
Operator :
Sample :
Misc :
ALS Vial : 4 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

%#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			EXANE $$ ETHYL CYCLOHEXANE $$ ETHY			
			LCYCLOHEXAN			
			CYCLOHEXANE, ETHYL- $$ ETHYLCYCLOH	141561	001678-91-7	76
			EXANE $$ ETHYL CYCLOHEXANE $$ ETHY			
			LCYCLOHEXAN			
			ETHYLCYCLOHEXANE $$ ETHYLCYCLOHEXA	54425	001678-91-7	76
8	34.541	0.14	D:\DATABASE\DEMO.L			
			CIS-TRICYCLO[7.5.0.0(2,8)]TETRADEC	161352	000000-00-0	30
			A-7,9-DIENE			
			1,1'-BI(SPIRO[2.5]OCTYLIDENE	162904	000000-00-0	30
			Naphthalene, 1-butyl-1,2,3,4-tetra	283065	029138-93-0	25
			hydro-4-pentyl- $$ 1-Butyl-4-panty			
			1-1,2,3,4-tetrahydronaphthalene #			
9	35.470	0.12	D:\DATABASE\DEMO.L			
			Chromium, carbonyl-(.eta.-4-1,3-bu	398828	999398-83-2	35
			tadiene)(.eta.-5-pentamethylcyclop			
			entadienyl)-			
			KAUR-16-EN-18-OIC ACID $$ KAUR-16-	168418	020316-84-1	30
			EN-18-OIC ACID, (4.BETA.)- $$ (-)-			
			KAURNENOIC ACID $$ (4-BETA)-KAUR-1			
			6-EN-18-OIC ACID			
			CADMIUM[II] BIS(DIBUTYLDITHIOPHOSP	283924	043159-11-1	22
			HATE)			
10	35.757	0.06	D:\DATABASE\DEMO.L			
			DEHYDROABIETIC ACID	464556	000000-00-0	98
			METHYL ABIETA-8,11,13-TRIEN-18-OAT	464549	001235-74-1	95
			E $$ 1-PHENANTHRENECARBOXYLIC ACID			
			, 1,2,3,4,4A,9,10,10A-OCTAHYDRO-1,			
			4A-DIMETHYL-7-(1-METHYLETHYL)-, ME			
			THYL ESTER, [1R-(1.ALPHA.,4A.BETA.			
			,10A.ALPHA.)]- $$ DEHYDROABIETIC A			
			CID METHYL ESTER $$ METHYL DEHYDRO			
			ABIETATE			
			1-Phenanthrenecarboxylic acid, 1,2	464538	001235-74-1	95
			,3,4,4a,9,10,10a-octahydro-1,4a-di			
			methyl-7-(1-methylethyl)-, methyl			
			ester, [1R-(1.alpha.,4a.beta.,10a.			
			alpha.)]- $$ Podocarpa-8,11,13-tri			
			en-15-oic acid, 13-isopropyl-, met			
			hyl ester $$ Methyl dehydroabietat			
11	36.092	0.21	D:\DATABASE\DEMO.L			
			PIMARA-8(14),15-DIEN-18-OIC ACID $	504608	000127-27-5	70
			$ 1-PHENANTHRENECARBOXYLIC ACID, 7			
			-ETHENYL-1,2,3,4,4A,4B,5,6,7,9,10,			
			10A-DODECAHYDRO-1,4A,7-TRIMETHYL-,			
			[1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,			
			7.BETA.,10A.ALPHA.)]- $$ (+)-PIMAR			
			IC ACID $$ .ALPHA.-PIMARIC ACID			
			KAUR-16-EN-18-OIC ACID $$ KAUR-16-	168418	020316-84-1	53
			EN-18-OIC ACID, (4.BETA.)- $$ (-)-			
			KAURNENOIC ACID $$ (4-BETA)-KAUR-1			
			6-EN-18-OIC ACID			
			(4-Ethylphenyl)-(2-methylbenzo[4,5	504586	999504-59-8	50
			]imidazo[1,2-a] pyrimidin-4-yl)ami			
			ne			

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Data File : WLM-10prsan-140c-1jm.D
Acq On    : 10 Oct 2019  13:01
Operator  :
Sample    :
Misc      :
ALS Vial  : 4   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e
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#	RT	Area%	Library/ID	Ref#	CAS#	Qual
2	36.383	0.08	D:\DATABASE\DEMO.L METHYL ABIETA-7,13-DIEN-18-OATE $$ 1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL)-, METHYL ESTER, [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A.ALPHA.)]- $$ ABALYN $$ ABIETIC ACID METHYL ESTER	480551	000127-25-3	99
			METHYL ABIETA-7,13-DIEN-18-OATE $$ 1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL)-, METHYL ESTER, [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A.ALPHA.)]- $$ ABALYN $$ ABIETIC ACID METHYL ESTER	258918	000127-25-3	99
			Methyl abietate $$ 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,4b,5,6,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, methyl ester, [1R-(1.alpha.,4a.beta.,4b.alpha.,10a.alpha.)]- $$ Podocarpa-7,13-dien-15-oic acid, 13-isopropyl-, methyl ester $$ Abalyn	258889	000127-25-3	99
3	36.594	0.62	D:\DATABASE\DEMO.L 1-PHENANTHRENECARBOXYLIC ACID, 7-ETHENYL-1,2,3,4,4A,4B,5,6,7,8,10,10A-DODECAHYDRO-1,4A,7-TRIMETHYL-, [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,7.ALPHA.,10A.ALPHA.)]- $$ ISOPIMARIC ACID $$ PODOCARP-7-EN-15-OIC ACID, 13.BETA.-METHYL-13-VINYL-	466436	005835-26-7	91
			KAUR-16-EN-18-OIC ACID $$ KAUR-16-EN-18-OIC ACID, (4.BETA.)- $$ (-)-KAURNENOIC ACID $$ (4-BETA)-KAUR-16-EN-18-OIC ACID	168418	020316-84-1	83
			4-Androsten-6.beta.-ol-3,17-dione	513437	999513-45-0	59
4	36.950	0.31	D:\DATABASE\DEMO.L 1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,9,10,10A-OCTAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL)-, [1R-(1.ALPHA.,4A.BETA.,10A.ALPHA.)]- $$ (-)-DEHYDROABIETIC ACID $$ 1,2,3,4,4A,9,10,10A-OCTAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL)-1-PHENANTHRENECARBOXYLIC ACID	503110	001740-19-8	90
			1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1R-(1.alpha.,4a.beta.,10a.alpha.)]- $$ Podocarpa-8,11,13-trien-15-oic acid, 13-isopropyl- $$ Abieta-8,11,13-trien-18-oic acid $$ Abietic acid, dehydro-	503093	001740-19-8	90
			1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1R-(1.	503081	001740-19-8	89

Library Search Report

ata Path : F:\DATA MS\daa\
ata File : WLM-10prsan-140c-1jm.D
cq On : 10 Oct 2019 13:01
perator :
ample :
isc :
LS Vial : 4 Sample Multiplier: 1

earch Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

nknown Spectrum: Apex
ntegration Events: ChemStation Integrator - autoint1.e

RT	Area%	Library/ID	Ref#	CAS#	Qual
		alpha.,4a.beta.,10a.alpha.)]- $$ P odocarpa-8,11,13-trien-15-oic acid , 13-isopropyl- $$ Abieta-8,11,13- trien-18-oic acid $$ Abietic acid, dehydro-			
37.204	0.02	D:\DATABASE\DEMO.L 1-Phenanthrenecarboxylic acid, 1,2 ,3,4,4a,9,10,10a-octahydro-1,4a-di methyl-7-(1-methylethyl)-, [1S-(1. alpha.,4a.alpha.,10a.beta.)]- $$ P odocarpa-8,11,13-trien-16-oic acid , 13-isopropyl- $$ Callitrisic aci d $$ 4-Epiabietic acid, dehydro-	503094	005155-70-4	91
		ABIETA-8,11,13-TRIEN-18-OIC ACID $ $ 1-PHENANTHRENECARBOXYLIC ACID, 1 ,2,3,4,4A,9,10,10A-OCTAHYDRO-1,4A- DIMETHYL-7-(1-METHYLETHYL)-, [1S-(1.ALPHA.,4A.ALPHA.,10A.BETA.)]- $$ 13-ISOPROPYLPODOCARPA-8,11,13-TRI EN-16-OIC ACID $$ 4-EPIABIETIC ACI D, DEHYDRO-	503112	005155-70-4	91
		ABIETA-7,13-DIEN-18-OIC ACID $$ 1- PHENANTHRENECARBOXYLIC ACID, 1,2,3 ,4,4A,4B,5,6,10,10A-DECAHYDRO- $$ 1-PHENANTHRENECARBOXYLIC ACID, 1,2 ,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1, 4A-DIMETHYL-7-(1-METHYLETHYL)-, [1 R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A .ALPHA.)]-	168419	000514-10-3	70
37.312	0.02	D:\DATABASE\DEMO.L ABIETA-7,13-DIEN-18-OIC ACID $$ 1- PHENANTHRENECARBOXYLIC ACID, 1,2,3 ,4,4A,4B,5,6,10,10A-DECAHYDRO- $$ 1-PHENANTHRENECARBOXYLIC ACID, 1,2 ,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1, 4A-DIMETHYL-7-(1-METHYLETHYL)-, [1 R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A .ALPHA.)]-	168420	000514-10-3	86
		Palustric acid $$ Podocarpa-8,13-d ien-15-oic acid, 13-isopropyl- $$ 1-Phenanthrenecarboxylic acid, 1,2 ,3,4,4a,5,6,9,10,10a-decahydro-1,4 a-dimethyl-7-(1-methylethyl)-, (1R -(1.alpha.,4a.beta.,10a.alpha.))- $$ 8,13-Abietadien-18-oic acid	513439	001945-53-5	56
		1-PHENANTHRENECARBOXYLIC ACID, 7-E THENYL-1,2,3,4,4A,4B,5,6,7,8,10,10 A-DODECAHYDRO-1,4A,7-TRIMETHYL-, [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,7. ALPHA.,10A.ALPHA.)]- $$ ISOPIMARIC ACID $$ PODOCARP-7-EN-15-OIC ACID , 13.BETA.-METHYL-13-VINYL-	466436	005835-26-7	55
37.350	0.00	D:\DATABASE\DEMO.L ABIETA-7,13-DIEN-18-OIC ACID $$ 1- PHENANTHRENECARBOXYLIC ACID, 1,2,3 ,4,4A,4B,5,6,10,10A-DECAHYDRO- $$	168420	000514-10-3	90

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsen-140c-1jm.D
Acq On : 10 Oct 2019 13:01
Operator :
Sample :
Misc :
ALS Vial : 4 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autointl.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			1-PHENANTHRENECARBOXYLIC ACID, 1,2 ,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1, 4A-DIMETHYL-7-(1-METHYLETHYL)-, [1 R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A .ALPHA.)]-			
			Palustric acid $$ Podocarpa-8,13-d ien-15-oic acid, 13-isopropyl- $$ 1-Phenanthrenecarboxylic acid, 1,2 ,3,4,4a,5,6,9,10,10a-decahydro-1,4 a-dimethyl-7-(1-methylethyl)-, (1R -(1.alpha.,4a.beta.,10a.alpha.))- $$ 8,13-Abietadien-18-oic acid	513439	001945-53-5	86
			ABIETA-7,13-DIEN-18-OIC ACID $$ 1- PHENANTHRENECARBOXYLIC ACID, 1,2,3 ,4,4A,4B,5,6,10,10A-DECAHYDRO- $$ 1-PHENANTHRENECARBOXYLIC ACID, 1,2 ,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1, 4A-DIMETHYL-7-(1-METHYLETHYL)-, [1 R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A .ALPHA.)]-	168419	000514-10-3	83
18	37.696	2.19	D:\DATABASE\DEMO.L			
			Abietic acid $$ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid	513378	000514-10-3	99
			Abietic acid $$ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid	513344	000514-10-3	95
			Abietic acid $$ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid	513347	000514-10-3	91
19	39.003	0.11	D:\DATABASE\DEMO.L			
			.beta.-Pimaric acid $$ .delta.6,8(14)-Abietadienoic acid $$ 1-Pimari c acid $$ 1-Sapietic acid	513374	000079-54-9	64
			Abietic acid $$ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid	513347	000514-10-3	64
			Abietic acid $$ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet	513344	000514-10-3	55

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-140c-1jm.D
Acq On : 10 Oct 2019 13:01
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Sample :
Misc :
ALS Vial : 4 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			a.,4b.alpha.,10a.alpha.)]- $$ Podocarpa-7,13-dien-15-oic acid, 13-isopropyl- $$ L-abietic acid			

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Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-140c-2jm.D
Acq On    : 12 Oct 2019    9:38
Operator  :
Sample    :
Misc      :
ALS Vial  : 3   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e
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k#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	1.962	4.82	D:\DATABASE\DEMO.L			
			Methyl Alcohol $$ Methanol $$ Carbinol $$ Methyl hydroxide	5073	000067-56-1	2
			METHANOL $$ HYDROXYMETHANE $$ ALCOHOL, METHYL $$ ALCOOL METHYLIQUE	5075	000067-56-1	2
			Methyl Alcohol $$ Methanol $$ Carbinol $$ Methyl hydroxide	5072	000067-56-1	2
2	2.135	0.14	D:\DATABASE\DEMO.L			
			Pentane, 2,4-dimethyl- $$ 2,4-Dimethylpentane	18753	000108-08-7	90
			PENTANE, 2,4-DIMETHYL- $$ 2,4-DIMETHYLPENTANE $$ PENTANE, 2,4-DIMETHYL	18833	000108-08-7	80
			PENTANE, 2,4-DIMETHYL- $$ 2,4-DIMETHYLPENTANE $$ PENTANE, 2,4-DIMETHYL	19002	000108-08-7	80
3	2.205	10.92	D:\DATABASE\DEMO.L			
			HEXANE, 3-METHYL- $$ 3-METHYLHEXANE $$ 2-ETHYLPENTANE $$ HEXANE, 3-METHYL	18994	000589-34-4	87
			Hexane, 3-methyl- $$ 2-Ethylpentane $$ 3-Methylhexane	18811	000589-34-4	80
			Hexane, 3-methyl- $$ 2-Ethylpentane $$ 3-Methylhexane	18743	000589-34-4	64
4	2.243	4.25	D:\DATABASE\DEMO.L			
			1,3-DIMETHYLCYCLOPENTANE $$ CYCLOPENTANE, 1,3-DIMETHYL-, CIS- $$ 1,3-DIMETHYLCYCLOPENTANE (CIS) $$ 1,3-DIMETHYLCYCLOPENTANE CIS	62286	002532-58-3	91
			Cyclopentane, 1,3-dimethyl-, cis- $$ cis-1,3-Dimethylcyclopentane $$ 1,3-Dimethylcyclopentane cis $$ 1,3-Dimethylcyclopentane #	62231	002532-58-3	91
			Cyclopentane, 1,3-dimethyl- $$ 1,3-Dimethylcyclopentane	101343	002453-00-1	91
5	2.335	6.48	D:\DATABASE\DEMO.L			
			CYCLOHEXANE, METHYL- $$ METHYLCYCLOHEXANE $$ 1-METHYLCYCLOHEXANE $$ CYCLOHEXANE, METHYL	141469	000108-87-2	96
			Cyclohexane, methyl- $$ Cyclohexylmethane $$ Hexahydrotoluene $$ Methylcyclohexane	141386	000108-87-2	94
			CYCLOHEXANE, METHYL- $$ METHYLCYCLOHEXANE $$ 1-METHYLCYCLOHEXANE $$ CYCLOHEXANE, METHYL	141470	000108-87-2	94
6	2.421	63.14	D:\DATABASE\DEMO.L			
			Toluene $$ Benzene, methyl $$ Methacide $$ Methylbenzene	158580	000108-88-3	91
			Toluene $$ Benzene, methyl $$ Methacide $$ Methylbenzene	158579	000108-88-3	91
			BENZENE, METHYL- $$ METHYLBENZENE $$ TOLUENE $$ ANTISAL 1A	158625	000108-88-3	91
7	2.745	1.12	D:\DATABASE\DEMO.L			

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-140c-2jm.D
Acq On : 12 Oct 2019 9:38
Operator :
Sample :
Misc :
ALS Vial : 3 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			Cyclohexane, ethyl- $$ Ethylcycloh exane	141508	001678-91-7	93
			CYCLOHEXANE, ETHYL- $$ ETHYLCYCLOH EXANE $$ ETHYL CYCLOHEXANE $$ ETHY LCYCLOHEXAN	141561	001678-91-7	76
			Cyclohexane, ethyl- $$ Ethylcycloh exane	141503	001678-91-7	76
8	2.870	0.58	D:\DATABASE\DEMO.L			
			BENZENE, METHYL- $$ METHYLBENZENE $$ TOLUENE $$ ANTISAL 1A	158623	000108-88-3	91
			1,3,5-CYCLOHEPTATRIENE $$ CYCLOHEP TA-1,3,5-TRIENE $$ CYCLOHEPTATRIEN E $$ CYCLOHEPTATRIENE [UN2603] [FL AMMABLE LIQUID]	158639	000544-25-2	91
			1,3,5-Cycloheptatriene $$ Tropilid ene $$ Cyclohepta-1,3,5-triene $$ Cycloheptatriene	158600	000544-25-2	90
9	4.614	0.01	D:\DATABASE\DEMO.L			
			Eucalyptol $$ Cineole $$ 2-Oxabicy clo[2.2.2]octane, 1,3,3-trimethyl- $$ p-Menthane, 1,8-epoxy-	23206	000470-82-6	94
			2-OXABICYCLO[2.2.2]OCTANE, 1,3,3-T RIMETHYL- $$ 1, 8-CINEOL $$ 1,3,3-TRIMETHYL-2-OXABICYCLO(2.2.2)OCTAN E $$ 1,3,3-TRIMETHYL-2-OXABICYCLO[2.2.2]OCTANE	23288	000470-82-6	93
			2-OXABICYCLO[2.2.2]OCTANE, 1,3,3-T RIMETHYL- $$ 1, 8-CINEOL $$ 1,3,3-TRIMETHYL-2-OXABICYCLO(2.2.2)OCTAN E $$ 1,3,3-TRIMETHYL-2-OXABICYCLO[2.2.2]OCTANE	23420	000470-82-6	93
10	16.753	0.01	D:\DATABASE\DEMO.L			
			4-BROMO-N-[(6-METHYL-2-PYRIDYL)AMI NOMETHYL]PHTHALIMIDE $$ 5-BROMO-2-{[(6-METHYL-2-PYRIDINYL)AMINO]METH YL}-1H-ISOINDOLE-1,3(2H)-DIONE	7473	999007-47-4	9
			2-METHOXY-4-(METHOXYMETHYL)-6-METH YLNICOTINONITRILE $$ PYRIDINE-3-CA RBONITRILE, 2,4-DIMETHOXY-6-METHYL	7347	063644-84-8	9
			3-(3-OXO-3H-BENZO[F]CHROMEN-2-YL)- 2,4(1H,3H)-QUINOLINEDIONE $$ 4-HYD ROXY-3-(2-OXO-2H-1-OXA-3-PHENANTHR YL)-2(1H)-QUINOLINONE	7476	999007-47-7	4
11	17.309	0.02	D:\DATABASE\DEMO.L			
			2H-2,4A-METHANONAPHTHALENE, 1,3,4, 5,6,7-HEXAHYDRO-1,1,5,5-TETRAMETHY L-, (2S)- $$ (-)-ISOLONGIFOLENE $$ (-)-ISOLONGIFOLINE $$ (2S)-1,3,4, 5,6,7-HEXAHYDRO-1,1,5,5-TETRAMETHY L-2H-2,4A-METHANONAPHTHALENE	350805	001135-66-6	97
			2H-2,4a-Methanonaphthalene, 1,3,4, 5,6,7-hexahydro-1,1,5,5-tetramethy 1-, (2S)- $$ 2H-2,4a-Methanonaphth alene, 1,3,4,5,6,7-hexahydro-1,1,5 ,5-tetramethyl-, (2S,4aR)-(-)- $$	350641	001135-66-6	97

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Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-140c-2jm.D
Acq On    : 12 Oct 2019    9:38
Operator  :
Sample    :
Misc      :
ALS Vial  : 3   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e
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#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			Isolongifolene $$ (-)-Isolongifol1 ne			
			2H-2,4A-METHANONAPHTHALENE, 1,3,4, 5,6,7-HEXAHYDRO-1,1,5,5-TETRAMETHY L-, (2S)- $$ (-)-ISOLONGIFOLENE $$ (-)-ISOLONGIFOLINE $$ (2S)-1,3,4, 5,6,7-HEXAHYDRO-1,1,5,5-TETRAMETHY L-2H-2,4A-METHANONAPHTHALENE	350804	001135-66-6	95
2	17.709	0.01	D:\DATABASE\DEMO.L			
			3-AMINOOXY-4-CHLORO-BUTYRIC ACID E THYL ESTER $$ ETHYL 3-(AMINOOXY)-4 -CHLOROBUTANOATE	2831	999002-83-2	9
			Taurolidine $$ 2H-1,2,4-Thiadiazin e, 4,4'-methylenebis[tetrahydro-, 1,1,1',1'-tetraoxide $$ 4,4'-Methy lenebis(tetrahydro-1,2,4-thiadiazi ne 1,1-dioxide) $$ Taurolin	4983	019388-87-5	9
			3-Aminooxy-4-chlorobutyric acid, e thyl ester	2829	999002-83-0	9
3	17.838	0.01	D:\DATABASE\DEMO.L			
			1,4,5,6,7,8-HEXAHYDROCYCLOHEPTA[C] PYRAZOLE $$ 4,5-PENTANOPYRAZOLE	1149	999001-14-9	10
			2-METHOXY-4-(METHOXYMETHYL)-6-METH YLNICOTINONITRILE $$ PYRIDINE-3-CA RBONITRILE, 2,4-DIMETHOXY-6-METHYL	7347	063644-84-8	9
			BENZENE, 1-(2-CYCLOHEXEN-1-YL-2-D) -4-METHOXY- $$ 3-(P-METHOXYPHENYL) (2-2H1)CYCLOHEX-1-ENE	7344	086426-62-2	7
4	28.939	0.00	D:\DATABASE\DEMO.L			
			4-(METHOXYMETHYL)-6-METHYL-2-PHENO XYNICOTINONITRILE $$ PYRIDINE-3-CA RBONITRILE, 4-METHOXYMETHYL-6-METH YL-2-PHENOXY-	7413	332057-36-0	16
			1-DODECANAMINE $$ 1-AMINODODECANE $$ 1-DODECYLAMINE $$ ALAMINE 4	4661	000124-22-1	9
			1-Dodecanamine $$ Dodecylamine $$ n-Dodecylamine $$ Alamine 4	4652	000124-22-1	9
5	30.301	0.03	D:\DATABASE\DEMO.L			
			ENT-PIMARA-8,15-DIENE	481166	021561-92-2	96
			Phenanthrene, 7-ethenyl-1,2,3,4,4a ,5,6,7,8,9,10,10a-dodecahydro-1,1, 4a,7-tetramethyl- $$ Pimara-8,15-d iene #	481092	055255-56-6	90
			PIMARA-8,15-DIENE $$ PHENANTHRENE, 7-ETHENYL-1,2,3,4,4A,5,6,7,8,9,10 ,10A-DODECAHYDRO-1,1,4A,7-TETRAMET HYL- $$ 7.ALPHA.-ETHENYL-1,1,4A,7. BETA.-TETRAMETHYL-1,2,3,4,4A,5,6,7 ,8,9,10,10A-DODECAHYDROPHENANTHREN	481165	055255-56-6	90
6	30.717	0.00	D:\DATABASE\DEMO.L			
			4-(METHOXYMETHYL)-6-METHYL-2-PHENO XYNICOTINONITRILE $$ PYRIDINE-3-CA RBONITRILE, 4-METHOXYMETHYL-6-METH YL-2-PHENOXY-	7413	332057-36-0	27

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Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-140c-2jm.D
Acq On    : 12 Oct 2019    9:38
Operator  :
Sample    :
Misc      :
ALS Vial  : 3   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e
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Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			3-(3-OXO-3H-BENZO[F]CHROMEN-2-YL)-2,4(1H,3H)-QUINOLINEDIONE $$ 4-HYDROXY-3-(2-OXO-2H-1-OXA-3-PHENANTHRYL)-2(1H)-QUINOLINONE	7476	999007-47-7	12
			4-BROMO-N-[(6-METHYL-2-PYRIDYL)AMINOMETHYL]PHTHALIMIDE $$ 5-BROMO-2-{[(6-METHYL-2-PYRIDINYL)AMINO]METHYL}-1H-ISOINDOLE-1,3(2H)-DIONE	7473	999007-47-4	9
17	31.251	0.01	D:\DATABASE\DEMO.L 4-(METHOXYMETHYL)-6-METHYL-2-PHENOXYNICOTINONITRILE $$ PYRIDINE-3-CARBONITRILE, 4-METHOXYMETHYL-6-METHYL-2-PHENOXY-	7413	332057-36-0	12
			D.G.R.B.A.	454	000000-00-0	9
			3-(3-OXO-3H-BENZO[F]CHROMEN-2-YL)-2,4(1H,3H)-QUINOLINEDIONE $$ 4-HYDROXY-3-(2-OXO-2H-1-OXA-3-PHENANTHRYL)-2(1H)-QUINOLINONE	7476	999007-47-7	9
18	31.705	0.02	D:\DATABASE\DEMO.L 4-(METHOXYMETHYL)-6-METHYL-2-PHENOXYNICOTINONITRILE $$ PYRIDINE-3-CARBONITRILE, 4-METHOXYMETHYL-6-METHYL-2-PHENOXY-	7413	332057-36-0	14
			6-ETHYL-2-METHYL-4,6-DIHYDRO-2H-[1,4]OXAZINO[3,2-C]QUINOLINE-3,5-DIONE $$ 6-ETHYL-2-METHYL-2H-1-OXA-4,6-PHENANTHROLINE-3,5(4H,6H)-DIONE $$ 6-ETHYL-2-METHYL-6,10B-DIHYDRO-2H-[1,4]OXAZINO[3,2-C]QUINOLINE-3,5-DIONE	7414	334023-40-4	12
			Ethanedicarboxamide, N-allyl-N'-(2,5-dimethylphenyl)-	7392	331864-72-3	10
19	31.829	0.01	D:\DATABASE\DEMO.L 4-(METHOXYMETHYL)-6-METHYL-2-PHENOXYNICOTINONITRILE $$ PYRIDINE-3-CARBONITRILE, 4-METHOXYMETHYL-6-METHYL-2-PHENOXY-	7413	332057-36-0	22
			2,2'-(1,4-Piperazinediyl)bis[N-(4-methoxyphenyl)succinimide]	7524	293766-05-9	9
			1-Tetradecanamine $$ Tetradecylamine $$ Armeen 14 $$ Myristylamine	4817	002016-42-4	7
20	32.067	0.01	D:\DATABASE\DEMO.L 9-(4-HYDROXYPHENYL)-3,3,6,6-TETRAMETHYL-3,4,6,7,8A,9-HEXAHYDRO-1,8(2H,5H)-ACRIDINEDIONE	7482	999007-48-3	10
			4-(METHOXYMETHYL)-6-METHYL-2-PHENOXYNICOTINONITRILE $$ PYRIDINE-3-CARBONITRILE, 4-METHOXYMETHYL-6-METHYL-2-PHENOXY-	7413	332057-36-0	10
			2,2'-(1,4-Piperazinediyl)bis[N-(4-methoxyphenyl)succinimide]	7524	293766-05-9	9
21	32.197	0.00	D:\DATABASE\DEMO.L 4-(METHOXYMETHYL)-6-METHYL-2-PHENOXYNICOTINONITRILE $$ PYRIDINE-3-CA	7413	332057-36-0	35

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Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-140c-2jm.D
Acq On    : 12 Oct 2019    9:38
Operator  :
Sample    :
Misc      :
ALS Vial  : 3   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autointl.e
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#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			RBONITRILE, 4-METHOXYMETHYL-6-METH YL-2-PHENOXY-			
			L-Alanine, N-glycyl- $$ Alanine, N -glycyl-, L- $$ Glcylalanine $$ Gl y-ala	4366	003695-73-6	9
			Glycyl-dl-alanine $$ DL-Alanine, N -glycyl- $$ N-(Aminoacetyl)alanine #1	4361	000926-77-2	5
2	32.413	0.02	D:\DATABASE\DEMO.L			
			4-(METHOXYMETHYL)-6-METHYL-2-PHENO XYNICOTINONITRILE $$ PYRIDINE-3-CA RBONITRILE, 4-METHOXYMETHYL-6-METH YL-2-PHENOXY-	7413	332057-36-0	12
			3-(3-OXO-3H-BENZO[F]CHROMEN-2-YL)- 2,4(1H,3H)-QUINOLINEDIONE $$ 4-HYD ROXY-3-(2-OXO-2H-1-OXA-3-PHENANTHR YL)-2(1H)-QUINOLINONE	7476	999007-47-7	10
			1-DODECANAMINE $$ 1-AMINODODECANE $$ 1-DODECYLAMINE $$ ALAMINE 4	4661	000124-22-1	10
3	32.969	0.00	D:\DATABASE\DEMO.L			
			4-(METHOXYMETHYL)-6-METHYL-2-PHENO XYNICOTINONITRILE $$ PYRIDINE-3-CA RBONITRILE, 4-METHOXYMETHYL-6-METH YL-2-PHENOXY-	7413	332057-36-0	27
			2,2,3,3,4,4,5,5-OCTAFLUORO-N-(3-ME THOXYPHENYL)PENTANAMIDE $$ PENTANA MIDE, 2,2,3,3,4,4,5,5-OCTAFLUORO-N -(3-METHOXYPHENYL)-	7474	339166-43-7	10
			9-(4-HYDROXYPHENYL)-3,3,6,6-TETRAM ETHYL-3,4,6,7,8A,9-HEXAHYDRO-1,8(2 H,5H)-ACRIDINEDIONE	7482	999007-48-3	10
4	33.369	0.01	D:\DATABASE\DEMO.L			
			2,2'-(1,4-PIPERAZINEDIYL)BIS[N-(4- METHOXYPHENYL)SUCCINIMIDE]	7525	293766-05-9	17
			2,2'-(1,4-Piperazinediyl)bis[N-(4- methoxyphenyl)succinimide]	7524	293766-05-9	17
			4-(METHOXYMETHYL)-6-METHYL-2-PHENO XYNICOTINONITRILE $$ PYRIDINE-3-CA RBONITRILE, 4-METHOXYMETHYL-6-METH YL-2-PHENOXY-	7413	332057-36-0	12
5	33.493	0.08	D:\DATABASE\DEMO.L			
			PIMARA-8(14),15-DIEN-18-AL $$ 1-PH ENANTHRENECARBOXALDEHYDE, 7-ETHENY L-1,2,3,4,4A,4B,5,6,7,9,10,10A-DOD ECAHYDRO-1,4A,7-TRIMETHYL-, [1R-(1 .ALPHA.,4A.BETA.,4B.ALPHA.,7.BETA. ,10A.ALPHA.)]- $$ CRYPTOPINON $$ C RYPTOPINONE	481208	000472-39-9	83
			1-Phenanthrenecarboxaldehyde, 7-et henyl-1,2,3,4,4a,4b,5,6,7,9,10,10a -dodecahydro-1,4a,7-trimethyl-, [1 R-(1.alpha.,4a.beta.,4b.alpha.,7.b eta.,10a.alpha.)]- $$ Podocarp-8(1 4)-en-15-al, 13.alpha.-methyl-13-v inyl- $$ Cryptopinon $$ Cryptopino	481182	000472-39-9	83

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsen-140c-2jm.D
Acq On : 12 Oct 2019 9:38
Operator :
Sample :
Misc :
ALS Vial : 3 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			ne			
			KAURA-5,16-DIEN-18-OL $$ KAURA-5,1	492904	023837-99-2	80
			6-DIEN-18(OR 19)-OL $$ KAURA-5,16-			
			DIEN-19-OL			
26	33.677	0.01	D:\DATABASE\DEMO.L			
			3-PHENYL-2-ACETYL-1-HYDROXYCYCLOHE	45247	088483-84-5	27
			XENE-4-CARBONITRILE			
			2,4-Bis(hydroxylamino)-5-nitropyri	44521	999044-52-3	14
			midine			
			Sarcosine, n-hexanoyl-, butyl este	45268	999045-27-0	14
27	33.785	0.02	D:\DATABASE\DEMO.L			
			No matches found			
28	33.855	0.06	D:\DATABASE\DEMO.L			
			1-Methyl-10,18-bisnorabieta-8,11,1	466158	999466-16-6	93
			3-triene			
			4-(N-METHYLAMINO)-6,7-(1,2,3,4-TET	466219	000000-00-0	78
			RAHYDRO-1,1,4,4-TETRAMETHYLBENZO)I			
			NDOLE			
			1-[4-METHOXY-3-(4-METHYLPHENOXY)PH	466181	116345-94-9	62
			ENYL]ETHANONE $$ ETHANONE, 1-[4-ME			
			THOXY-3-(4-METHYLPHENOXY)PHENYL]-			
29	34.131	0.02	D:\DATABASE\DEMO.L			
			KAUR-16-EN-18-OIC ACID $$ KAUR-16-	168418	020316-84-1	15
			EN-18-OIC ACID, (4.BETA.)- $$ (-)-			
			KAURNENOIC ACID $$ (4-BETA)-KAUR-1			
			6-EN-18-OIC ACID			
			ABIETA-7,13-DIEN-18-OIC ACID $$ 1-	168420	000514-10-3	11
			PHENANTHRENECARBOXYLIC ACID, 1,2,3			
			,4,4A,4B,5,6,10,10A-DECAHYDRO- $$			
			1-PHENANTHRENECARBOXYLIC ACID, 1,2			
			,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,			
			4A-DIMETHYL-7-(1-METHYLETHYL)-, [1			
			R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A			
			.ALPHA.)]-			
			7-ANTI-METHYL-N-PHENYL-7-SYN-VINYL	167018	118205-81-5	9
			-5,6-DIAZABICYCLO[2.2.1]HEPT-2-ENE			
			-5,6-DICARBOXIMIDE			
30	34.185	0.02	D:\DATABASE\DEMO.L			
			Benzaldehyde, 4-(1-methylethyl)- $	286032	000122-03-2	46
			$ Benzaldehyde, p-isopropyl- $$ p-			
			Cumic aldehyde $$ p-Isopropylbenza			
			ldehyde			
			BENZALDEHYDE, 4-(1-METHYLETHYL)- $	286114	000122-03-2	46
			$ 4-ISOPROPYLBENZALDEHYDE $$ 4-(1-			
			METHYLETHYL)-BENZALDEHYDE $$ 4-(1-			
			METHYLETHYL)BENZALDEHYDE			
			1-(2-PROPYL)-2,3,5-TRIMETHYLCYCLOP	286083	999286-08-6	45
			ENTA-2,4-DIEN $$ 5-ALLYL-1,2,4-TRI			
			METHYL-1,3-CYCLOPENTADIENE			
31	34.309	0.03	D:\DATABASE\DEMO.L			
			METHYL PIMARA-8,15-DIEN-18-OATE $$	466513	003582-26-1	60
			1-PHENANTHRENECARBOXYLIC ACID, 7-			
			ETHENYL-1,2,3,4,4A,5,6,7,8,9,10,10			

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Data Path : F:\DATA MS\daa\
Data File : WLM-10prsen-140c-2jm.D
Acq On    : 12 Oct 2019    9:38
Operator  :
Sample    :
Misc      :
ALS Vial  : 3   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e
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%#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			A-DODECAHYDRO-1,4A,7-TRIMETHYL-, METHYL ESTER, [1R-(1.ALPHA.,4A.BETA.,7.BETA.,10A.ALPHA.)]- $$ METHYL 8,15-PIMARADIEN-18-OATE			
			1-Phenanthrenecarboxylic acid, 7-ethenyl-1,2,3,4,4a,5,6,7,8,9,10,10a-dodecahydro-1,4a,7-trimethyl-, methyl ester, [1R-(1.alpha.,4a.beta.,7.alpha.,10a.alpha.)]- $$ Podocarp-8-en-15-oic acid, 13.beta.-methyl-13-vinyl-, methyl ester	466506	019907-21-2	46
			METHYL PIMARA-8,15-DIEN-18-OATE $$ 1-PHENANTHRENECARBOXYLIC ACID, 7-ETHENYL-1,2,3,4,4A,5,6,7,8,9,10,10A-DODECAHYDRO-1,4A,7-TRIMETHYL-, METHYL ESTER, [1R-(1.ALPHA.,4A.BETA.,7.ALPHA.,10A.ALPHA.)]- $$ METHYL 8,15-ISOPIMARADIEN-18-OATE	466512	019907-21-2	46
32	34.530	0.13	D:\DATABASE\DEMO.L 2H-1,4-BENZODIAZEPIN-2-ONE, 7-CHLORO-1,3-DIHYDRO-3-HYDROXY-5-PHENYL- $$ (+-)-OXAZEPAM $$ (RS)-OXAZEPAM $$ 1,3-DIHYDRO-7-CHLORO-3-HYDROXY-5-PHENYL-2H-1,4-BENZODIAZEPIN-2-ONE	481202	000604-75-1	64
			1,5-CYCLODODECADIENE, 8,10-BIS(METHYLENE)- $$ MIXTURE OF TRANS,TRANS-1,3-DIMETHYLENECYCLODODECA-5,9-DIENE AND TRANS,TRANS-1,10-DIMETHYLENECYCLODODECA-3,7-DIENE (ISOMER A)	161342	066405-18-3	42
			1-Phenanthrenecarboxaldehyde, 7-ethenyl-1,2,3,4,4a,4b,5,6,7,9,10,10a-dodecahydro-1,4a,7-trimethyl-, [1R-(1.alpha.,4a.beta.,4b.alpha.,7.beta.,10a.alpha.)]- $$ Podocarp-8(14)-en-15-al, 13.alpha.-methyl-13-vinyl- $$ Cryptopinon $$ Cryptopinone	481182	000472-39-9	41
33	34.644	0.00	D:\DATABASE\DEMO.L Ethyl 2-((diethoxyphosphoryl)oxy)-3,3,3-trifluoropropanoate	3375	999003-37-6	1
34	34.687	0.00	D:\DATABASE\DEMO.L 1-Tetradecanamine $$ Tetradecylamine $$ Armeen 14 $$ Myristylamine	4817	002016-42-4	10
			1-Undecanamine $$ Undecylamine $$ n-Undecylamine $$ Hendecylamine	4554	007307-55-3	9
			4-(METHOXYMETHYL)-6-METHYL-2-PHENOXYNICOTINONITRILE $$ PYRIDINE-3-CARBONITRILE, 4-METHOXYMETHYL-6-METHYL-2-PHENOXY-	7413	332057-36-0	9
35	34.779	0.02	D:\DATABASE\DEMO.L Benzonitrile, m-phenethyl- $$ 3-(2-Phenylethyl)benzonitrile #	162409	034176-91-5	11
			3-(2-PHENYLETHYL)BENZONITRILE $$ BENZONITRILE, M-PHENETHYL- $$ 1-(3-	162420	034176-91-5	11

Data Path : F:\DATA MS\daa\
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Acq On : 12 Oct 2019 9:38
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Sample :
Misc :
ALS Vial : 3 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			CYANOPHENYL)-2-PHENYLETHANE $$ M-CYANO-1,2-DIPHENYLETHANE			
			2H-3,9A-METHANO-1-BENZOXEPIN, OCTAHYDRO-2,2,5A,9-TETRAMETHYL-, [3R-(3.ALPHA.,5A.ALPHA.,9.ALPHA.,9A.ALPHA.)]- $$ .BETA.-AGAROFURAN, DIHYDRO- $$ .BETA.-DIHYDROAGAROFURAN $$ 2H-3,9A-METHANO-1-BENZOXEPIN, OCTAHYDRO-2,2,5A,9-TETRAMETHYL-	3110	005956-09-2	10
36	34.919	0.01	D:\DATABASE\DEMO.L			
			Diethyl 3-chloro-2-hydroxypropylmalonate	3235	999003-23-6	9
			DIETHYL 2-(3-CHLORO-2-HYDROXYPROPYL)MALONATE $$ DIETHYL 3-CHLORO-2-HYDROXYPROPYLMALONATE	3236	999003-23-7	9
			2H-3,9A-METHANO-1-BENZOXEPIN, OCTAHYDRO-2,2,5A,9-TETRAMETHYL-, [3R-(3.ALPHA.,5A.ALPHA.,9.ALPHA.,9A.ALPHA.)]- $$ .BETA.-AGAROFURAN, DIHYDRO- $$ .BETA.-DIHYDROAGAROFURAN $$ 2H-3,9A-METHANO-1-BENZOXEPIN, OCTAHYDRO-2,2,5A,9-TETRAMETHYL-	3110	005956-09-2	8
37	34.984	0.01	D:\DATABASE\DEMO.L			
			4-(Phenylthioxomethyl)morpholine $$ Morpholine, 4-(thiobenzoyl)- $$ Morpholinylthiobenzamide $$ 4-(Thiobenzoyl)morpholine	256918	002032-36-2	25
			(1S*,2S*,5R*,10R*)-1,6-DIMETHYL-10-ETHOXY-11-OXATRICYCLO[5.3.0.1(2,5)]UNDEC-6-ENE	257280	124780-75-2	23
			(1S*,2S*,5R*,6R*,10R*)-1,6-DIMETHYL-10-ETHOXY-11-OXATRICYCLO[5.3.0.1(2,5)]UNDEC-6-ENE	257281	124780-76-3	17
38	35.027	0.02	D:\DATABASE\DEMO.L			
			2-Cyclohexyldimethylsilyloxyoct-3-ene	123545	999123-54-8	62
			1,1-DIMETHOXYUNDECANE $$ UNDECANAL, DIMETHYL ACETAL $$ UNDECANE, 1,1-DIMETHOXY- $$ UNDECANAL DIMETHYL ACETAL	123009	052517-67-6	53
			1-Ethyl-2-pentamethyldisilanyloxycyclohexane	123454	999123-45-7	53
39	35.141	0.02	D:\DATABASE\DEMO.L			
			KAUR-16-EN-18-OIC ACID $$ KAUR-16-EN-18-OIC ACID, (4.BETA.)- $$ (-)-KAURNENOIC ACID $$ (4-BETA)-KAUR-16-EN-18-OIC ACID	168418	020316-84-1	38
			2-METHYL-3-PHENYL-1H-INDOLE $$ 1H-INDOLE, 2-METHYL-3-PHENYL- $$ 2-METHYL-3-PHENYLINDOLE $$ 3 PHENYL-2-METHYLINDOLE	428173	004757-69-1	25
			PYRIMIDINE, 2-(4-NITRO-2-THIENYL)- $$ 2-(4'-NITRO-2'-THIENYL)PYRIMIDINE	428101	057059-15-1	25

Data Path : F:\DATA MS\daa\
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Sample :
Misc :
ALS Vial : 3 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autointl.e

k#	RT	Area%	Library/ID	Ref#	CAS#	Qual
40	35.163	0.02	D:\DATABASE\DEMO.L			
			KAUR-16-EN-18-OIC ACID $$ KAUR-16-EN-18-OIC ACID, (4.BETA.)- $$ (-)-KAURNENOIC ACID $$ (4-BETA)-KAUR-16-EN-18-OIC ACID	168418	020316-84-1	38
			BUTYL 2-(METHYLAMINO)BENZOATE $$ ANTHRANILIC ACID, N-METHYL-, BUTYL ESTER $$ N-BUTYL O-METHYLAMINOBENZOATE	209256	015236-34-7	35
			1H-Pyrazole-1-acetamide, 4-iodo-N-(phenylmethyl)-	170579	999170-58-2	16
41	35.276	0.01	D:\DATABASE\DEMO.L			
			CIS-4-ETHOXY-B-METHYL-B-NITROSTYRENE	428132	000000-00-0	48
			2-PROPENE-1-SULFONIC ACID, 3-(3,4,5-TRIMETHOXYPHENYL)-, METHYL ESTER, (E)- $$ METHYL-3-(3',4',5'-TRIMETHOXYPHENYL)-2-PROPENE-1-SULPHONAT	428799	104503-96-0	38
			BUTYL 2-(METHYLAMINO)BENZOATE $$ ANTHRANILIC ACID, N-METHYL-, BUTYL ESTER $$ N-BUTYL O-METHYLAMINOBENZOATE	209256	015236-34-7	38
42	35.298	0.01	D:\DATABASE\DEMO.L			
			KAUR-16-EN-18-OIC ACID $$ KAUR-16-EN-18-OIC ACID, (4.BETA.)- $$ (-)-KAURNENOIC ACID $$ (4-BETA)-KAUR-16-EN-18-OIC ACID	168418	020316-84-1	35
			ABIETA-7,13-DIEN-18-OIC ACID $$ 1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,4B,5,6,10,10A-DECAHYDRO- $$ 1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL)-, [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A.ALPHA.)]-	168420	000514-10-3	11
			Benzenepropanoic acid, tert-butyldimethylsilyl ester $$ tert-Butyl(dimethyl)silyl 3-phenylpropanoate #	123517	078324-01-3	10
43	35.395	0.04	D:\DATABASE\DEMO.L			
			Pyridine, 4-[5-[[(4-fluorophenyl)methyl]thio]-1,3,4-oxadiazol-2-yl]-	229059	999229-06-2	27
			6-(3-BROMOPROPYL)-2(1H)-PYRIDINONE	228227	101773-69-7	25
			2(1H)-PYRIDINONE, 6-METHYL- $$ 2(1H)-PYRIDINONE, 6-METHYL- $$ 2(1H)-PYRIDONE, 6-METHYL- $$ 2(1H)-PYRIDONE, 6-METHYL-	226818	003279-76-3	25
44	35.470	0.57	D:\DATABASE\DEMO.L			
			Phenol, 2,4-bis(1-phenylethyl)- $$ 2,4-Bis(1-phenylethyl)phenol #	504578	002769-94-0	51
			ROSIN ACIDS	504611	000000-00-0	45
			PIMARA-8(14),15-DIEN-18-OIC ACID $$ 1-PHENANTHRENECARBOXYLIC ACID, 7-ETHENYL-1,2,3,4,4A,4B,5,6,7,9,10,10A-DODECAHYDRO-1,4A,7-TRIMETHYL-, [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,	504609	000127-27-5	42

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-140c-2jm.D
Acq On : 12 Oct 2019 9:38
Operator :
Sample :
Misc :
ALS Vial : 3 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

%#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			7.BETA.,10A.ALPHA.)]- $$ (+)-PIMAR IC ACID $$ .ALPHA.-PIMARIC ACID			
45	35.649	0.07	D:\DATABASE\DEMO.L			
			1H-NAPHTHO[2,3-C]PYRAN-5,10-DIONE, 3,4-DIHYDRO-7,9-DIMETHOXY-1,3-DIM ETHYL-, CIS-(.+-.)- $$ (+,-)-CIS-7 ,9-DIMETHOXY-1,3-DIMETHYL-3,4,5,10 -TETRAHYDRONAPHTHO[2,3-C]PYRAN-5,1 0-DIONE	513558	084018-43-9	52
			1H-NAPHTHO[2,3-C]PYRAN-5,10-DIONE, 3,4-DIHYDRO-7,9-DIMETHOXY-1,3-DIM ETHYL-, TRANS-(.+-.)- $$ (+,-)-DEO XYQUINONE A DIMETHYL ETHER $$ (+,-)-TRANS-7,9-DIMETHOXY-1,3-DIMETHYL -3,4,5,10-TETRAHYDRONAPHTHO[2,3-C] PYRAN-5,10-DIONE	513557	084018-44-0	50
			Methanone, [1,4-dimethyl-7-(1-meth ylethyl)-2-azulenyl]phenyl- $$ 2-B enzoylguaiazulene $$ (7-Isopropyl- 1,4-dimethyl-2-azulenyl)(phenyl)me thanone #	513367	039665-56-0	43
46	35.751	0.17	D:\DATABASE\DEMO.L			
			DEHYDROABIETIC ACID	464556	000000-00-0	97
			METHYL ABIETA-8,11,13-TRIEN-18-OAT E $$ 1-PHENANTHRENECARBOXYLIC ACID , 1,2,3,4,4A,9,10,10A-OCTAHYDRO-1, 4A-DIMETHYL-7-(1-METHYLETHYL)-, ME THYL ESTER, [1R-(1.ALPHA.,4A.BETA. ,10A.ALPHA.)]- $$ DEHYDROABIETIC A CID METHYL ESTER $$ METHYL DEHYDRO ABIETATE	464549	001235-74-1	95
			1-Phenanthrenecarboxylic acid, 1,2 ,3,4,4a,9,10,10a-octahydro-1,4a-di methyl-7-(1-methylethyl)-, methyl ester, [1R-(1.alpha.,4a.beta.,10a. alpha.)]- $$ Podocarpa-8,11,13-tri en-15-oic acid, 13-isopropyl-, met hyl ester $$ Methyl dehydroabietat	464538	001235-74-1	94
47	35.913	0.06	D:\DATABASE\DEMO.L			
			KAUR-16-EN-18-OIC ACID $$ KAUR-16- EN-18-OIC ACID, (4.BETA.)- $$ (-)- KAURNENOIC ACID $$ (4-BETA)-KAUR-1 6-EN-18-OIC ACID	168418	020316-84-1	58
			Androst-5-en-17-ol, 4,4-dimethyl-	513436	999513-44-9	51
			Abietic acid $$ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid	513378	000514-10-3	38
48	35.989	0.08	D:\DATABASE\DEMO.L			
			1-CYCLOHEXENE-1-METHANOL, .ALPHA., 2-DIETHENYL- $$ 1-(2'-ETHENYL-1'-C YCLOHEXENYL)-2-PROPEN-1-OL	160335	115691-99-1	59

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsen-140c-2jm.D
Acq On : 12 Oct 2019 9:38
Operator :
Sample :
Misc :
ALS Vial : 3 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

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			Silane, dimethyl(undec-2-enyloxy)i	123856	999123-85-9	55
			sobutoxy-			
			2-Methyl-1-propanol, tert-butyldim	122637	999122-64-0	35
			ethylsilyl ether			
49	36.092	0.48	D:\DATABASE\DEMO.L			
			INDOLIZINO[1,2-B]QUINOLIN-9(11H)-O	504762	054318-62-6	92
			NE, 8-[(FORMYLOXY)METHYL]-7-(1-OXO			
			PROPYL)- $$ 8-FORMYLOXYMETHYL-7-(1			
			-OXOPROPYL)INDOLIZINO)1,2-B)QUINOL			
			IN-9(11H)-ONE			
			PIMARA-8(14),15-DIEN-18-OIC ACID $	504609	000127-27-5	70
			$ 1-PHENANTHRENECARBOXYLIC ACID, 7			
			-ETHENYL-1,2,3,4,4A,4B,5,6,7,9,10,			
			10A-DODECAHYDRO-1,4A,7-TRIMETHYL-,			
			[1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,			
			7.BETA.,10A.ALPHA.)]- $$ (+)-PIMAR			
			IC ACID $$ .ALPHA.-PIMARIC ACID			
			1-Hydroxy-6-(3-isopropenyl-cyclopr	257257	999257-26-0	42
			op-1-enyl)-6-methyl-heptan-2-one			
50	36.313	0.02	D:\DATABASE\DEMO.L			
			PIMARA-8(14),15-DIEN-18-OIC ACID $	504608	000127-27-5	90
			$ 1-PHENANTHRENECARBOXYLIC ACID, 7			
			-ETHENYL-1,2,3,4,4A,4B,5,6,7,9,10,			
			10A-DODECAHYDRO-1,4A,7-TRIMETHYL-,			
			[1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,			
			7.BETA.,10A.ALPHA.)]- $$ (+)-PIMAR			
			IC ACID $$ .ALPHA.-PIMARIC ACID			
			Pimaric acid $$ 1-Phenanthrenecarb	504569	000127-27-5	90
			oxylic acid, 7-ethenyl-1,2,3,4,4a,			
			4b,5,6,7,9,10,10a-dodecahydro-1,4a			
			,7-trimethyl-, [1R-(1.alpha.,4a.be			
			ta.,4b.alpha.,7.beta.,10a.alpha.)]			
			- $$ Podocarp-8(14)-en-15-oic acid			
			, 13.alpha.-methyl-13-vinyl- $$ D-			
			pimaric acid			
			PIMARA-8(14),15-DIEN-18-OIC ACID $	504609	000127-27-5	59
			$ 1-PHENANTHRENECARBOXYLIC ACID, 7			
			-ETHENYL-1,2,3,4,4A,4B,5,6,7,9,10,			
			10A-DODECAHYDRO-1,4A,7-TRIMETHYL-,			
			[1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,			
			7.BETA.,10A.ALPHA.)]- $$ (+)-PIMAR			
			IC ACID $$ .ALPHA.-PIMARIC ACID			
51	36.383	0.22	D:\DATABASE\DEMO.L			
			METHYL ABIETA-7,13-DIEN-18-OATE $$	258918	000127-25-3	98
			1-PHENANTHRENECARBOXYLIC ACID, 1,			
			2,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1			
			,4A-DIMETHYL-7-(1-METHYLETHYL)-, M			
			ETHYL ESTER, [1R-(1.ALPHA.,4A.BETA			
			.,4B.ALPHA.,10A.ALPHA.)]- $$ ABALY			
			N $$ ABIETIC ACID METHYL ESTER			
			Methyl abietate $$ 1-Phenanthrenec	258889	000127-25-3	98
			arboxylic acid, 1,2,3,4,4a,4b,5,6,			
			10,10a-decahydro-1,4a-dimethyl-7-(			
			1-methylethyl)-, methyl ester, [1R			
			-(1.alpha.,4a.beta.,4b.alpha.,10a.			
			alpha.)]- $$ Podocarpa-7,13-dien-1			

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsen-140c-2jm.D
Acq On : 12 Oct 2019 9:38
Operator :
Sample :
Misc :
ALS Vial : 3 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

%#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			5-oic acid, 13-isopropyl-, methyl ester $$ Abalyn			
			METHYL ABIETA-7,13-DIEN-18-OATE $$ 1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL)-, METHYL ESTER, [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A.ALPHA.)]- $$ ABALYN $$ ABIETIC ACID METHYL ESTER	480551	000127-25-3	94
52	36.589	0.74	D:\DATABASE\DEMO.L			
			1-PHENANTHRENECARBOXYLIC ACID, 7-ETHENYL-1,2,3,4,4A,4B,5,6,7,8,10,10A-DODECAHYDRO-1,4A,7-TRIMETHYL-, [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,7.ALPHA.,10A.ALPHA.)]- $$ ISOPIMARIC ACID $$ PODOCARP-7-EN-15-OIC ACID, 13.BETA.-METHYL-13-VINYL-	466436	005835-26-7	89
			BENZ[A]ANTHRACENONE	513655	099707-96-7	87
			Phenol, 2,4-bis(1-phenylethyl)- $$ 2,4-Bis(1-phenylethyl)phenol #	504578	002769-94-0	86
53	36.740	0.27	D:\DATABASE\DEMO.L			
			1H-NAPHTHO[2,3-C]PYRAN-5,10-DIONE, 3,4-DIHYDRO-7,9-DIMETHOXY-1,3-DIMETHYL-, TRANS-(.+-.)- $$ (+,-)-DEOXYQUINONE A DIMETHYL ETHER $$ (+,-)-TRANS-7,9-DIMETHOXY-1,3-DIMETHYL-3,4,5,10-TETRAHYDRONAPHTHO[2,3-C]PYRAN-5,10-DIONE	513557	084018-44-0	90
			1H-NAPHTHO[2,3-C]PYRAN-5,10-DIONE, 3,4-DIHYDRO-7,9-DIMETHOXY-1,3-DIMETHYL-, CIS-(.+-.)- $$ (+,-)-CIS-7,9-DIMETHOXY-1,3-DIMETHYL-3,4,5,10-TETRAHYDRONAPHTHO[2,3-C]PYRAN-5,10-DIONE	513558	084018-43-9	90
			Androst-5-en-17-ol, 4,4-dimethyl-	513436	999513-44-9	86
54	36.870	0.04	D:\DATABASE\DEMO.L			
			Palustric acid $$ Podocarpa-8,13-dien-15-oic acid, 13-isopropyl- $$ 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,5,6,9,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, (1R-(1.alpha.,4a.beta.,10a.alpha.))- $$ 8,13-Abietadien-18-oic acid	513439	001945-53-5	55
			Androst-5-en-17-ol, 4,4-dimethyl-	513436	999513-44-9	53
			1-Hydroxy-3,7,8-trimethoxyxanthen-9-one $$ 8-Hydroxy-1,2,6-trimethoxy-9H-xanthen-9-one #	504580	020882-69-3	50
55	36.945	0.87	D:\DATABASE\DEMO.L			
			1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1R-(1.alpha.,4a.beta.,10a.alpha.)]- $$ Podocarpa-8,11,13-trien-15-oic acid, 13-isopropyl- $$ Abieta-8,11,13-trien-18-oic acid $$ Abietic acid,	503093	001740-19-8	99

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-140c-2jm.D
Acq On : 12 Oct 2019 9:38
Operator :
Sample :
Misc :
ALS Vial : 3 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

k#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			dehydro- ABIETA-8,11,13-TRIEN-18-OIC ACID $	503106	999503-11-8	99
			$ PODOCARPA-8,11,13-TRIEN-15-SAEUR E, 13-ISOPROPYL-			
			1-PHENANTHRENECARBOXYLIC ACID, 1,2	503110	001740-19-8	99
			,3,4,4A,9,10,10A-OCTAHYDRO-1,4A-DI METHYL-7-(1-METHYLETHYL)-, [1R-(1. ALPHA.,4A.BETA.,10A.ALPHA.)]- $$ (-)-DEHYDROABIETIC ACID $$ 1,2,3,4, 4A,9,10,10A-OCTAHYDRO-1,4A-DIMETHY L-7-(1-METHYLETHYL)-1-PHENANTHRENE CARBOXYLIC ACID			
56	37.161	0.04	D:\DATABASE\DEMO.L			
			1-Phenanthrenecarboxylic acid, 1,2	503094	005155-70-4	93
			,3,4,4a,9,10,10a-octahydro-1,4a-di methyl-7-(1-methylethyl)-, [1S-(1. alpha.,4a.alpha.,10a.beta.)]- $$ P odocarpa-8,11,13-trien-16-oic acid , 13-isopropyl- $$ Callitrisic aci d $$ 4-Epiabietic acid, dehydro-			
			ABIETA-8,11,13-TRIEN-18-OIC ACID $	503112	005155-70-4	93
			$ 1-PHENANTHRENECARBOXYLIC ACID, 1 ,2,3,4,4A,9,10,10A-OCTAHYDRO-1,4A- DIMETHYL-7-(1-METHYLETHYL)-, [1S-(1.ALPHA.,4A.ALPHA.,10A.BETA.)]- $$ 13-ISOPROPYLPODOCARPA-8,11,13-TRI EN-16-OIC ACID $$ 4-EPIABIETIC ACI D, DEHYDRO-			
			ABIETA-7,13-DIEN-18-OIC ACID $$ 1-	168419	000514-10-3	70
			PHENANTHRENECARBOXYLIC ACID, 1,2,3 ,4,4A,4B,5,6,10,10A-DECAHYDRO- $$ 1-PHENANTHRENECARBOXYLIC ACID, 1,2 ,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1, 4A-DIMETHYL-7-(1-METHYLETHYL)-, [1 R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A .ALPHA.)]-			
57	37.242	0.24	D:\DATABASE\DEMO.L			
			ABIETA-7,13-DIEN-18-OIC ACID $$ 1-	168420	000514-10-3	86
			PHENANTHRENECARBOXYLIC ACID, 1,2,3 ,4,4A,4B,5,6,10,10A-DECAHYDRO- $$ 1-PHENANTHRENECARBOXYLIC ACID, 1,2 ,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1, 4A-DIMETHYL-7-(1-METHYLETHYL)-, [1 R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A .ALPHA.)]-			
			ABIETA-7,13-DIEN-18-OIC ACID $$ 1-	168419	000514-10-3	70
			PHENANTHRENECARBOXYLIC ACID, 1,2,3 ,4,4A,4B,5,6,10,10A-DECAHYDRO- $$ 1-PHENANTHRENECARBOXYLIC ACID, 1,2 ,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1, 4A-DIMETHYL-7-(1-METHYLETHYL)-, [1 R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A .ALPHA.)]-			
			Abietic acid $$ 1-Phenanthrenecarb	513378	000514-10-3	70
			oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet			

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Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-140c-2jm.D
Acq On    : 12 Oct 2019    9:38
Operator  :
Sample    :
Misc      :
ALS Vial  : 3   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e

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                a.,4b.alpha.,10a.alpha.)]- $$ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- $$ L-abietic acid

58  37.291  0.18 D:\DATABASE\DEMO.L
                ABIETA-7,13-DIEN-18-OIC ACID $$ 1- 168419 000514-10-3 90
                PHENANTHRENECARBOXYLIC ACID, 1,2,3
                ,4,4A,4B,5,6,10,10A-DECAHYDRO- $$
                1-PHENANTHRENECARBOXYLIC ACID, 1,2
                ,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,
                4A-DIMETHYL-7-(1-METHYLETHYL)-, [1
                R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A
                .ALPHA.)]-
                Abietic acid $$ 1-Phenanthrenecarb 513378 000514-10-3 78
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- $$ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- $$ L-abietic acid
                Palustric acid $$ Podocarpa-8,13-d 513439 001945-53-5 70
                ien-15-oic acid, 13-isopropyl- $$
                1-Phenanthrenecarboxylic acid, 1,2
                ,3,4,4a,5,6,9,10,10a-decahydro-1,4
                a-dimethyl-7-(1-methylethyl)-, (1R
                -(1.alpha.,4a.beta.,10a.alpha.))-
                $$ 8,13-Abietadien-18-oic acid

59  37.388  0.13 D:\DATABASE\DEMO.L
                ABIETA-8,11,13-TRIEN-18-OIC ACID $ 503112 005155-70-4 90
                $ 1-PHENANTHRENECARBOXYLIC ACID, 1
                ,2,3,4,4A,9,10,10A-OCTAHYDRO-1,4A-
                DIMETHYL-7-(1-METHYLETHYL)-, [1S-(
                1.ALPHA.,4A.ALPHA.,10A.BETA.)]- $$
                 13-ISOPROPYLPODOCARPA-8,11,13-TRI
                EN-16-OIC ACID $$ 4-EPIABIETIC ACI
                D, DEHYDRO-
                1-Phenanthrenecarboxylic acid, 1,2 503094 005155-70-4 90
                ,3,4,4a,9,10,10a-octahydro-1,4a-di
                methyl-7-(1-methylethyl)-, [1S-(1.
                alpha.,4a.alpha.,10a.beta.)]- $$ P
                odocarpa-8,11,13-trien-16-oic acid
                , 13-isopropyl- $$ Callitrisic aci
                d $$ 4-Epiabietic acid, dehydro-
                ABIETA-7,13-DIEN-18-OIC ACID $$ 1- 168419 000514-10-3 86
                PHENANTHRENECARBOXYLIC ACID, 1,2,3
                ,4,4A,4B,5,6,10,10A-DECAHYDRO- $$
                1-PHENANTHRENECARBOXYLIC ACID, 1,2
                ,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,
                4A-DIMETHYL-7-(1-METHYLETHYL)-, [1
                R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A
                .ALPHA.)]-

60  37.448  0.07 D:\DATABASE\DEMO.L
                1-Phenanthrenecarboxylic acid, 1,2 503094 005155-70-4 92
                ,3,4,4a,9,10,10a-octahydro-1,4a-di
                methyl-7-(1-methylethyl)-, [1S-(1.
                alpha.,4a.alpha.,10a.beta.)]- $$ P
                odocarpa-8,11,13-trien-16-oic acid
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Data Path : F:\DATA MS\daa\
Data File : WLM-10prsen-140c-2jm.D
Acq On    : 12 Oct 2019   9:38
Operator  :
Sample    :
Misc      :
ALS Vial  : 3   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L              Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#      RT  Area%          Library/ID                Ref#      CAS#   Qual
_______________________________________________________________________________
                   , 13-isopropyl- $$ Callitrisic aci
                   d $$ 4-Epiabietic acid, dehydro-
                   ABIETA-8,11,13-TRIEN-18-OIC ACID $ 503112 005155-70-4 92
                   $ 1-PHENANTHRENECARBOXYLIC ACID, 1
                   ,2,3,4,4A,9,10,10A-OCTAHYDRO-1,4A-
                   DIMETHYL-7-(1-METHYLETHYL)-, [1S-(
                   1.ALPHA.,4A.ALPHA.,10A.BETA.)]- $$
                    13-ISOPROPYLPODOCARPA-8,11,13-TRI
                   EN-16-OIC ACID $$ 4-EPIABIETIC ACI
                   D, DEHYDRO-
                   ABIETA-7,13-DIEN-18-OIC ACID $$ 1- 168419 000514-10-3 90
                   PHENANTHRENECARBOXYLIC ACID, 1,2,3
                   ,4,4A,4B,5,6,10,10A-DECAHYDRO- $$
                   1-PHENANTHRENECARBOXYLIC ACID, 1,2
                   ,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,
                   4A-DIMETHYL-7-(1-METHYLETHYL)-, [1
                   R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A
                   .ALPHA.)]-

 61  37.696   3.22 D:\DATABASE\DEMO.L
                   Abietic acid $$ 1-Phenanthrenecarb 513378 000514-10-3 99
                   oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                   10a-decahydro-1,4a-dimethyl-7-(1-m
                   ethylethyl)-, [1R-(1.alpha.,4a.bet
                   a.,4b.alpha.,10a.alpha.)]- $$ Podo
                   carpa-7,13-dien-15-oic acid, 13-is
                   opropyl- $$ L-abietic acid
                   Abietic acid $$ 1-Phenanthrenecarb 513347 000514-10-3 94
                   oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                   10a-decahydro-1,4a-dimethyl-7-(1-m
                   ethylethyl)-, [1R-(1.alpha.,4a.bet
                   a.,4b.alpha.,10a.alpha.)]- $$ Podo
                   carpa-7,13-dien-15-oic acid, 13-is
                   opropyl- $$ L-abietic acid
                   Abietic acid $$ 1-Phenanthrenecarb 513344 000514-10-3 93
                   oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                   10a-decahydro-1,4a-dimethyl-7-(1-m
                   ethylethyl)-, [1R-(1.alpha.,4a.bet
                   a.,4b.alpha.,10a.alpha.)]- $$ Podo
                   carpa-7,13-dien-15-oic acid, 13-is
                   opropyl- $$ L-abietic acid

 62  38.485   0.09 D:\DATABASE\DEMO.L
                   Abietic acid $$ 1-Phenanthrenecarb 513378 000514-10-3 92
                   oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                   10a-decahydro-1,4a-dimethyl-7-(1-m
                   ethylethyl)-, [1R-(1.alpha.,4a.bet
                   a.,4b.alpha.,10a.alpha.)]- $$ Podo
                   carpa-7,13-dien-15-oic acid, 13-is
                   opropyl- $$ L-abietic acid
                   Abietic acid $$ 1-Phenanthrenecarb 513344 000514-10-3 55
                   oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                   10a-decahydro-1,4a-dimethyl-7-(1-m
                   ethylethyl)-, [1R-(1.alpha.,4a.bet
                   a.,4b.alpha.,10a.alpha.)]- $$ Podo
                   carpa-7,13-dien-15-oic acid, 13-is
                   opropyl- $$ L-abietic acid
                   Palustric acid $$ Podocarpa-8,13-d 513439 001945-53-5 53
                   ien-15-oic acid, 13-isopropyl- $$
```

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-140c-2jm.D
Acq On : 12 Oct 2019 9:38
Operator :
Sample :
Misc :
ALS Vial : 3 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,5,6,9,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, (1R-(1.alpha.,4a.beta.,10a.alpha.))- $$ 8,13-Abietadien-18-oic acid			
63	38.825	0.08	D:\DATABASE\DEMO.L			
			Abietic acid $$ 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,4b,5,6,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1R-(1.alpha.,4a.beta.,4b.alpha.,10a.alpha.)]- $$ Podocarpa-7,13-dien-15-oic acid, 13-isopropyl- $$ L-abietic acid	513378	000514-10-3	83
			Abietic acid $$ 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,4b,5,6,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1R-(1.alpha.,4a.beta.,4b.alpha.,10a.alpha.)]- $$ Podocarpa-7,13-dien-15-oic acid, 13-isopropyl- $$ L-abietic acid	513344	000514-10-3	83
			CYCLOTETRADECA[B]FURAN-7(4H)-ONE, 2,5,6,8,9,12,13,15A-OCTAHYDRO-3,6,10,14-TETRAMETHYL- $$ (3Z,10E,14E)-6,7-EPOXY-3,6,10,14-TETRAMETHYL-2,4,5,6,7,8,9,12,13,15A-DECAHYDROCYCLOTETRADECA(B)FURAN	294174	070701-53-0	62
64	39.003	0.18	D:\DATABASE\DEMO.L			
			Abietic acid $$ 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,4b,5,6,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1R-(1.alpha.,4a.beta.,4b.alpha.,10a.alpha.)]- $$ Podocarpa-7,13-dien-15-oic acid, 13-isopropyl- $$ L-abietic acid	513347	000514-10-3	70
			Abietic acid $$ 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,4b,5,6,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1R-(1.alpha.,4a.beta.,4b.alpha.,10a.alpha.)]- $$ Podocarpa-7,13-dien-15-oic acid, 13-isopropyl- $$ L-abietic acid	513378	000514-10-3	46
			.beta.-Pimaric acid $$ .delta.6,8(14)-Abietadienoic acid $$ 1-Pimaric acid $$ 1-Sapietic acid	513374	000079-54-9	43

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-140c-3jm.D
Acq On : 12 Oct 2019 13:19
Operator :
Sample :
Misc :
ALS Vial : 3 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

k#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	1.962	5.29	D:\DATABASE\DEMO.L			
			Methyl Alcohol $$ Methanol $$ Carbinol $$ Methyl hydroxide	5073	000067-56-1	2
			METHANOL $$ HYDROXYMETHANE $$ ALCOHOL, METHYL $$ ALCOOL METHYLIQUE	5075	000067-56-1	2
			Methyl Alcohol $$ Methanol $$ Carbinol $$ Methyl hydroxide	5072	000067-56-1	2
2	2.070	0.01	D:\DATABASE\DEMO.L			
			Decyl trifluoroacetate $$ Decyl 2,2,2-trifluoroacetate $$ 1-Decanol, trifluoroacetate $$ Acetic acid, trifluoro-, decyl ester	32006	000333-88-0	64
			L-Talose, 6-deoxy-3-C-methyl-2-O-methyl- $$ Talose, 6-deoxy-3-C-methyl-2-O-methyl-, L- $$ L-Vinalose $$ Vinalose	27022	027208-98-6	33
			6-DEOXY-3-C-METHYL-2-O-METHYLHEXOSE $$ L-TALOSE, 6-DEOXY-3-C-METHYL-2-O-METHYL- $$ 6-DEOXY-3-C-METHYL-2-O-METHYLTALOSE $$ L-VINELOSE	27067	027208-98-6	33
3	2.135	0.15	D:\DATABASE\DEMO.L			
			Pentane, 2,4-dimethyl- $$ 2,4-Dimethylpentane	18753	000108-08-7	90
			Pentane, 2,4-dimethyl- $$ 2,4-Dimethylpentane	18750	000108-08-7	87
			HEPTANE, 3-METHYL- $$ 3-METHYLHEPTANE $$ 2-ETHYLHEXANE	19876	000589-81-1	72
4	2.200	11.25	D:\DATABASE\DEMO.L			
			HEXANE, 3-METHYL- $$ 3-METHYLHEXANE $$ 2-ETHYLPENTANE $$ HEXANE, 3-METHYL	18994	000589-34-4	64
			1-PENTANOL, 2-METHYL- $$ 2-METHYLPENTAN-1-OL $$ (+-)-2-METHYL-1-PENTANOL $$ (+-)-2-METHYLPENTANOL	19228	000105-30-6	59
			Hexane, 3-methyl- $$ 2-Ethylpentane $$ 3-Methylhexane	18754	000589-34-4	58
5	2.243	4.42	D:\DATABASE\DEMO.L			
			Cyclopentane, 1,3-dimethyl-, cis- $$ cis-1,3-Dimethylcyclopentane $$ 1,3-Dimethylcyclopentane cis $$ 1,3-Dimethylcyclopentane #	62231	002532-58-3	91
			1,3-DIMETHYLCYCLOPENTANE $$ CYCLOPENTANE, 1,3-DIMETHYL-, CIS- $$ 1,3-DIMETHYLCYCLOPENTANE (CIS) $$ 1,3-DIMETHYLCYCLOPENTANE CIS	62286	002532-58-3	91
			Cyclopentane, 1,3-dimethyl- $$ 1,3-Dimethylcyclopentane	101343	002453-00-1	91
6	2.335	6.68	D:\DATABASE\DEMO.L			
			CYCLOHEXANE, METHYL- $$ METHYLCYCLOHEXANE $$ 1-METHYLCYCLOHEXANE $$ CYCLOHEXANE, METHYL	141469	000108-87-2	96
			CYCLOHEXANE, METHYL- $$ METHYLCYCLOHEXANE $$ 1-METHYLCYCLOHEXANE $$ CYCLOHEXANE, METHYL	141470	000108-87-2	95

Library Search Report

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-140c-3jm.D
Acq On : 12 Oct 2019 13:19
Operator :
Sample :
Misc :
ALS Vial : 3 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autointl.e

%#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			CYCLOHEXANE, METHYL- $$ METHYLCYCL OHEXANE $$ 1-METHYLCYCLOHEXANE $$ CYCLOHEXANE, METHYL	141467	000108-87-2	95
7	2.421	61.30	D:\DATABASE\DEMO.L			
			Toluene $$ Benzene, methyl $$ Meth acide $$ Methylbenzene	158580	000108-88-3	91
			BENZENE, METHYL- $$ METHYLBENZENE $$ TOLUENE $$ ANTISAL 1A	158625	000108-88-3	91
			Toluene $$ Benzene, methyl $$ Meth acide $$ Methylbenzene	158579	000108-88-3	91
8	2.746	1.12	D:\DATABASE\DEMO.L			
			Cyclohexane, ethyl- $$ Ethylcycloh exane	141506	001678-91-7	93
			CYCLOHEXANE, ETHYL- $$ ETHYLCYCLOH EXANE $$ ETHYL CYCLOHEXANE $$ ETHY LCYCLOHEXAN	141561	001678-91-7	93
			Cyclohexane, ethyl- $$ Ethylcycloh exane	141508	001678-91-7	93
9	2.870	0.50	D:\DATABASE\DEMO.L			
			BENZENE, METHYL- $$ METHYLBENZENE $$ TOLUENE $$ ANTISAL 1A	158623	000108-88-3	90
			1,3,5-CYCLOHEPTATRIENE $$ CYCLOHEP TA-1,3,5-TRIENE $$ CYCLOHEPTATRIEN E $$ CYCLOHEPTATRIENE [UN2603] [FL AMMABLE LIQUID]	158636	000544-25-2	90
			1,3,5-Cycloheptatriene $$ Tropilid ene $$ Cyclohepta-1,3,5-triene $$ Cycloheptatriene	158600	000544-25-2	90
10	4.615	0.02	D:\DATABASE\DEMO.L			
			2-OXABICYCLO[2.2.2]OCTANE, 1,3,3-T RIMETHYL- $$ 1, 8-CINEOL $$ 1,3,3- TRIMETHYL-2-OXABICYCLO(2.2.2)OCTAN E $$ 1,3,3-TRIMETHYL-2-OXABICYCLO[2.2.2]OCTANE	23420	000470-82-6	95
			2-OXABICYCLO[2.2.2]OCTANE, 1,3,3-T RIMETHYL- $$ 1, 8-CINEOL $$ 1,3,3- TRIMETHYL-2-OXABICYCLO(2.2.2)OCTAN E $$ 1,3,3-TRIMETHYL-2-OXABICYCLO[2.2.2]OCTANE	23430	000470-82-6	95
			2-OXABICYCLO[2.2.2]OCTANE, 1,3,3-T RIMETHYL- $$ 1, 8-CINEOL $$ 1,3,3- TRIMETHYL-2-OXABICYCLO(2.2.2)OCTAN E $$ 1,3,3-TRIMETHYL-2-OXABICYCLO[2.2.2]OCTANE	23426	000470-82-6	93
11	17.315	0.04	D:\DATABASE\DEMO.L			
			2H-2,4A-METHANONAPHTHALENE, 1,3,4, 5,6,7-HEXAHYDRO-1,1,5,5-TETRAMETHY L-, (2S)- $$ (-)-ISOLONGIFOLENE $$ (-)-ISOLONGIFOLINE $$ (2S)-1,3,4, 5,6,7-HEXAHYDRO-1,1,5,5-TETRAMETHY L-2H-2,4A-METHANONAPHTHALENE	350800	001135-66-6	98
			2H-2,4a-Methanonaphthalene, 1,3,4, 5,6,7-hexahydro-1,1,5,5-tetramethy 1-, (2S)- $$ 2H-2,4a-Methanonaphth	350640	001135-66-6	98

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Data Path : F:\DATA MS\daa\
Data File : WLM-10prsen-140c-3jm.D
Acq On    : 12 Oct 2019  13:19
Operator  :
Sample    :
Misc      :
ALS Vial  : 3   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e
```

#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			alene, 1,3,4,5,6,7-hexahydro-1,1,5,5-tetramethyl-, (2S,4aR)-(-)- $$ Isolongifolene $$ (-)-Isolongifolina			
			2H-2,4a-Methanonaphthalene, 1,3,4,5,6,7-hexahydro-1,1,5,5-tetramethyl-, (2S)- $$ 2H-2,4a-Methanonaphthalene, 1,3,4,5,6,7-hexahydro-1,1,5,5-tetramethyl-, (2S,4aR)-(-)- $$ Isolongifolene $$ (-)-Isolongifolina	350641	001135-66-6	98
2	17.720	0.01	D:\DATABASE\DEMO.L			
			2,2,3,3,4,4,5,5-OCTAFLUORO-N-(3-METHOXYPHENYL)PENTANAMIDE $$ PENTANAMIDE, 2,2,3,3,4,4,5,5-OCTAFLUORO-N-(3-METHOXYPHENYL)-	7474	339166-43-7	9
			3-(3-OXO-3H-BENZO[F]CHROMEN-2-YL)-2,4(1H,3H)-QUINOLINEDIONE $$ 4-HYDROXY-3-(2-OXO-2H-1-OXA-3-PHENANTHRYL)-2(1H)-QUINOLINONE	7476	999007-47-7	9
			BENZENE, 1-(2-CYCLOHEXEN-1-YL-2-D)-4-METHOXY- $$ 3-(P-METHOXYPHENYL)(2-2H1)CYCLOHEX-1-ENE	7344	086426-62-2	9
3	17.849	0.00	D:\DATABASE\DEMO.L			
			1,3-OXATHIOL-1-IUM, 4-HYDROXY-2-[(1-METHYLETHYL)THIO]-5-(TRIFLUOROACETYL)-, HYDROXIDE, INNER SALT $$ 2-ISOPROPYLTHIO-5-TRIFLUORACETYL-1,3-OXATHIOLYIUM-4-OLAT	7423	096088-83-4	9
			4-BROMO-N-[(6-METHYL-2-PYRIDYL)AMINOMETHYL]PHTHALIMIDE $$ 5-BROMO-2-{[(6-METHYL-2-PYRIDINYL)AMINO]METHYL}-1H-ISOINDOLE-1,3(2H)-DIONE	7473	999007-47-4	9
			Propanedioic acid, (hydroxyimino)-, diethyl ester $$ Bis-(ethoxycarbonyl)hydroxyiminomethane $$ Diethyl 2-(hydroxyimino)malonate #	2893	006829-41-0	4
4	28.610	0.01	D:\DATABASE\DEMO.L			
			4-(METHOXYMETHYL)-6-METHYL-2-PHENOXYNICOTINONITRILE $$ PYRIDINE-3-CARBONITRILE, 4-METHOXYMETHYL-6-METHYL-2-PHENOXY-	7413	332057-36-0	12
			Diethyl diethylmalonate $$ Diethylmalonic acid diethyl ester $$ Propanedioic acid, diethyl-, diethyl ester $$ Diethylmalonate diethyl ester	3074	000077-25-8	9
			4-BROMO-N-[(6-METHYL-2-PYRIDYL)AMINOMETHYL]PHTHALIMIDE $$ 5-BROMO-2-{[(6-METHYL-2-PYRIDINYL)AMINO]METHYL}-1H-ISOINDOLE-1,3(2H)-DIONE	7473	999007-47-4	9
5	28.929	0.01	D:\DATABASE\DEMO.L			
			1,3-OXATHIOL-1-IUM, 4-HYDROXY-2-[(1-METHYLETHYL)THIO]-5-(TRIFLUOROACETYL)-, HYDROXIDE, INNER SALT $$ 2	7423	096088-83-4	9

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Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-140c-3jm.D
Acq On    : 12 Oct 2019  13:19
Operator  :
Sample    :
Misc      :
ALS Vial  : 3   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e

#     RT  Area%          Library/ID                    Ref#     CAS#   Qual
                -ISOPROPYLTHIO-5-TRIFLUOROACETYL-1,
                3-OXATHIOLYIUM-4-OLAT
                PHENOL, 2-SEC-BUTYL-4-(METHYLTHIO)     132 000000-00-0  9
                -6-NITRO-
                9-(4-HYDROXYPHENYL)-3,3,6,6-TETRAM    7482 999007-48-3  9
                ETHYL-3,4,6,7,8A,9-HEXAHYDRO-1,8(2
                H,5H)-ACRIDINEDIONE

6  30.306  0.04 D:\DATABASE\DEMO.L
                PIMARA-8,15-DIENE $$ PHENANTHRENE, 481165 055255-56-6 93
                 7-ETHENYL-1,2,3,4,4A,5,6,7,8,9,10
                ,10A-DODECAHYDRO-1,1,4A,7-TETRAMET
                HYL- $$ 7.ALPHA.-ETHENYL-1,1,4A,7.
                BETA.-TETRAMETHYL-1,2,3,4,4A,5,6,7
                ,8,9,10,10A-DODECAHYDROPHENANTHREN
                PHENANTHRENE, 7-ETHENYL-1,2,3,4,4A 481161 018319-61-4 93
                ,5,6,7,8,9,10,10A-DODECAHYDRO-1,1,
                4A,7-TETRAMETHYL-, [4AS-(4A.ALPHA.
                ,7.ALPHA.,10A.BETA.)]- $$ PIMARA-8
                (9),15-DIENE $$ PODOCARP-8-ENE, 13
                .ALPHA.-METHYL-13-VINYL-
                Phenanthrene, 7-ethenyl-1,2,3,4,4a 481092 055255-56-6 91
                ,5,6,7,8,9,10,10a-dodecahydro-1,1,
                4a,7-tetramethyl- $$ Pimara-8,15-d
                iene #

7  30.717  0.01 D:\DATABASE\DEMO.L
                4-(METHOXYMETHYL)-6-METHYL-2-PHENO    7413 332057-36-0 27
                XYNICOTINONITRILE $$ PYRIDINE-3-CA
                RBONITRILE, 4-METHOXYMETHYL-6-METH
                YL-2-PHENOXY-
                1,3-OXATHIOL-1-IUM, 4-HYDROXY-2-[(    7423 096088-83-4  9
                1-METHYLETHYL)THIO]-5-(TRIFLUOROAC
                ETYL)-, HYDROXIDE, INNER SALT $$ 2
                -ISOPROPYLTHIO-5-TRIFLUOROACETYL-1,
                3-OXATHIOLYIUM-4-OLAT
                9-(4-HYDROXYPHENYL)-3,3,6,6-TETRAM    7482 999007-48-3  9
                ETHYL-3,4,6,7,8A,9-HEXAHYDRO-1,8(2
                H,5H)-ACRIDINEDIONE

8  31.268  0.01 D:\DATABASE\DEMO.L
                4-(METHOXYMETHYL)-6-METHYL-2-PHENO    7413 332057-36-0 27
                XYNICOTINONITRILE $$ PYRIDINE-3-CA
                RBONITRILE, 4-METHOXYMETHYL-6-METH
                YL-2-PHENOXY-
                L-Alanine, N-glycyl- $$ Alanine, N    4366 003695-73-6  7
                -glycyl-, L- $$ Glycylalanine $$ Gl
                y-ala
                1-Nonanamine $$ Nonylamine $$ n-No    4312 000112-20-9  7
                nylamine $$ 1-Aminononane

9  31.311  0.00 D:\DATABASE\DEMO.L
                ACETIC ACID, TRICHLORO-, ETHYL EST    2904 000515-84-4  2
                ER $$ ACETIC ACID, 2,2,2-TRICHLORO
                ETHYL ESTER $$ ACETIC ACID, ESTER
                WITH TRICHLOROETHANOL $$ ACETIC AC
                ID, TRICHLORO-, ETHYL ESTE
                Acetic acid, trichloro-, ethyl est    2897 000515-84-4  2
                er $$ Ethyl trichloroacetate $$ Ac
```

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-140c-3jm.D
Acq On : 12 Oct 2019 13:19
Operator :
Sample :
Misc :
ALS Vial : 3 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			etic acid, ester with trichloroeth anol $$ Acetic acid, 2,2,2-trichlo roethyl ester			
			2-BUTENE, 1-BROMO-3-METHYL- $$ 1-B ROMO-3-METHYL-BUT-2-ENE $$ .GAMMA. ,.GAMMA.-DIMETHYLALLYL BROMIDE $$ 1-BROMO-3-METHYL-2-BUTENE	673	000870-63-3	2
20	31.700	0.02	D:\DATABASE\DEMO.L			
			Ethanedicarboxamide, N-allyl-N'-(2 ,5-dimethylphenyl)-	7392	331864-72-3	2
			.ALPHA.-METHYL-4-METHOXY-STYRENE $ $ 1-ISOPROPENYL-4-METHOXYBENZENE $ $ 4-ISOPROPENYLPHENYL METHYL ETHER	1191	999001-19-1	2
			13-OXABICYCLO[8.2.1]TRIDEC-1(12)-E N-11-ONE	7353	000000-00-0	1
21	31.835	0.01	D:\DATABASE\DEMO.L			
			2,2,3,3,4,4,4-Heptafluoro-butanol $$ 2,2,3,3,4,4,4,-Heptafluoro-1-bu tanol $$ 1H,1H-Heptafluoro-1-butan ol $$ Perfluoro-1,1-dihydrobutanol	5574	000375-01-9	1
			2,2,3,3,4,4,4-Heptafluoro-butanol $$ 2,2,3,3,4,4,4,-Heptafluoro-1-bu tanol $$ 1H,1H-Heptafluoro-1-butan ol $$ Perfluoro-1,1-dihydrobutanol	5572	000375-01-9	1
22	32.019	0.01	D:\DATABASE\DEMO.L			
			Triethyl 1,2,3-tricarbonitrile-1,2 ,3-tricarboxylate	3424	999003-42-5	1
23	32.089	0.02	D:\DATABASE\DEMO.L			
			4-(METHOXYMETHYL)-6-METHYL-2-PHENO XYNICOTINONITRILE $$ PYRIDINE-3-CA RBONITRILE, 4-METHOXYMETHYL-6-METH YL-2-PHENOXY-	7413	332057-36-0	22
			9-(4-HYDROXYPHENYL)-3,3,6,6-TETRAM ETHYL-3,4,6,7,8A,9-HEXAHYDRO-1,8(2 H,5H)-ACRIDINEDIONE	7482	999007-48-3	17
			1-Undecanamine $$ Undecylamine $$ n-Undecylamine $$ Hendecylamine	4551	007307-55-3	9
24	32.402	0.01	D:\DATABASE\DEMO.L			
			Carbamic acid, 1-naphthalenyl-, me thyl ester $$ Methyl N-.alpha.-nap hthylcarbamate $$ Methyl N-(1-naph thyl)carbamate $$ Methyl 1-naphtha lenecarbamate	419171	005449-00-3	25
			Carbamic acid, 1-naphthalenyl-, me thyl ester $$ Methyl N-.alpha.-nap hthylcarbamate $$ Methyl N-(1-naph thyl)carbamate $$ Methyl 1-naphtha lenecarbamate	419116	005449-00-3	25
			Pyrimidine, 2,4-diamino-5-(3-pyrid ylmethyl)- $$ 2,4-Diamino-5-(3-pyr idylmethyl)-pyrimidine $$ 2,4-Pyri midinediamine, 5-(3-pyridinylmethy l)- $$ 2,4-Diamino-5-[3-pyridylmet hyl]pyrimidine	419153	052606-04-9	25

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Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
25	32.451	0.01	D:\DATABASE\DEMO.L			
			2-CHLORO-4-NITROBENZOIC ACID	339	000099-60-5	7
			Acetic acid, 1-cyano-1-(cyclohexen-1-yl)-1-(3-oxocyclopent-1-en-1-yl)-, ethyl ester	3292	999003-29-3	1
			CYCLOPROPANECARBONYL CHLORIDE, 2,2-DIBROMO-1-METHYL- $$ 2,2-DIBROMO-1-METHYLCYCLOPROPANECARBONYL CHLORIDE	7425	005365-22-0	1
26	32.975	0.01	D:\DATABASE\DEMO.L			
			4-(METHOXYMETHYL)-6-METHYL-2-PHENOXYNICOTINONITRILE $$ PYRIDINE-3-CARBONITRILE, 4-METHOXYMETHYL-6-METHYL-2-PHENOXY-	7413	332057-36-0	12
			1-Tetradecanamine $$ Tetradecylamine $$ Armeen 14 $$ Myristylamine	4817	002016-42-4	9
			1-Dodecanamine $$ Dodecylamine $$ n-Dodecylamine $$ Alamine 4	4652	000124-22-1	9
27	33.386	0.01	D:\DATABASE\DEMO.L			
			L-Alanine, N-glycyl- $$ Alanine, N-glycyl-, L- $$ Glcylalanine $$ Gly-ala	4366	003695-73-6	14
			4-(METHOXYMETHYL)-6-METHYL-2-PHENOXYNICOTINONITRILE $$ PYRIDINE-3-CARBONITRILE, 4-METHOXYMETHYL-6-METHYL-2-PHENOXY-	7413	332057-36-0	12
			N-(CYCLOHEXYLCARBONYL)-4-MORPHOLINECARBOXAMIDE $$ CYCLOHEXANECARBOXAMIDE, N-(4-MORPHOLYLCARBONYL)- $$ N-(4-MORPHOLINYLCARBONYL)CYCLOHEXANECARBOXAMIDE	7397	339162-13-9	10
28	33.499	0.12	D:\DATABASE\DEMO.L			
			Phenanthrene, 7-ethenyl-1,2,3,4,4a,5,6,7,8,9,10,10a-dodecahydro-1,1,4a,7-tetramethyl- $$ Pimara-8,15-diene #	481092	055255-56-6	86
			PIMARA-8,15-DIENE $$ PHENANTHRENE, 7-ETHENYL-1,2,3,4,4A,5,6,7,8,9,10,10A-DODECAHYDRO-1,1,4A,7-TETRAMETHYL- $$ 7.ALPHA.-ETHENYL-1,1,4A,7.BETA.-TETRAMETHYL-1,2,3,4,4A,5,6,7,8,9,10,10A-DODECAHYDROPHENANTHREN	481165	055255-56-6	86
			PHENANTHRENE, 7-ETHENYL-1,2,3,4,4A,5,6,7,8,9,10,10A-DODECAHYDRO-1,1,4A,7-TETRAMETHYL-, [4AS-(4A.ALPHA.,7.ALPHA.,10A.BETA.)]- $$ PIMARA-8(9),15-DIENE $$ PODOCARP-8-ENE, 13.ALPHA.-METHYL-13-VINYL-	481161	018319-61-4	84
29	33.623	0.00	D:\DATABASE\DEMO.L			
			1-Hexadecanamine $$ Hexadecylamine $$ n-Cetylamine $$ n-Hexadecylamine	4902	000143-27-1	27
			2-METHOXY-4-(METHOXYMETHYL)-6-METHYLNICOTINONITRILE $$ PYRIDINE-3-CA	7347	063644-84-8	22

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Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

%#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			RBONITRILE, 2,4-DIMETHOXY-6-METHYL			
			Taurolidine $$ 2H-1,2,4-Thiadiazin	4983	019388-87-5	16
			e, 4,4'-methylenebis[tetrahydro-,			
			1,1,1',1'-tetraoxide $$ 4,4'-Methy			
			lenebis(tetrahydro-1,2,4-thiadiazi			
			ne 1,1-dioxide) $$ Taurolin			
30	33.683	0.00	D:\DATABASE\DEMO.L			
			1-Hexadecanamine $$ Hexadecylamine	4902	000143-27-1	22
			$$ n-Cetylamine $$ n-Hexadecylami			
			ne			
			1-Tetradecanamine $$ Tetradecylami	4817	002016-42-4	10
			ne $$ Armeen 14 $$ Myristylamine			
			1-Tetradecanamine $$ Tetradecylami	4815	002016-42-4	9
			ne $$ Armeen 14 $$ Myristylamine			
31	33.710	0.00	D:\DATABASE\DEMO.L			
			1-Hexadecanamine $$ Hexadecylamine	4902	000143-27-1	23
			$$ n-Cetylamine $$ n-Hexadecylami			
			ne			
			2-METHOXY-4-(METHOXYMETHYL)-6-METH	7347	063644-84-8	22
			YLNICOTINONITRILE $$ PYRIDINE-3-CA			
			RBONITRILE, 2,4-DIMETHOXY-6-METHYL			
			2-(3-BUTOXY-2-HYDROXYPROPYL)MALONO	7415	331648-87-4	10
			HYDRAZIDE $$ MALONODIHYDRAZIDE, 2-			
			(3-BUTOXY-2-HYDROXYPROPYL)-			
32	33.796	0.03	D:\DATABASE\DEMO.L			
			KAUR-16-EN-18-OIC ACID $$ KAUR-16-	168418	020316-84-1	41
			EN-18-OIC ACID, (4.BETA.)- $$ (-)-			
			KAURNENOIC ACID $$ (4-BETA)-KAUR-1			
			6-EN-18-OIC ACID			
			ABIETA-7,13-DIEN-18-OIC ACID $$ 1-	168420	000514-10-3	15
			PHENANTHRENECARBOXYLIC ACID, 1,2,3			
			,4,4A,4B,5,6,10,10A-DECAHYDRO- $$			
			1-PHENANTHRENECARBOXYLIC ACID, 1,2			
			,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,			
			4A-DIMETHYL-7-(1-METHYLETHYL)-, [1			
			R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A			
			.ALPHA.)]-			
			ABIETA-7,13-DIEN-18-OIC ACID $$ 1-	168419	000514-10-3	11
			PHENANTHRENECARBOXYLIC ACID, 1,2,3			
			,4,4A,4B,5,6,10,10A-DECAHYDRO- $$			
			1-PHENANTHRENECARBOXYLIC ACID, 1,2			
			,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,			
			4A-DIMETHYL-7-(1-METHYLETHYL)-, [1			
			R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A			
			.ALPHA.)]-			
33	33.866	0.06	D:\DATABASE\DEMO.L			
			10,13-DIMETHYL-4,5,6,7,8,9,10,11,1	466180	999466-18-8	95
			2,13,14,15-DODECAHYDRO-1H-CYCLOPEN			
			TA[A]PHENANTHRENE $$ ANDROSTA-2,16			
			-DIENE			
			1-Methyl-10,18-bisnorabieta-8,11,1	466158	999466-16-6	94
			3-triene			
			4-(N-METHYLAMINO)-6,7-(1,2,3,4-TET	466219	000000-00-0	90
			RAHYDRO-1,1,4,4-TETRAMETHYLBENZO)I			
			NDOLE			

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Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autointl.e

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34	34.142	0.02	D:\DATABASE\DEMO.L			
			Taurolidine $$ 2H-1,2,4-Thiadiazin	4983	019388-87-5	9
			e, 4,4'-methylenebis[tetrahydro-,			
			1,1,1',1'-tetraoxide $$ 4,4'-Methy			
			lenebis(tetrahydro-1,2,4-thiadiazi			
			ne 1,1-dioxide) $$ Taurolin			
			Ethyl 2-((diethoxyphosphoryl)oxy)-	3375	999003-37-6	4
			3,3,3-trifluoropropanoate			
35	34.207	0.02	D:\DATABASE\DEMO.L			
			Ethanedicarboxamide, N-allyl-N'-(2	7392	331864-72-3	10
			,5-dimethylphenyl)-			
			.ALPHA.-METHYL-4-METHOXY-STYRENE $	1191	999001-19-1	2
			$ 1-ISOPROPENYL-4-METHOXYBENZENE $			
			$ 4-ISOPROPENYLPHENYL METHYL ETHER			
			Ethyl 2-((diethoxyphosphoryl)oxy)-	3375	999003-37-6	1
			3,3,3-trifluoropropanoate			
36	34.320	0.03	D:\DATABASE\DEMO.L			
			1-Phenanthrenecarboxylic acid, 7-e	466507	003582-26-1	83
			thenyl-1,2,3,4,4a,5,6,7,8,9,10,10a			
			-dodecahydro-1,4a,7-trimethyl-, me			
			thyl ester, [1R-(1.alpha.,4a.beta.			
			,7.beta.,10a.alpha.)]- $$ Podocarp			
			-8-en-15-oic acid, 13.alpha.-methy			
			l-13-vinyl-, methyl ester			
			METHYL PIMARA-8,15-DIEN-18-OATE $$	466513	003582-26-1	64
			1-PHENANTHRENECARBOXYLIC ACID, 7-			
			ETHENYL-1,2,3,4,4A,5,6,7,8,9,10,10			
			A-DODECAHYDRO-1,4A,7-TRIMETHYL-, M			
			ETHYL ESTER, [1R-(1.ALPHA.,4A.BETA			
			.,7.BETA.,10A.ALPHA.)]- $$ METHYL			
			8,15-PIMARADIEN-18-OATE			
			ISOPIMARA-7,15-DIEN-18-OIC ACID ME	466522	000000-00-0	58
			THYL ESTER			
37	34.428	0.00	D:\DATABASE\DEMO.L			
			2H-3,9A-METHANO-1-BENZOXEPIN, OCTA	3110	005956-09-2	7
			HYDRO-2,2,5A,9-TETRAMETHYL-, [3R-(			
			3.ALPHA.,5A.ALPHA.,9.ALPHA.,9A.ALP			
			HA.)]- $$ .BETA.-AGAROFURAN, DIHYD			
			RO- $$ .BETA.-DIHYDROAGAROFURAN $$			
			2H-3,9A-METHANO-1-BENZOXEPIN, OCT			
			AHYDRO-2,2,5A,9-TETRAMETHYL-			
			2-METHOXY-4-(METHOXYMETHYL)-6-METH	7347	063644-84-8	2
			YLNICOTINONITRILE $$ PYRIDINE-3-CA			
			RBONITRILE, 2,4-DIMETHOXY-6-METHYL			
			QUINUCLIDINIUM-METHANESULFONATE	3027	126821-96-3	1
38	34.536	0.10	D:\DATABASE\DEMO.L			
			1,2,4-TRIAZOLO(3,4-C)(1,2,4)-BENZO	282352	000000-00-0	53
			TRIAZIN-1(5H)-ONE			
			15-OXABICYCLO[12.1.0]PENTADECA-4,8	181486	079897-31-7	47
			-DIENE, 1,5,9-TRIMETHYL-12-(1-METH			
			YLETHENYL)-, [1S-(1R*,4E,8E,12S*,1			
			4R*)]- $$ (1R,3S,4S,7E,11E)-3,4-EP			
			OXYCEMBRA-7,11,15-TRIENE			
			1,4,8-CYCLODODECATRIENE-1-CARBOXYL	164771	057709-14-5	38

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Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autointl.e

%#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			IC ACID, 12-ETHENYL-, METHYL ESTER , (E,E,E)- $$ METHYL 12-VINYLCYCLO DODECA-1,4,8-TRIENECARBOXYLATE			
39	34.785	0.02	D:\DATABASE\DEMO.L			
			2H-3,9A-METHANO-1-BENZOXEPIN, OCTA HYDRO-2,2,5A,9-TETRAMETHYL-, [3R-(3.ALPHA.,5A.ALPHA.,9.ALPHA.,9A.ALP HA.)]- $$ .BETA.-AGAROFURAN, DIHYD RO- $$ .BETA.-DIHYDROAGAROFURAN $$ 2H-3,9A-METHANO-1-BENZOXEPIN, OCT AHYDRO-2,2,5A,9-TETRAMETHYL-	3110	005956-09-2	25
			3-Benzyl-2-(2-furyl)-3,4-dihydro-4 -quinazolinone $$ 3-Benzyl-2-(2-fu ryl)-4(3H)-quinazolinone #	168374	256954-79-7	11
			3-BENZYL-2-(2-FURYL)-4(3H)-QUINAZO LINONE $$ 3-BENZYL-2-(2-FURYL)-3,4 -DIHYDRO-4-QUINAZOLINONE	168393	256954-79-7	11
40	34.914	0.02	D:\DATABASE\DEMO.L			
			2H-3,9A-METHANO-1-BENZOXEPIN, OCTA HYDRO-2,2,5A,9-TETRAMETHYL-, [3R-(3.ALPHA.,5A.ALPHA.,9.ALPHA.,9A.ALP HA.)]- $$ .BETA.-AGAROFURAN, DIHYD RO- $$ .BETA.-DIHYDROAGAROFURAN $$ 2H-3,9A-METHANO-1-BENZOXEPIN, OCT AHYDRO-2,2,5A,9-TETRAMETHYL-	3110	005956-09-2	7
			ETHYL 2,2-DIFLUORO-4-IODOOCTANOATE	3430	127224-09-3	4
			Diethyl 3-chloro-2-hydroxypropylma lonate	3235	999003-23-6	2
41	35.033	0.03	D:\DATABASE\DEMO.L			
			1-ACETYLAMINO-5,5-DIMETHOXY-2,3-DI METHYL-2(E)-PENTENE	122973	000000-00-0	59
			2-Methylbutanoic acid, 3-(t-butyld imethylsilyloxy)- $$ 3-([tert-Buty l(dimethyl)silyl]oxy)-2-methylbuta noic acid #	123203	108782-00-9	53
			Benzene, 1-[(dimethoxymethyl)-1-et hyl]-4-methoxycarbonyl-1-ethyl-	123523	999123-52-6	53
42	35.168	0.03	D:\DATABASE\DEMO.L			
			KAUR-16-EN-18-OIC ACID $$ KAUR-16- EN-18-OIC ACID, (4.BETA.)- $$ (-)- KAURNENOIC ACID $$ (4-BETA)-KAUR-1 6-EN-18-OIC ACID	168418	020316-84-1	49
			ABIETA-7,13-DIEN-18-OIC ACID $$ 1- PHENANTHRENECARBOXYLIC ACID, 1,2,3 ,4,4A,4B,5,6,10,10A-DECAHYDRO- $$ 1-PHENANTHRENECARBOXYLIC ACID, 1,2 ,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1, 4A-DIMETHYL-7-(1-METHYLETHYL)-, [1 R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A .ALPHA.)]-	168420	000514-10-3	15
			BUTYL 2-(METHYLAMINO)BENZOATE $$ A NTHRANILIC ACID, N-METHYL-, BUTYL ESTER $$ N-BUTYL O-METHYLAMINOBENZ OATE	209256	015236-34-7	14

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Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

%k#	RT	Area%	Library/ID	Ref#	CAS#	Qual
43	35.303	0.01	D:\DATABASE\DEMO.L			
			2-((E)-[((E)-2-([(E)-(2-HYDROXYPHENYL)METHYLIDENE]AMINO)PROPYL)IMINO]METHYL)PHENOL $$ .ALPHA.,.ALPHA.'-(1-METHYLETHYLENEDIIMINO)DI-ORTHO-CRESOL $$ .ALPHA.,.ALPHA.'-DIPROPYLENEDINITRILODI-O-CRESOL $$ ALPHA,ALPHA'-(1-METHYLETHYLENEDIIMINO)DI-ORTHO-CRESOL	45719	000094-91-7	40
			3-Methylindole-2-carboxylic acid, 4,5,6,7-tetrahydro-, ethyl ester $$ Ethyl 3-methyl-4,5,6,7-tetrahydro-1H-indole-2-carboxylate #	428008	037945-37-2	25
			1-Dimethylisopropylsilyloxy-3-methylbut-2-ene	122592	999122-59-5	18
44	35.400	0.03	D:\DATABASE\DEMO.L			
			2-(ACETYLAMINO)PHENYL ACETATE $$ ACETIC ACID 2-ACETYLAMINO-PHENYL ESTER	227934	999227-93-7	38
			1,3,4-Thiadiazol-2-amine, 5-[[(4-fluorophenyl)methyl]thio]-	228627	999228-63-0	38
			PHENOL, 3-AMINO- $$ 3-AMINOPHENOL $$ 1-AMINO-3-HYDROXYBENZENE $$ 3-AMINO-1-HYDROXYBENZENE	226836	000591-27-5	30
45	35.487	0.85	D:\DATABASE\DEMO.L			
			BENZ[A]ANTHRACENONE	513655	099707-96-7	83
			(4-Ethylphenyl)-(2-methylbenzo[4,5]imidazo[1,2-a] pyrimidin-4-yl)amine	504586	999504-59-8	72
			ROSIN ACIDS	504611	000000-00-0	64
46	35.665	0.08	D:\DATABASE\DEMO.L			
			1-PHENANTHRENECARBOXYLIC ACID, 7-ETHENYL-1,2,3,4,4A,4B,5,6,7,8,10,10A-DODECAHYDRO-1,4A,7-TRIMETHYL-, [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,7.ALPHA.,10A.ALPHA.)]- $$ ISOPIMARIC ACID $$ PODOCARP-7-EN-15-OIC ACID, 13.BETA.-METHYL-13-VINYL-	466436	005835-26-7	45
			(7-ISOPROPYL-1,4-DIMETHYL-2-AZULENYL)(PHENYL)METHANONE $$ METHANONE, [1,4-DIMETHYL-7-(1-METHYLETHYL)-2-AZULENYL]PHENYL- $$ 2-BENZOYLGUAIAZULENE	513663	039665-56-0	40
			Androst-5-en-17-ol, 4,4-dimethyl-	513436	999513-44-9	38
47	35.762	0.24	D:\DATABASE\DEMO.L			
			DEHYDROABIETIC ACID	464556	000000-00-0	97
			1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methylethyl)-, methyl ester, [1R-(1.alpha.,4a.beta.,10a.alpha.)]- $$ Podocarpa-8,11,13-trien-15-oic acid, 13-isopropyl-, methyl ester $$ Methyl dehydroabietat	464538	001235-74-1	93
			1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-di	464536	001235-74-1	93

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Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e
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%#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			methyl-7-(1-methylethyl)-, methyl ester, [1R-(1.alpha.,4a.beta.,10a.alpha.)]- $$ Podocarpa-8,11,13-trien-15-oic acid, 13-isopropyl-, methyl ester $$ Methyl dehydroabietat			
48	35.930	0.08	D:\DATABASE\DEMO.L Palustric acid $$ Podocarpa-8,13-dien-15-oic acid, 13-isopropyl- $$ 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,5,6,9,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, (1R-(1.alpha.,4a.beta.,10a.alpha.))- $$ 8,13-Abietadien-18-oic acid	513439	001945-53-5	43
			2-ACETYL-4,9-DIMETHOXY-7-METHYL-5H-FURO[3,2-G][1]-BENZOPYRAN-5-ONE	513538	092611-83-1	38
			CYCLOPROPANECARBONITRILE, 1,1'-[IMINOBIS(METHYLENE)]BIS[2,2,3,3-TETRAMETHYL- $$ 2,2,2',2',3,3,3',3'-OCTAMETHYL-1,1'-IMINEBIS(METHYLENE)DICYCLOPROPANE-1,1'-DICARBONITRILE	504526	090594-32-4	27
49	36.011	0.08	D:\DATABASE\DEMO.L Kaura-9(11),16-dien-18-oic acid, (4.alpha.)- $$ Kaura-5,16-dien-18(or 19)-oic acid $$ (-)-Kaur-9(11),16-dien-19-oic acid $$ Grandiflorenic acid	503103	022338-67-6	64
			KAURA-9(11),16-DIEN-18-OIC ACID, (4.ALPHA.)- $$ (-)-KAUR-9(11),16-DIEN-19-OIC ACID $$ GRANDIFLORENIC ACID $$ KAURA-5,16-DIEN-18(OR 19)-OIC ACID	503118	022338-67-6	60
			1-Hydroxy-3,7,8-trimethoxyxanthen-9-one $$ 8-Hydroxy-1,2,6-trimethoxy-9H-xanthen-9-one #	504580	020882-69-3	53
50	36.103	0.47	D:\DATABASE\DEMO.L INDOLIZINO[1,2-B]QUINOLIN-9(11H)-ONE, 8-[(FORMYLOXY)METHYL]-7-(1-OXOPROPYL)- $$ 8-FORMYLOXYMETHYL-7-(1-OXOPROPYL)INDOLIZINO)1,2-B)QUINOLIN-9(11H)-ONE	504762	054318-62-6	70
			KAUR-16-EN-18-OIC ACID $$ KAUR-16-EN-18-OIC ACID, (4.BETA.)- $$ (-)-KAURNENOIC ACID $$ (4-BETA)-KAUR-16-EN-18-OIC ACID	168418	020316-84-1	53
			Phenol, 2,4-bis(1-phenylethyl)- $$ 2,4-Bis(1-phenylethyl)phenol #	504578	002769-94-0	45
51	36.389	0.24	D:\DATABASE\DEMO.L METHYL ABIETA-7,13-DIEN-18-OATE $$ 1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL)-, METHYL ESTER, [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A.ALPHA.)]- $$ ABALYN $$ ABIETIC ACID METHYL ESTER	258918	000127-25-3	97
			Methyl abietate $$ 1-Phenanthrenec	258889	000127-25-3	97

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Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-140c-3jm.D
Acq On    : 12 Oct 2019  13:19
Operator  :
Sample    :
Misc      :
ALS Vial  : 3   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e
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Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			arboxylic acid, 1,2,3,4,4a,4b,5,6, 10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, methyl ester, [1R -(1.alpha.,4a.beta.,4b.alpha.,10a. alpha.)]- $$ Podocarpa-7,13-dien-1 5-oic acid, 13-isopropyl-, methyl ester $$ Abalyn			
			METHYL ABIETA-7,13-DIEN-18-OATE $$ 1-PHENANTHRENECARBOXYLIC ACID, 1, 2,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1 ,4A-DIMETHYL-7-(1-METHYLETHYL)-, M ETHYL ESTER, [1R-(1.ALPHA.,4A.BETA .,4B.ALPHA.,10A.ALPHA.)]- $$ ABALY N $$ ABIETIC ACID METHYL ESTER	480551	000127-25-3	94
52	36.600	0.63	D:\DATABASE\DEMO.L			
			Phenol, 2,4-bis(1-phenylethyl)- $$ 2,4-Bis(1-phenylethyl)phenol #	504578	002769-94-0	94
			KAUR-16-EN-18-OIC ACID $$ KAUR-16- EN-18-OIC ACID, (4.BETA.)- $$ (-)- KAURNENOIC ACID $$ (4-BETA)-KAUR-1 6-EN-18-OIC ACID	168418	020316-84-1	91
			O-HYDROGEN PERDEUTERIO HEXADECANOI C ACID	504545	039756-30-4	90
53	36.756	0.33	D:\DATABASE\DEMO.L			
			1H-NAPHTHO[2,3-C]PYRAN-5,10-DIONE, 3,4-DIHYDRO-7,9-DIMETHOXY-1,3-DIM ETHYL-, TRANS-(.+-.)- $$ (+,-)-DEO XYQUINONE A DIMETHYL ETHER $$ (+,-)-TRANS-7,9-DIMETHOXY-1,3-DIMETHYL -3,4,5,10-TETRAHYDRONAPHTHO[2,3-C] PYRAN-5,10-DIONE	513557	084018-44-0	91
			1H-NAPHTHO[2,3-C]PYRAN-5,10-DIONE, 3,4-DIHYDRO-7,9-DIMETHOXY-1,3-DIM ETHYL-, CIS-(.+-.)- $$ (+,-)-CIS-7 ,9-DIMETHOXY-1,3-DIMETHYL-3,4,5,10 -TETRAHYDRONAPHTHO[2,3-C]PYRAN-5,1 0-DIONE	513558	084018-43-9	91
			3-ACETYL-1-METHYL-2-(1'-METHYL-1H- INDOL-2'-YL)-1H-INDOLE	513641	000000-00-0	80
54	36.967	0.53	D:\DATABASE\DEMO.L			
			1-Phenanthrenecarboxylic acid, 1,2 ,3,4,4a,9,10,10a-octahydro-1,4a-di methyl-7-(1-methylethyl)-, [1R-(1. alpha.,4a.beta.,10a.alpha.)]- $$ P odocarpa-8,11,13-trien-15-oic acid , 13-isopropyl- $$ Abieta-8,11,13- trien-18-oic acid $$ Abietic acid, dehydro-	503093	001740-19-8	97
			1-PHENANTHRENECARBOXYLIC ACID, 1,2 ,3,4,4A,9,10,10A-OCTAHYDRO-1,4A-DI METHYL-7-(1-METHYLETHYL)-, [1R-(1. ALPHA.,4A.BETA.,10A.ALPHA.)]- $$ (-)-DEHYDROABIETIC ACID $$ 1,2,3,4, 4A,9,10,10A-OCTAHYDRO-1,4A-DIMETHY L-7-(1-METHYLETHYL)-1-PHENANTHRENE CARBOXYLIC ACID	503110	001740-19-8	97

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Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-140c-3jm.D
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Operator  :
Sample    :
Misc      :
ALS Vial  : 3   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autointl.e

%#     RT  Area%          Library/ID                    Ref#     CAS#   Qual
                ABIETA-8,11,13-TRIEN-18-OIC ACID $ 503106 999503-11-8 97
                $ PODOCARPA-8,11,13-TRIEN-15-SARUR
                E, 13-ISOPROPYL-

55  37.032  0.60 D:\DATABASE\DEMO.L
                ABIETA-8,11,13-TRIEN-18-OIC ACID $ 503106 999503-11-8 83
                $ PODOCARPA-8,11,13-TRIEN-15-SARUR
                E, 13-ISOPROPYL-
                1-Phenanthrenecarboxylic acid, 1,2 503093 001740-19-8 83
                ,3,4,4a,9,10,10a-octahydro-1,4a-di
                methyl-7-(1-methylethyl)-, [1R-(1.
                alpha.,4a.beta.,10a.alpha.)]- $$ P
                odocarpa-8,11,13-trien-15-oic acid
                , 13-isopropyl- $$ Abieta-8,11,13-
                trien-18-oic acid $$ Abietic acid,
                 dehydro-
                1-PHENANTHRENECARBOXYLIC ACID, 1,2 503110 001740-19-8 83
                ,3,4,4A,9,10,10A-OCTAHYDRO-1,4A-DI
                METHYL-7-(1-METHYLETHYL)-, [1R-(1.
                ALPHA.,4A.BETA.,10A.ALPHA.)]- $$ (
                -)-DEHYDROABIETIC ACID $$ 1,2,3,4,
                4A,9,10,10A-OCTAHYDRO-1,4A-DIMETHY
                L-7-(1-METHYLETHYL)-1-PHENANTHRENE
                CARBOXYLIC ACID

56  37.237  0.28 D:\DATABASE\DEMO.L
                ABIETA-7,13-DIEN-18-OIC ACID $$ 1- 168419 000514-10-3 86
                PHENANTHRENECARBOXYLIC ACID, 1,2,3
                ,4,4A,4B,5,6,10,10A-DECAHYDRO- $$
                1-PHENANTHRENECARBOXYLIC ACID, 1,2
                ,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,
                4A-DIMETHYL-7-(1-METHYLETHYL)-, [1
                R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A
                .ALPHA.)]-
                Abietic acid $$ 1-Phenanthrenecarb 513378 000514-10-3 60
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- $$ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- $$ L-abietic acid
                1H-NAPHTHO[2,3-C]PYRAN-5,10-DIONE, 513558 084018-43-9 58
                 3,4-DIHYDRO-7,9-DIMETHOXY-1,3-DIM
                ETHYL-, CIS-(.+-.)- $$ (+,-)-CIS-7
                ,9-DIMETHOXY-1,3-DIMETHYL-3,4,5,10
                -TETRAHYDRONAPHTHO[2,3-C]PYRAN-5,1
                0-DIONE

57  37.270  0.26 D:\DATABASE\DEMO.L
                ABIETA-7,13-DIEN-18-OIC ACID $$ 1- 168419 000514-10-3 93
                PHENANTHRENECARBOXYLIC ACID, 1,2,3
                ,4,4A,4B,5,6,10,10A-DECAHYDRO- $$
                1-PHENANTHRENECARBOXYLIC ACID, 1,2
                ,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,
                4A-DIMETHYL-7-(1-METHYLETHYL)-, [1
                R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A
                .ALPHA.)]-
                ABIETA-7,13-DIEN-18-OIC ACID $$ 1- 168420 000514-10-3 83
                PHENANTHRENECARBOXYLIC ACID, 1,2,3
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Data Path : F:\DATA MS\daa\
Data File : WLM-10prsen-140c-3jm.D
Acq On : 12 Oct 2019 13:19
Operator :
Sample :
Misc :
ALS Vial : 3 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			,4,4A,4B,5,6,10,10A-DECAHYDRO- $$ 1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL)-, [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A.ALPHA.)]-			
			Abietic acid $$ 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,4b,5,6,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1R-(1.alpha.,4a.beta.,4b.alpha.,10a.alpha.)]- $$ Podocarpa-7,13-dien-15-oic acid, 13-isopropyl- $$ L-abietic acid	513344	000514-10-3	70
58	37.378	0.14	D:\DATABASE\DEMO.L			
			ABIETA-7,13-DIEN-18-OIC ACID $$ 1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,4B,5,6,10,10A-DECAHYDRO- $$ 1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL)-, [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A.ALPHA.)]-	168419	000514-10-3	70
			Abietic acid $$ 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,4b,5,6,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1R-(1.alpha.,4a.beta.,4b.alpha.,10a.alpha.)]- $$ Podocarpa-7,13-dien-15-oic acid, 13-isopropyl- $$ L-abietic acid	513378	000514-10-3	70
			ABIETA-7,13-DIEN-18-OIC ACID $$ 1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,4B,5,6,10,10A-DECAHYDRO- $$ 1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL)-, [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A.ALPHA.)]-	168420	000514-10-3	68
59	37.410	0.05	D:\DATABASE\DEMO.L			
			ABIETA-7,13-DIEN-18-OIC ACID $$ 1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,4B,5,6,10,10A-DECAHYDRO- $$ 1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL)-, [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A.ALPHA.)]-	168420	000514-10-3	83
			ABIETA-7,13-DIEN-18-OIC ACID $$ 1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,4B,5,6,10,10A-DECAHYDRO- $$ 1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL)-, [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A.ALPHA.)]-	168419	000514-10-3	78
			Abietic acid $$ 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,4b,5,6,10,10a-decahydro-1,4a-dimethyl-7-(1-m	513344	000514-10-3	70

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-140c-3jm.D
Acq On : 12 Oct 2019 13:19
Operator :
Sample :
Misc :
ALS Vial : 3 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autointl.e

%#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid			
60	37.437	0.23	D:\DATABASE\DEMO.L ABIETA-7,13-DIEN-18-OIC ACID $$ 1- PHENANTHRENECARBOXYLIC ACID, 1,2,3 ,4,4A,4B,5,6,10,10A-DECAHYDRO- $$ 1-PHENANTHRENECARBOXYLIC ACID, 1,2 ,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1, 4A-DIMETHYL-7-(1-METHYLETHYL)-, [1 R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A .ALPHA.)]-	168420	000514-10-3	86
			Abietic acid $$ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid	513344	000514-10-3	66
			Palustric acid $$ Podocarpa-8,13-d ien-15-oic acid, 13-isopropyl- $$ 1-Phenanthrenecarboxylic acid, 1,2 ,3,4,4a,5,6,9,10,10a-decahydro-1,4 a-dimethyl-7-(1-methylethyl)-, (1R -(1.alpha.,4a.beta.,10a.alpha.))- $$ 8,13-Abietadien-18-oic acid	513439	001945-53-5	64
61	37.707	3.08	D:\DATABASE\DEMO.L Abietic acid $$ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid	513378	000514-10-3	99
			Abietic acid $$ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid	513347	000514-10-3	94
			2,2'-DIMETHYL-4,4',5,5'-TETRAMETHO XYBIPHENYL $$ 4,4',5,5'-TETRAMETHO XY-2,2'-DIMETHYL-1,1'-BIPHENYL	513577	062012-51-5	90
62	38.485	0.04	D:\DATABASE\DEMO.L Abietic acid $$ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid	513344	000514-10-3	91
			Abietic acid $$ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m	513347	000514-10-3	89

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-140c-3jm.D
Acq On : 12 Oct 2019 13:19
Operator :
Sample :
Misc :
ALS Vial : 3 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid			
			Palustric acid $$ Podocarpa-8,13-d ien-15-oic acid, 13-isopropyl- $$ 1-Phenanthrenecarboxylic acid, 1,2 ,3,4,4a,5,6,9,10,10a-decahydro-1,4 a-dimethyl-7-(1-methylethyl)-, (1R -(1.alpha.,4a.beta.,10a.alpha.))- $$ 8,13-Abietadien-18-oic acid	513439	001945-53-5	86
63	38.523	0.06	D:\DATABASE\DEMO.L			
			Abietic acid $$ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid	513378	000514-10-3	96
			Abietic acid $$ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid	513344	000514-10-3	90
			Abietic acid $$ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid	513347	000514-10-3	89
64	38.842	0.08	D:\DATABASE\DEMO.L			
			Abietic acid $$ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid	513347	000514-10-3	70
			2,3,4,5-TETRAMETHYL-6,6-DIPHENYL-2 ,4-CYCLOHEXADIEN-1-ONE $$ 2,4-CYCL OHEXADIEN-1-ONE, 2,3,4,5-TETRAMETH YL-6,6-DIPHENYL- $$ 2,4-CYCLOHEXAD IENONE, TETRAMETHYL-6,6-DIPHENYL-	513665	074764-49-1	62
			2,4-Cyclohexadien-1-one, 2,3,4,5-t etramethyl-6,6-diphenyl- $$ 2,3,4, 5-Tetramethyl-6,6-diphenyl-2,4-cyc lohexadien-1-one #	513431	074764-49-1	62
65	39.014	0.16	D:\DATABASE\DEMO.L			
			Abietic acid $$ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo	513347	000514-10-3	66

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-140c-3jm.D
Acq On : 12 Oct 2019 13:19
Operator :
Sample :
Misc :
ALS Vial : 3 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			carpa-7,13-dien-15-oic acid, 13-is			
			opropyl- $$ L-abietic acid			
			Abietic acid $$ 1-Phenanthrenecarb	513378	000514-10-3	50
			oxylic acid, 1,2,3,4,4a,4b,5,6,10,			
			10a-decahydro-1,4a-dimethyl-7-(1-m			
			ethylethyl)-, [1R-(1.alpha.,4a.bet			
			a.,4b.alpha.,10a.alpha.)]- $$ Podo			
			carpa-7,13-dien-15-oic acid, 13-is			
			opropyl- $$ L-abietic acid			
			4-Androsten-6.beta.-ol-3,17-dione	513437	999513-45-0	46

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsen-140c-4jm.D
Acq On : 12 Oct 2019 14:08
Operator :
Sample :
Misc :
ALS Vial : 4 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

%k#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	1.962	4.48	D:\DATABASE\DEMO.L			
			Methyl Alcohol $$ Methanol $$ Carb inol $$ Methyl hydroxide	5073	000067-56-1	2
			METHANOL $$ HYDROXYMETHANE $$ ALCO HOL, METHYL $$ ALCOOL METHYLIQUE	5075	000067-56-1	2
			Methyl Alcohol $$ Methanol $$ Carb inol $$ Methyl hydroxide	5072	000067-56-1	2
2	2.135	0.13	D:\DATABASE\DEMO.L			
			Pentane, 2,4-dimethyl- $$ 2,4-Dime thylpentane	18753	000108-08-7	90
			Pentane, 2,4-dimethyl- $$ 2,4-Dime thylpentane	18750	000108-08-7	87
			PENTANE, 2,4-DIMETHYL- $$ 2,4-DIME THYLPENTANE $$ PENTANE, 2,4-DIMETH YL	19002	000108-08-7	80
3	2.205	10.81	D:\DATABASE\DEMO.L			
			HEXANE, 3-METHYL- $$ 3-METHYLHEXAN E $$ 2-ETHYLPENTANE $$ HEXANE, 3-M ETHYL	18994	000589-34-4	83
			Hexane, 3-methyl- $$ 2-Ethylpentan e $$ 3-Methylhexane	18811	000589-34-4	80
			Hexane, 3-methyl- $$ 2-Ethylpentan e $$ 3-Methylhexane	18754	000589-34-4	64
4	2.243	4.26	D:\DATABASE\DEMO.L			
			1,3-DIMETHYLCYCLOPENTANE $$ CYCLOP ENTANE, 1,3-DIMETHYL-, CIS- $$ 1,3 -DIMETHYLCYCLOPENTANE (CIS) $$ 1,3 -DIMETHYLCYCLOPENTANE CIS	62286	002532-58-3	91
			Cyclopentane, 1,3-dimethyl- $$ 1,3 -Dimethylcyclopentane	101343	002453-00-1	91
			Cyclopentane, 1,3-dimethyl-, cis- $$ cis-1,3-Dimethylcyclopentane $$ 1,3-Dimethylcyclopentane cis $$ 1 ,3-Dimethylcyclopentane #	62231	002532-58-3	91
5	2.335	6.55	D:\DATABASE\DEMO.L			
			CYCLOHEXANE, METHYL- $$ METHYLCYCL OHEXANE $$ 1-METHYLCYCLOHEXANE $$ CYCLOHEXANE, METHYL	141469	000108-87-2	96
			Cyclohexane, methyl- $$ Cyclohexyl methane $$ Hexahydrotoluene $$ Met hylcyclohexane	141386	000108-87-2	94
			CYCLOHEXANE, METHYL- $$ METHYLCYCL OHEXANE $$ 1-METHYLCYCLOHEXANE $$ CYCLOHEXANE, METHYL	141467	000108-87-2	94
6	2.421	61.85	D:\DATABASE\DEMO.L			
			Toluene $$ Benzene, methyl $$ Meth acide $$ Methylbenzene	158579	000108-88-3	91
			BENZENE, METHYL- $$ METHYLBENZENE $$ TOLUENE $$ ANTISAL 1A	158625	000108-88-3	91
			Toluene $$ Benzene, methyl $$ Meth acide $$ Methylbenzene	158580	000108-88-3	91
7	2.745	1.12	D:\DATABASE\DEMO.L			
			Cyclohexane, ethyl- $$ Ethylcycloh	141506	001678-91-7	93

```
Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-140c-4jm.D
Acq On    : 12 Oct 2019  14:08
Operator  :
Sample    :
Misc      :
ALS Vial  : 4   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L              Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e
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t#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			exane			
			CYCLOHEXANE, ETHYL- $$ ETHYLCYCLOH	141561	001678-91-7	93
			EXANE $$ ETHYL CYCLOHEXANE $$ ETHY			
			LCYCLOHEXAN			
			ETHYLCYCLOHEXANE $$ ETHYLCYCLOHEXA	54425	001678-91-7	81
8	2.875	0.38	D:\DATABASE\DEMO.L			
			1,3,5-CYCLOHEPTATRIENE $$ CYCLOHEP	158639	000544-25-2	90
			TA-1,3,5-TRIENE $$ CYCLOHEPTATRIEN			
			E $$ CYCLOHEPTATRIENE [UN2603] [FL			
			AMMABLE LIQUID]			
			1,3,5-Cycloheptatriene $$ Tropilid	158600	000544-25-2	90
			ene $$ Cyclohepta-1,3,5-triene $$			
			Cycloheptatriene			
			1,3,5-CYCLOHEPTATRIENE $$ CYCLOHEP	158610	000544-25-2	87
			TA-1,3,5-TRIENE $$ CYCLOHEPTATRIEN			
			E $$ CYCLOHEPTATRIENE [UN2603] [FL			
			AMMABLE LIQUID]			
9	4.609	0.01	D:\DATABASE\DEMO.L			
			Eucalyptol $$ Cineole $$ 2-Oxabicy	23207	000470-82-6	96
			clo[2.2.2]octane, 1,3,3-trimethyl-			
			$$ p-Menthane, 1,8-epoxy-			
			Eucalyptol $$ Cineole $$ 2-Oxabicy	23252	000470-82-6	96
			clo[2.2.2]octane, 1,3,3-trimethyl-			
			$$ p-Menthane, 1,8-epoxy-			
			2-OXABICYCLO[2.2.2]OCTANE, 1,3,3-T	23424	000470-82-6	96
			RIMETHYL- $$ 1, 8-CINEOL $$ 1,3,3-			
			TRIMETHYL-2-OXABICYCLO(2.2.2)OCTAN			
			E $$ 1,3,3-TRIMETHYL-2-OXABICYCLO[			
			2.2.2]OCTANE			
10	17.315	0.04	D:\DATABASE\DEMO.L			
			2H-2,4a-Methanonaphthalene, 1,3,4,	350641	001135-66-6	99
			5,6,7-hexahydro-1,1,5,5-tetramethy			
			1-, (2S)- $$ 2H-2,4a-Methanonaphth			
			alene, 1,3,4,5,6,7-hexahydro-1,1,5			
			,5-tetramethyl-, (2S,4aR)-(-)- $$			
			Isolongifolene $$ (-)-Isolongifoli			
			ne			
			2H-2,4A-METHANONAPHTHALENE, 1,3,4,	350804	001135-66-6	98
			5,6,7-HEXAHYDRO-1,1,5,5-TETRAMETHY			
			L-, (2S)- $$ (-)-ISOLONGIFOLENE $$			
			(-)-ISOLONGIFOLINE $$ (2S)-1,3,4,			
			5,6,7-HEXAHYDRO-1,1,5,5-TETRAMETHY			
			L-2H-2,4A-METHANONAPHTHALENE			
			1,4-METHANOAZULENE, DECAHYDRO-4,8,	350758	000475-20-7	97
			8-TRIMETHYL-9-METHYLENE-, [1S-(1.A			
			LPHA.,3A.BETA.,4.ALPHA.,8A.BETA.)]			
			- $$ (+)-LONGIFOLEN $$ (+)-LONGIFO			
			LENE $$ (+)-LONGOFOLENE			
11	17.725	0.01	D:\DATABASE\DEMO.L			
			3,6,8-NONATRIENOIC ACID, 5-METHYL-	2933	000000-00-0	10
			, ETHYLESTER			
			3,6,8-Nonatrienoic acid, 5-methyl-	2929	999002-93-0	10
			, ethyl ester			
			2-PHENYLETHANAMINE $$ BENZENEETHAN	4100	000064-04-0	9
			AMINE $$ (2-AMINOETHYL)BENZENE $$			

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsen-140c-4jm.D
Acq On : 12 Oct 2019 14:08
Operator :
Sample :
Misc :
ALS Vial : 4 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

%#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			.BETA.-AMINOETHYLBENZENE			
12	28.616	0.01	D:\DATABASE\DEMO.L			
			4-(METHOXYMETHYL)-6-METHYL-2-PHENOXYNICOTINONITRILE $$ PYRIDINE-3-CARBONITRILE, 4-METHOXYMETHYL-6-METHYL-2-PHENOXY-	7413	332057-36-0	38
			3-(3-OXO-3H-BENZO[F]CHROMEN-2-YL)-2,4(1H,3H)-QUINOLINEDIONE $$ 4-HYDROXY-3-(2-OXO-2H-1-OXA-3-PHENANTHRYL)-2(1H)-QUINOLINONE	7476	999007-47-7	23
			METHYL 1A,7B-DIHYDRO-1H-CYCLOPROPA[A]NAPHTHALENE-1-CARBOXYLATE $$ 1H-CYCLOPROPA[A]NAPHTHALENE-1-CARBOXYLIC ACID, 1A,7B-DIHYDRO-, METHYL ESTER $$ 2,3-BENZO-7-METHOXYCARBONYL-BICYCLO(4.1.0)-HEPTA-4-ENE	7363	023398-50-7	9
13	28.934	0.01	D:\DATABASE\DEMO.L			
			PHENOL, 2-SEC-BUTYL-4-(METHYLTHIO)-6-NITRO-	132	000000-00-0	35
			4-BROMO-N-[(6-METHYL-2-PYRIDYL)AMINOMETHYL]PHTHALIMIDE $$ 5-BROMO-2-{[(6-METHYL-2-PYRIDINYL)AMINO]METHYL}-1H-ISOINDOLE-1,3(2H)-DIONE	7473	999007-47-4	9
			3-(3-OXO-3H-BENZO[F]CHROMEN-2-YL)-2,4(1H,3H)-QUINOLINEDIONE $$ 4-HYDROXY-3-(2-OXO-2H-1-OXA-3-PHENANTHRYL)-2(1H)-QUINOLINONE	7476	999007-47-7	9
14	30.306	0.03	D:\DATABASE\DEMO.L			
			ENT-PIMARA-8,15-DIENE	481166	021561-92-2	95
			1,2-DIAZA-3-SILACYCLOPENT-5-ENE, 2-(1,1-DIMETHYLETHYL)-3,3,5-TRIMETHYL-4-(PHENYLMETHYLENE)-, (Z)- $$ 4-BENZYLIDENE-2-TERT-BUTYL-3,3,5-TRIMETHYL-1,2-DIAZA-3-SILA-5-CYCLOPENTENE	481139	085226-13-7	83
			4H,8H-BENZO[1,2-B:3,4-B']DIPYRAN-4-ONE, 5-METHOXY-2,8,8-TRIMETHYL- $$ 5-METHOXY-2,8,8-TRIMETHYL-4H,8H-BENZO[1,2-B:3,4-B']DIPYRAN-4-ONE $$ 5-O-METHYLALLOPTAEROXYLIN $$ ALLOPTAEROXYLIN METHYL ETHER	481134	035930-31-5	83
15	30.712	0.01	D:\DATABASE\DEMO.L			
			4-(METHOXYMETHYL)-6-METHYL-2-PHENOXYNICOTINONITRILE $$ PYRIDINE-3-CARBONITRILE, 4-METHOXYMETHYL-6-METHYL-2-PHENOXY-	7413	332057-36-0	35
			1,3-OXATHIOL-1-IUM, 4-HYDROXY-2-[(1-METHYLETHYL)THIO]-5-(TRIFLUOROACETYL)-, HYDROXIDE, INNER SALT $$ 2-ISOPROPYLTHIO-5-TRIFLUORACETYL-1,3-OXATHIOLYIUM-4-OLAT	7423	096088-83-4	10
			1-Tetradecanamine $$ Tetradecylamine $$ Armeen 14 $$ Myristylamine	4817	002016-42-4	9
16	31.257	0.00	D:\DATABASE\DEMO.L			

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-140c-4jm.D
Acq On : 12 Oct 2019 14:08
Operator :
Sample :
Misc :
ALS Vial : 4 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

k#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			4-(METHOXYMETHYL)-6-METHYL-2-PHENOXYNICOTINONITRILE $$ PYRIDINE-3-CARBONITRILE, 4-METHOXYMETHYL-6-METHYL-2-PHENOXY-	7413	332057-36-0	10
			2,2'-(1,4-PIPERAZINEDIYL)BIS[N-(4-METHOXYPHENYL)SUCCINIMIDE]	7525	293766-05-9	9
			2-(3-BUTOXY-2-HYDROXYPROPYL)MALONOHYDRAZIDE $$ MALONODIHYDRAZIDE, 2-(3-BUTOXY-2-HYDROXYPROPYL)-	7415	331648-87-4	9
17	31.311	0.01	D:\DATABASE\DEMO.L			
			4-(METHOXYMETHYL)-6-METHYL-2-PHENOXYNICOTINONITRILE $$ PYRIDINE-3-CARBONITRILE, 4-METHOXYMETHYL-6-METHYL-2-PHENOXY-	7413	332057-36-0	27
			9-(4-HYDROXYPHENYL)-3,3,6,6-TETRAMETHYL-3,4,6,7,8A,9-HEXAHYDRO-1,8(2H,5H)-ACRIDINEDIONE	7482	999007-48-3	23
			3-(3-OXO-3H-BENZO[F]CHROMEN-2-YL)-2,4(1H,3H)-QUINOLINEDIONE $$ 4-HYDROXY-3-(2-OXO-2H-1-OXA-3-PHENANTHRYL)-2(1H)-QUINOLINONE	7476	999007-47-7	12
18	31.700	0.02	D:\DATABASE\DEMO.L			
			6-ETHYL-2-METHYL-4,6-DIHYDRO-2H-[1,4]OXAZINO[3,2-C]QUINOLINE-3,5-DIONE $$ 6-ETHYL-2-METHYL-2H-1-OXA-4,6-PHENANTHROLINE-3,5(4H,6H)-DIONE $$ 6-ETHYL-2-METHYL-6,10B-DIHYDRO-2H-[1,4]OXAZINO[3,2-C]QUINOLINE-3,5-DIONE	7414	334023-40-4	14
			2-METHOXY-4-(METHOXYMETHYL)-6-METHYLNICOTINONITRILE $$ PYRIDINE-3-CARBONITRILE, 2,4-DIMETHOXY-6-METHYL	7347	063644-84-8	10
			1,3-OXATHIOL-1-IUM, 4-HYDROXY-2-[(1-METHYLETHYL)THIO]-5-(TRIFLUOROACETYL)-, HYDROXIDE, INNER SALT $$ 2-ISOPROPYLTHIO-5-TRIFLUORACETYL-1,3-OXATHIOLYIUM-4-OLAT	7423	096088-83-4	9
19	31.830	0.01	D:\DATABASE\DEMO.L			
			4-(METHOXYMETHYL)-6-METHYL-2-PHENOXYNICOTINONITRILE $$ PYRIDINE-3-CARBONITRILE, 4-METHOXYMETHYL-6-METHYL-2-PHENOXY-	7413	332057-36-0	12
			1,3-OXATHIOL-1-IUM, 4-HYDROXY-2-[(1-METHYLETHYL)THIO]-5-(TRIFLUOROACETYL)-, HYDROXIDE, INNER SALT $$ 2-ISOPROPYLTHIO-5-TRIFLUORACETYL-1,3-OXATHIOLYIUM-4-OLAT	7423	096088-83-4	9
			1-Tetradecanamine $$ Tetradecylamine $$ Armeen 14 $$ Myristylamine	4817	002016-42-4	9
20	32.019	0.01	D:\DATABASE\DEMO.L			
			4-(METHOXYMETHYL)-6-METHYL-2-PHENOXYNICOTINONITRILE $$ PYRIDINE-3-CARBONITRILE, 4-METHOXYMETHYL-6-METHYL-2-PHENOXY-	7413	332057-36-0	14
			2,2'-(1,4-PIPERAZINEDIYL)BIS[N-(4-	7525	293766-05-9	10

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsen-140c-4jm.D
Acq On : 12 Oct 2019 14:08
Operator :
Sample :
Misc :
ALS Vial : 4 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autointl.e

%k#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			METHOXYPHENYL)SUCCINIMIDE]			
			2,2'-(1,4-Piperazinediyl)bis[N-(4-methoxyphenyl)succinimide]	7524	293766-05-9	10
21	32.105	0.02	D:\DATABASE\DEMO.L			
			1,2-DIAZA-3-SILACYCLOPENT-5-ENE, 2-(1,1-DIMETHYLETHYL)-3,3,5-TRIMETHYL-4-(PHENYLMETHYLENE)-, (Z)- $$ 4-BENZYLIDENE-2-TERT-BUTYL-3,3,5-TRIMETHYL-1,2-DIAZA-3-SILA-5-CYCLOPENTENE	481139	085226-13-7	64
			PIMARA-8,15-DIENE $$ PHENANTHRENE, 7-ETHENYL-1,2,3,4,4A,5,6,7,8,9,10,10A-DODECAHYDRO-1,1,4A,7-TETRAMETHYL- $$ 7.ALPHA.-ETHENYL-1,1,4A,7.BETA.-TETRAMETHYL-1,2,3,4,4A,5,6,7,8,9,10,10A-DODECAHYDROPHENANTHREN	481165	055255-56-6	60
			Naphthalene, decahydro-1,1,4a-trimethyl-6-methylene-5-(3-methylene-4-pentenyl)-, [4aS-(4a.alpha.,5.alpha.,8a.beta.)]- $$ Labda-8(20),13(16),14-triene $$ Sclaren $$ Sclarene	481093	000511-02-4	46
22	32.305	0.00	D:\DATABASE\DEMO.L			
			Taurolidine $$ 2H-1,2,4-Thiadiazine, 4,4'-methylenebis[tetrahydro-, 1,1,1',1'-tetraoxide $$ 4,4'-Methylenebis(tetrahydro-1,2,4-thiadiazine 1,1-dioxide) $$ Taurolin	4983	019388-87-5	12
			1-Dodecanamine $$ Dodecylamine $$ n-Dodecylamine $$ Alamine 4	4652	000124-22-1	12
			1-DODECANAMINE $$ 1-AMINODODECANE $$ 1-DODECYLAMINE $$ ALAMINE 4	4661	000124-22-1	12
23	32.402	0.01	D:\DATABASE\DEMO.L			
			3,5-DIETHYL-2-(2-FURYL)PYRIDINE $$ 3,5-DIETHYL-4-(2-FURYL)PYRIDINE	419329	078563-73-2	30
			2(1H)-Pyridone, 4-hydroxy-6-methyl-1-phenyl- $$ 2(1H)-Pyridinone, 4-hydroxy-6-methyl-1-phenyl- $$ N-Phenyl-4-hydroxy-6-methyl-2-pyridone $$ 4-Hydroxy-6-methyl-N-phenyl-2-pyridone	419190	015250-44-9	30
			4-NITRO-2-NAPHTHALDEHYDE	419272	000000-00-0	30
24	32.446	0.01	D:\DATABASE\DEMO.L			
			1-Hexadecanamine $$ Hexadecylamine $$ n-Cetylamine $$ n-Hexadecylamine	4902	000143-27-1	27
			4-(METHOXYMETHYL)-6-METHYL-2-PHENOXYNICOTINONITRILE $$ PYRIDINE-3-CARBONITRILE, 4-METHOXYMETHYL-6-METHYL-2-PHENOXY-	7413	332057-36-0	12
			1-Tetradecanamine $$ Tetradecylamine $$ Armeen 14 $$ Myristylamine	4815	002016-42-4	10
25	32.786	0.00	D:\DATABASE\DEMO.L			
			1-Hexadecanamine $$ Hexadecylamine	4902	000143-27-1	35

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsen-140c-4jm.D
Acq On : 12 Oct 2019 14:08
Operator :
Sample :
Misc :
ALS Vial : 4 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

%k#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			$$ n-Cetylamine $$ n-Hexadecylamine			
			4-(METHOXYMETHYL)-6-METHYL-2-PHENOXYNICOTINONITRILE $$ PYRIDINE-3-CARBONITRILE, 4-METHOXYMETHYL-6-METHYL-2-PHENOXY-	7413	332057-36-0	16
			1,12-DODECANEDIAMINE $$ DODECANE-1,12-DIAMINE	4751	999004-75-2	9
26	32.975	0.01	D:\DATABASE\DEMO.L			
			1-Tetradecanamine $$ Tetradecylamine $$ Armeen 14 $$ Myristylamine	4817	002016-42-4	14
			1-Hexadecanamine $$ Hexadecylamine $$ n-Cetylamine $$ n-Hexadecylamine	4902	000143-27-1	10
			Tridecylamine $$ n-Tridecylamine $$ 1-Aminotridecane $$ 1-Tridecanamine	4737	002869-34-3	10
27	33.369	0.01	D:\DATABASE\DEMO.L			
			4-(METHOXYMETHYL)-6-METHYL-2-PHENOXYNICOTINONITRILE $$ PYRIDINE-3-CARBONITRILE, 4-METHOXYMETHYL-6-METHYL-2-PHENOXY-	7413	332057-36-0	14
			1-PENTADECANAMINE $$ 1-PENTADECYLAMINE $$ N-PENTADECYLAMINE $$ PENTADECANE, 1-AMINO-	4879	002570-26-5	10
			L-Alanine, N-glycyl- $$ Alanine, N-glycyl-, L- $$ Glcylalanine $$ Gly-ala	4366	003695-73-6	9
28	33.494	0.14	D:\DATABASE\DEMO.L			
			PIMARA-8,15-DIENE $$ PHENANTHRENE, 7-ETHENYL-1,2,3,4,4A,5,6,7,8,9,10,10A-DODECAHYDRO-1,1,4A,7-TETRAMETHYL- $$ 7.ALPHA.-ETHENYL-1,1,4A,7.BETA.-TETRAMETHYL-1,2,3,4,4A,5,6,7,8,9,10,10A-DODECAHYDROPHENANTHREN	481165	055255-56-6	86
			1-Phenanthrenecarboxaldehyde, 7-ethenyl-1,2,3,4,4a,4b,5,6,7,9,10,10a-dodecahydro-1,4a,7-trimethyl-, [1R-(1.alpha.,4a.beta.,4b.alpha.,7.beta.,10a.alpha.)]- $$ Podocarp-8(14)-en-15-al, 13.alpha.-methyl-13-vinyl- $$ Cryptopinon $$ Cryptopinone	481182	000472-39-9	86
			PIMARA-8(14),15-DIEN-18-AL $$ 1-PHENANTHRENECARBOXALDEHYDE, 7-ETHENYL-1,2,3,4,4A,4B,5,6,7,9,10,10A-DODECAHYDRO-1,4A,7-TRIMETHYL-, [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,7.BETA.,10A.ALPHA.)]- $$ CRYPTOPINON $$ CRYPTOPINONE	481208	000472-39-9	86
29	33.688	0.01	D:\DATABASE\DEMO.L			
			1-PENTADECANAMINE $$ 1-PENTADECYLAMINE $$ N-PENTADECYLAMINE $$ PENTADECANE, 1-AMINO-	4879	002570-26-5	10
			1-Hexadecanamine $$ Hexadecylamine	4902	000143-27-1	10

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Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-140c-4jm.D
Acq On    : 12 Oct 2019  14:08
Operator  :
Sample    :
Misc      :
ALS Vial  : 4   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e
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%#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			$$ n-Cetylamine $$ n-Hexadecylamine			
			1,12-DODECANEDIAMINE $$ DODECANE-1,12-DIAMINE $$ DODECANDIAMIN-(1,12	4750	999004-75-1	9
30	33.791	0.03	D:\DATABASE\DEMO.L			
			Oxazol-5(4H)-one, 4-dichloromethylene-2-phenyl- $$ 4-(Dichloromethylene)-2-phenyl-1,3-oxazol-5(4H)-one	210766	054902-24-8	14
			#			
			SYN-1-(BENZYLOXY)-4-METHOXY-1-METHYL-4-(1,1,2,2,2-PENTAFLUOROETHYL)-2,5-CYCLOHEXADIENE	170976	000000-00-0	12
			KAUR-16-EN-18-OIC ACID $$ KAUR-16-EN-18-OIC ACID, (4.BETA.)- $$ (-)-KAURNENOIC ACID $$ (4-BETA)-KAUR-16-EN-18-OIC ACID	168418	020316-84-1	10
31	33.861	0.07	D:\DATABASE\DEMO.L			
			1-Methyl-10,18-bisnorabieta-8,11,13-triene	466158	999466-16-6	94
			10,13-DIMETHYL-4,5,6,7,8,9,10,11,12,13,14,15-DODECAHYDRO-1H-CYCLOPENTA[A]PHENANTHRENE $$ ANDROSTA-2,16-DIENE	466180	999466-18-8	90
			4b,8-Dimethyl-2-isopropylphenanthrene, 4b,5,6,7,8,8a,9,10-octahydro-	466159	999466-16-7	83
32	34.136	0.01	D:\DATABASE\DEMO.L			
			No matches found			
33	34.201	0.01	D:\DATABASE\DEMO.L			
			No matches found			
34	34.309	0.04	D:\DATABASE\DEMO.L			
			1-Phenanthrenecarboxylic acid, 7-ethenyl-1,2,3,4,4a,5,6,7,8,9,10,10a-dodecahydro-1,4a,7-trimethyl-, methyl ester, [1R-(1.alpha.,4a.beta.,7.beta.,10a.alpha.)]- $$ Podocarp-8-en-15-oic acid, 13.alpha.-methyl-13-vinyl-, methyl ester	466507	003582-26-1	64
			METHYL PIMARA-7,15-DIEN-18-OATE $$ 1-PHENANTHRENECARBOXYLIC ACID, 7-ETHENYL-1,2,3,4,4A,4B,5,6,7,8,10,10A-DODECAHYDRO-1,4A,7-TRIMETHYL-, METHYL ESTER, [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,7.ALPHA.,10A.ALPHA.)] - $$ ISOPIMARATE $$ ISOPIMARIC ACID, METHYL ESTER	466515	001686-62-0	49
			3,5-Bis(trifluoromethyl)benzamide $$ 3,5-di(Trifluoromethyl)benzamide $$ Benzamide, 3,5-bis(trifluoromethyl)-	466229	022227-26-5	49
35	34.525	0.08	D:\DATABASE\DEMO.L			
			PIMARA-8(14),15-DIEN-18-AL $$ 1-PHENANTHRENECARBOXALDEHYDE, 7-ETHENYL-1,2,3,4,4A,4B,5,6,7,9,10,10A-DOD	481208	000472-39-9	41

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Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-140c-4jm.D
Acq On    : 12 Oct 2019  14:08
Operator  :
Sample    :
Misc      :
ALS Vial  : 4   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autointl.e
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%#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			ECAHYDRO-1,4A,7-TRIMETHYL-, [1R-(1 .ALPHA.,4A.BETA.,4B.ALPHA.,7.BETA. ,10A.ALPHA.)]- $$ CRYPTOPINON $$ C RYPTOPINONE			
			(+)1A7,4A,9,10,10A-DODECAHYDRO-1,4 A,7-TRIMETHYL-7-VINYL-1-PHENANTHRE NCARBALDEHYDEHYL 4,AZC.BETA.THIOME THYL](12-YL2ETHYLTHIOYLENC1ETHYLDE THYL3-YLAPHTHC]TACXM.BETA.ANO6, [U CH0ALFPAL[YL9	481209	000000-00-0	38
			1-Phenanthrenecarboxaldehyde, 7-et henyl-1,2,3,4,4a,4b,5,6,7,9,10,10a -dodecahydro-1,4a,7-trimethyl-, [1 R-(1.alpha.,4a.beta.,4b.alpha.,7.b eta.,10a.alpha.)]- $$ Podocarp-8(1 4)-en-15-al, 13.alpha.-methyl-13-v inyl- $$ Cryptopinon $$ Cryptopino ne	481182	000472-39-9	38
36	34.666	0.00	D:\DATABASE\DEMO.L			
			4-(METHOXYMETHYL)-6-METHYL-2-PHENO XYNICOTINONITRILE $$ PYRIDINE-3-CA RBONITRILE, 4-METHOXYMETHYL-6-METH YL-2-PHENOXY-	7413	332057-36-0	10
			2-METHOXY-4-(METHOXYMETHYL)-6-METH YLNICOTINONITRILE $$ PYRIDINE-3-CA RBONITRILE, 2,4-DIMETHOXY-6-METHYL	7347	063644-84-8	10
			1-Hexadecanamine $$ Hexadecylamine $$ n-Cetylamine $$ n-Hexadecylami ne	4902	000143-27-1	10
37	34.693	0.00	D:\DATABASE\DEMO.L			
			2-((E)-[((E)-2-{[(E)-(2-HYDROXYPHE NYL)METHYLIDENE]AMINO}PROPYL)IMINO]METHYL)PHENOL $$ .ALPHA.,.ALPHA.' -(1-METHYLETHYLENEDIIMINO)DI-ORTHO -CRESOL $$ .ALPHA.,.ALPHA.'-DIPROP YLENEDINITRILODI-O-CRESOL $$ ALPHA ,ALPHA'-(1-METHYLETHYLENEDIIMINO)D I-ORTHO-CRESOL	45719	000094-91-7	35
			2-PYRIDINEPROPANOIC ACID, .ALPHA.-METHYL-.BETA.-OXO-, ETHYL ESTER $$ ETHYL 2-METHYL-3-OXO-3-(2-PYRIDIN YL)PROPANOATE	5863	999005-86-4	9
			2H-3,9A-METHANO-1-BENZOXEPIN, OCTA HYDRO-2,2,5A,9-TETRAMETHYL-, [3R-(3.ALPHA.,5A.ALPHA.,9.ALPHA.,9A.ALP HA.)]- $$ .BETA.-AGAROFURAN, DIHYD RO- $$ .BETA.-DIHYDROAGAROFURAN $$ 2H-3,9A-METHANO-1-BENZOXEPIN, OCT AHYDRO-2,2,5A,9-TETRAMETHYL-	3110	005956-09-2	7
38	34.790	0.02	D:\DATABASE\DEMO.L			
			3-BENZYL-2-(2-FURYL)-4(3H)-QUINAZO LINONE $$ 3-BENZYL-2-(2-FURYL)-3,4 -DIHYDRO-4-QUINAZOLINONE	168393	256954-79-7	25
			3-Benzyl-2-(2-furyl)-3,4-dihydro-4 -quinazolinone $$ 3-Benzyl-2-(2-fu ryl)-4(3H)-quinazolinone #	168374	256954-79-7	25

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-140c-4jm.D
Acq On : 12 Oct 2019 14:08
Operator :
Sample :
Misc :
ALS Vial : 4 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			2-((E)-[((E)-2-([(E)-(2-HYDROXYPHENYL)METHYLIDENE]AMINO)PROPYL)IMINO]METHYL)PHENOL $$ .ALPHA.,.ALPHA.'-(1-METHYLETHYLENEDIIMINO)DI-ORTHO-CRESOL $$ .ALPHA.,.ALPHA.'-DIPROPYLENEDINITRILODI-O-CRESOL $$ ALPHA,ALPHA'-(1-METHYLETHYLENEDIIMINO)DI-ORTHO-CRESOL	45719	000094-91-7	20
39	34.914	0.02	D:\DATABASE\DEMO.L HEXANOIC ACID, 6-AMINO- $$ 6-AMINO HEXANOIC ACID $$ .EPSILON. S $$ .EPSILON.-AMINO-N-CAPROIC ACID	4219	000060-32-2	1
40	35.028	0.04	D:\DATABASE\DEMO.L Benzene, 1-[(dimethoxymethyl)-1-ethyl]-4-methoxycarbonyl-1-ethyl-	123523	999123-52-6	53
			4,5-Bis-dimethoxymethyl-octanedioic acid, dimethyl ester	124248	999124-25-1	45
			1-Dimethyl(prop-2-enyl)silyloxy-10-undecene	123536	999123-53-9	45
41	35.152	0.02	D:\DATABASE\DEMO.L KAUR-16-EN-18-OIC ACID $$ KAUR-16-EN-18-OIC ACID, (4.BETA.)- $$ (-)-KAURNENOIC ACID $$ (4-BETA)-KAUR-16-EN-18-OIC ACID	168418	020316-84-1	62
			ABIETA-7,13-DIEN-18-OIC ACID $$ 1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,4B,5,6,10,10A-DECAHYDRO- $$ 1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL)-, [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A.ALPHA.)]-	168419	000514-10-3	15
			Silane, chlorotris(phenylmethyl)- $$ Tribenzylchlorosilane $$ Chlorotribenzylsilane $$ Silane, tribenzylchloro-	513117	018740-59-5	11
42	35.195	0.02	D:\DATABASE\DEMO.L ABIETA-7,13-DIEN-18-OIC ACID $$ 1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,4B,5,6,10,10A-DECAHYDRO- $$ 1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL)-, [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A.ALPHA.)]-	168419	000514-10-3	43
			KAUR-16-EN-18-OIC ACID $$ KAUR-16-EN-18-OIC ACID, (4.BETA.)- $$ (-)-KAURNENOIC ACID $$ (4-BETA)-KAUR-16-EN-18-OIC ACID	168418	020316-84-1	38
			BUTYL 2-(METHYLAMINO)BENZOATE $$ ANTHRANILIC ACID, N-METHYL-, BUTYL ESTER $$ N-BUTYL O-METHYLAMINOBENZOATE	209256	015236-34-7	22

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Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-140c-4jm.D
Acq On    : 12 Oct 2019  14:08
Operator  :
Sample    :
Misc      :
ALS Vial  : 4   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autointl.e

#     RT  Area%          Library/ID                    Ref#     CAS#   Qual

              KAUR-16-EN-18-OIC ACID $$ KAUR-16- 168418 020316-84-1 41
              EN-18-OIC ACID, (4.BETA.)- $$ (-)-
              KAURNENOIC ACID $$ (4-BETA)-KAUR-1
              6-EN-18-OIC ACID
              1,3-Propanediol, trimethylsilyl et 122171 999122-17-4 35
              her
              2-Pyrrol[tert-butyl(dimethyl)silyl 122672 999122-67-5 35
              ]oxymorphopropan-1-ol

4  35.395  0.04 D:\DATABASE\DEMO.L
              p-Heptyloxyaniline $$ 4-n-Heptylox 228109 039905-44-7 43
              yaniline
              2-(ACETYLAMINO)PHENYL ACETATE $$ A 227934 999227-93-7 43
              CETIC ACID 2-ACETYLAMINO-PHENYL ES
              TER
              1a,2,5,5-Tetramethyl-cis-1a,4a,5,6 227946 999227-94-9 41
              ,7,8-hexahydro-gamma-chromene

5  35.487  1.05 D:\DATABASE\DEMO.L
              Xanthen-9-one, 1-hydroxy-3,5,8-tri 504583 049599-09-9 70
              methoxy- $$ 5,8-Dimethylbellidifol
              in $$ 1-Hydroxy-3,5,8-trimethoxyxa
              nthen-9-one $$ 1-Hydroxy-3,5,8-tri
              methoxy-9H-xanthen-9-one #
              Phenol, 2,4-bis(1-phenylethyl)- $$ 504578 002769-94-0 53
               2,4-Bis(1-phenylethyl)phenol #
              1-[1-(4-METHYLTHIO)HEXYLIDENE]-4-P 504561 113035-73-7 53
              HENYLCYCLOHEXANE

6  35.654  0.09 D:\DATABASE\DEMO.L
              3-((1-Amino-2-naphthyl)methylene)- 504402 999504-41-4 45
              2-benzofuran-1(3H)-one peak 1
              4B-(P-DEUTEROPHENYL)-4B,10A-DIHYDR 504462 000000-00-0 40
              OBENZOCYCLOBUTADIENO(5,6B)-1,4-BEN
              ZODIOXAN
              PIMARA-8(14),15-DIEN-18-OIC ACID $ 504608 000127-27-5 38
              $ 1-PHENANTHRENECARBOXYLIC ACID, 7
              -ETHENYL-1,2,3,4,4A,4B,5,6,7,9,10,
              10A-DODECAHYDRO-1,4A,7-TRIMETHYL-,
               [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,
              7.BETA.,10A.ALPHA.)]- $$ (+)-PIMAR
              IC ACID $$ .ALPHA.-PIMARIC ACID

7  35.757  0.28 D:\DATABASE\DEMO.L
              DEHYDROABIETIC ACID               464556 000000-00-0 98
              METHYL ABIETA-8,11,13-TRIEN-18-OAT 464549 001235-74-1 94
              E $$ 1-PHENANTHRENECARBOXYLIC ACID
              , 1,2,3,4,4A,9,10,10A-OCTAHYDRO-1,
              4A-DIMETHYL-7-(1-METHYLETHYL)-, ME
              THYL ESTER, [1R-(1.ALPHA.,4A.BETA.
              ,10A.ALPHA.)]- $$ DEHYDROABIETIC A
              CID METHYL ESTER $$ METHYL DEHYDRO
              ABIETATE
              1-Phenanthrenecarboxylic acid, 1,2 464538 001235-74-1 93
              ,3,4,4a,9,10,10a-octahydro-1,4a-di
              methyl-7-(1-methylethyl)-, methyl
              ester, [1R-(1.alpha.,4a.beta.,10a.
              alpha.)]- $$ Podocarpa-8,11,13-tri
              en-15-oic acid, 13-isopropyl-, met
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Data Path : F:\DATA MS\daa\
Data File : WLM-10prsen-140c-4jm.D
Acq On    : 12 Oct 2019  14:08
Operator  :
Sample    :
Misc      :
ALS Vial  : 4   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e
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?k#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			hyl ester $$ Methyl dehydroabietat			
48	35.924	0.11	D:\DATABASE\DEMO.L			
			BENZ[A]ANTHRACENONE	513655	099707-96-7	52
			1H-NAPHTHO[2,3-C]PYRAN-5,10-DIONE, 3,4-DIHYDRO-7,9-DIMETHOXY-1,3-DIMETHYL-, CIS-(.+-.)- $$ (+,-)-CIS-7,9-DIMETHOXY-1,3-DIMETHYL-3,4,5,10-TETRAHYDRONAPHTHO[2,3-C]PYRAN-5,10-DIONE	513558	084018-43-9	52
			Palustric acid $$ Podocarpa-8,13-dien-15-oic acid, 13-isopropyl- $$ 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,5,6,9,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, (1R-(1.alpha.,4a.beta.,10a.alpha.))- $$ 8,13-Abietadien-18-oic acid	513439	001945-53-5	44
49	36.016	0.11	D:\DATABASE\DEMO.L			
			Pimaric acid $$ 1-Phenanthrenecarboxylic acid, 7-ethenyl-1,2,3,4,4a,4b,5,6,7,9,10,10a-dodecahydro-1,4a,7-trimethyl-, [1R-(1.alpha.,4a.beta.,4b.alpha.,7.beta.,10a.alpha.)]- $$ Podocarp-8(14)-en-15-oic acid, 13.alpha.-methyl-13-vinyl- $$ D-pimaric acid	466434	000127-27-5	64
			KAURA-9(11),16-DIEN-18-OIC ACID, (4.ALPHA.)- $$ (-)-KAUR-9(11),16-DIEN-19-OIC ACID $$ GRANDIFLORENIC ACID $$ KAURA-5,16-DIEN-18(OR 19)-OIC ACID	503118	022338-67-6	58
			ABIETA-7,13-DIEN-18-OIC ACID $$ 1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,4B,5,6,10,10A-DECAHYDRO- $$ 1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL)-, [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A.ALPHA.)]-	168420	000514-10-3	55
50	36.097	0.35	D:\DATABASE\DEMO.L			
			PHENOL, 5-[2-(3-HYDROXY-4-METHOXYPHENYL)ETHENYL]-2,3-DIMETHOXY-, (Z)- $$ 2,3-DIMETHOXY-5-[2-(3-HYDROXY-4-METHOXYPHENYL)ETHENYL]PHENOL (Z) $$ COMBRETASTATIN A3	513563	111394-45-7	86
			PIMARA-8(14),15-DIEN-18-OIC ACID $$ 1-PHENANTHRENECARBOXYLIC ACID, 7-ETHENYL-1,2,3,4,4A,4B,5,6,7,9,10,10A-DODECAHYDRO-1,4A,7-TRIMETHYL-, [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,7.BETA.,10A.ALPHA.)]- $$ (+)-PIMARIC ACID $$ .ALPHA.-PIMARIC ACID	504608	000127-27-5	60
			Abietic acid $$ 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,4b,5,6,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1R-(1.alpha.,4a.beta.,4b.alpha.,10a.alpha.)]- $$ Podo	513378	000514-10-3	58

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-140c-4jm.D
Acq On : 12 Oct 2019 14:08
Operator :
Sample :
Misc :
ALS Vial : 4 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

%#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid			
51	36.259	0.09	D:\DATABASE\DEMO.L			
			Pimaric acid $$ 1-Phenanthrenecarb oxylic acid, 7-ethenyl-1,2,3,4,4a, 4b,5,6,7,9,10,10a-dodecahydro-1,4a ,7-trimethyl-, [1R-(1.alpha.,4a.be ta.,4b.alpha.,7.beta.,10a.alpha.)] - $$ Podocarp-8(14)-en-15-oic acid , 13.alpha.-methyl-13-vinyl- $$ D- pimaric acid	466434	000127-27-5	87
			1H-NAPHTHO[2,3-C]PYRAN-5,10-DIONE, 3,4-DIHYDRO-7,9-DIMETHOXY-1,3-DIM ETHYL-, CIS-(.+-.)- $$ (+,-)-CIS-7 ,9-DIMETHOXY-1,3-DIMETHYL-3,4,5,10 -TETRAHYDRONAPHTHO[2,3-C]PYRAN-5,1 0-DIONE	513558	084018-43-9	72
			1H-NAPHTHO[2,3-C]PYRAN-5,10-DIONE, 3,4-DIHYDRO-7,9-DIMETHOXY-1,3-DIM ETHYL-, TRANS-(.+-.)- $$ (+,-)-DEO XYQUINONE A DIMETHYL ETHER $$ (+,-)-TRANS-7,9-DIMETHOXY-1,3-DIMETHYL -3,4,5,10-TETRAHYDRONAPHTHO[2,3-C] PYRAN-5,10-DIONE	513557	084018-44-0	72
52	36.384	0.24	D:\DATABASE\DEMO.L			
			METHYL ABIETA-7,13-DIEN-18-OATE $$ 1-PHENANTHRENECARBOXYLIC ACID, 1, 2,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1 ,4A-DIMETHYL-7-(1-METHYLETHYL)-, M ETHYL ESTER, [1R-(1.ALPHA.,4A.BETA .,4B.ALPHA.,10A.ALPHA.)]- $$ ABALY N $$ ABIETIC ACID METHYL ESTER	258918	000127-25-3	98
			Methyl abietate $$ 1-Phenanthrenec arboxylic acid, 1,2,3,4,4a,4b,5,6, 10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, methyl ester, [1R -(1.alpha.,4a.beta.,4b.alpha.,10a. alpha.)]- $$ Podocarpa-7,13-dien-1 5-oic acid, 13-isopropyl-, methyl ester $$ Abalyn	258889	000127-25-3	98
			METHYL ABIETA-7,13-DIEN-18-OATE $$ 1-PHENANTHRENECARBOXYLIC ACID, 1, 2,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1 ,4A-DIMETHYL-7-(1-METHYLETHYL)-, M ETHYL ESTER, [1R-(1.ALPHA.,4A.BETA .,4B.ALPHA.,10A.ALPHA.)]- $$ ABALY N $$ ABIETIC ACID METHYL ESTER	480551	000127-25-3	95
53	36.470	0.04	D:\DATABASE\DEMO.L			
			1H-2,10A-ETHANOPHENANTHRENE, KAUR- 16-EN-18-OIC ACID DERIV. $$ KAUR-1 6-EN-18-OIC ACID $$ KAUR-16-EN-18- OIC ACID, (4.ALPHA.)- $$ (-)-ENT-K AUR-16-EN-19-OIC ACID	513651	006730-83-2	53
			1-PHENANTHRENECARBOXYLIC ACID, 7-E THENYL-1,2,3,4,4A,4B,5,6,7,8,10,10 A-DODECAHYDRO-1,4A,7-TRIMETHYL-, [	466436	005835-26-7	51

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-140c-4jm.D
Acq On : 12 Oct 2019 14:08
Operator :
Sample :
Misc :
ALS Vial : 4 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autointl.e

%k#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,7.ALPHA.,10A.ALPHA.)]- $$ ISOPIMARIC ACID $$ PODOCARP-7-EN-15-OIC ACID, 13.BETA.-METHYL-13-VINYL-KAUR-16-EN-18-OIC ACID $$ KAUR-16-EN-18-OIC ACID, (4.BETA.)- $$ (-)-KAURNENOIC ACID $$ (4-BETA)-KAUR-16-EN-18-OIC ACID	168418	020316-84-1	49
54	36.508	0.05	D:\DATABASE\DEMO.L			
			1-PHENANTHRENECARBOXYLIC ACID, 7-ETHENYL-1,2,3,4,4A,4B,5,6,7,8,10,10A-DODECAHYDRO-1,4A,7-TRIMETHYL-, [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,7.ALPHA.,10A.ALPHA.)]- $$ ISOPIMARIC ACID $$ PODOCARP-7-EN-15-OIC ACID, 13.BETA.-METHYL-13-VINYL-	466436	005835-26-7	55
			2-ACETYL-4,9-DIMETHOXY-7-METHYL-5H-FURO[3,2-G][1]-BENZOPYRAN-5-ONE	513538	092611-83-1	49
			Palustric acid $$ Podocarpa-8,13-dien-15-oic acid, 13-isopropyl- $$ 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,5,6,9,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, (1R-(1.alpha.,4a.beta.,10a.alpha.))- $$ 8,13-Abietadien-18-oic acid	513439	001945-53-5	46
55	36.594	0.53	D:\DATABASE\DEMO.L			
			1H-NAPHTHO[2,3-C]PYRAN-5,10-DIONE, 3,4-DIHYDRO-7,9-DIMETHOXY-1,3-DIMETHYL-, CIS-(.+-.)- $$ (+,-)-CIS-7,9-DIMETHOXY-1,3-DIMETHYL-3,4,5,10-TETRAHYDRONAPHTHO[2,3-C]PYRAN-5,10-DIONE	513558	084018-43-9	91
			KAUR-16-EN-18-OIC ACID $$ KAUR-16-EN-18-OIC ACID, (4.BETA.)- $$ (-)-KAURNENOIC ACID $$ (4-BETA)-KAUR-16-EN-18-OIC ACID	168418	020316-84-1	90
			O-HYDROGEN PERDEUTERIO HEXADECANOIC ACID	504545	039756-30-4	90
56	36.746	0.38	D:\DATABASE\DEMO.L			
			1H-NAPHTHO[2,3-C]PYRAN-5,10-DIONE, 3,4-DIHYDRO-7,9-DIMETHOXY-1,3-DIMETHYL-, TRANS-(.+-.)- $$ (+,-)-DBOXYQUINONE A DIMETHYL ETHER $$ (+,-)-TRANS-7,9-DIMETHOXY-1,3-DIMETHYL-3,4,5,10-TETRAHYDRONAPHTHO[2,3-C]PYRAN-5,10-DIONE	513557	084018-44-0	91
			1H-NAPHTHO[2,3-C]PYRAN-5,10-DIONE, 3,4-DIHYDRO-7,9-DIMETHOXY-1,3-DIMETHYL-, CIS-(.+-.)- $$ (+,-)-CIS-7,9-DIMETHOXY-1,3-DIMETHYL-3,4,5,10-TETRAHYDRONAPHTHO[2,3-C]PYRAN-5,10-DIONE	513558	084018-43-9	91
			Abietic acid $$ 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,4b,5,6,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1R-(1.alpha.,4a.bet	513378	000514-10-3	86

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Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-140c-4jm.D
Acq On    : 12 Oct 2019  14:08
Operator  :
Sample    :
Misc      :
ALS Vial  : 4   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e
```

%#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid			
57	36.967	0.55	D:\DATABASE\DEMO.L 1-Phenanthrenecarboxylic acid, 1,2 ,3,4,4a,9,10,10a-octahydro-1,4a-di methyl-7-(1-methylethyl)-, [1R-(1. alpha.,4a.beta.,10a.alpha.)]- $$ P odocarpa-8,11,13-trien-15-oic acid , 13-isopropyl- $$ Abieta-8,11,13- trien-18-oic acid $$ Abietic acid, dehydro-	503081	001740-19-8	97
			ABIETA-8,11,13-TRIEN-18-OIC ACID $ $ PODOCARPA-8,11,13-TRIEN-15-SAKUR E, 13-ISOPROPYL-	503106	999503-11-8	97
			1-PHENANTHRENECARBOXYLIC ACID, 1,2 ,3,4,4A,9,10,10A-OCTAHYDRO-1,4A-DI METHYL-7-(1-METHYLETHYL)-, [1R-(1. ALPHA.,4A.BETA.,10A.ALPHA.)]- $$ (-)-DEHYDROABIETIC ACID $$ 1,2,3,4, 4A,9,10,10A-OCTAHYDRO-1,4A-DIMETHY L-7-(1-METHYLETHYL)-1-PHENANTHRENE CARBOXYLIC ACID	503110	001740-19-8	95
58	37.032	0.71	D:\DATABASE\DEMO.L 1-Phenanthrenecarboxylic acid, 1,2 ,3,4,4a,9,10,10a-octahydro-1,4a-di methyl-7-(1-methylethyl)-, [1S-(1. alpha.,4a.alpha.,10a.beta.)]- $$ P odocarpa-8,11,13-trien-16-oic acid , 13-isopropyl- $$ Callitrisic aci d $$ 4-Epiabietic acid, dehydro-	503094	005155-70-4	95
			ABIETA-8,11,13-TRIEN-18-OIC ACID $ $ 1-PHENANTHRENECARBOXYLIC ACID, 1 ,2,3,4,4A,9,10,10A-OCTAHYDRO-1,4A- DIMETHYL-7-(1-METHYLETHYL)-, [1S-(1.ALPHA.,4A.ALPHA.,10A.BETA.)]- $$ 13-ISOPROPYLPODOCARPA-8,11,13-TRI EN-16-OIC ACID $$ 4-EPIABIETIC ACI D, DEHYDRO-	503112	005155-70-4	95
			Abietic acid $$ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid	513344	000514-10-3	51
59	37.242	0.59	D:\DATABASE\DEMO.L ABIETA-7,13-DIEN-18-OIC ACID $$ 1- PHENANTHRENECARBOXYLIC ACID, 1,2,3 ,4,4A,4B,5,6,10,10A-DECAHYDRO- $$ 1-PHENANTHRENECARBOXYLIC ACID, 1,2 ,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1, 4A-DIMETHYL-7-(1-METHYLETHYL)-, [1 R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A .ALPHA.)]-	168420	000514-10-3	93
			ABIETA-7,13-DIEN-18-OIC ACID $$ 1-	168419	000514-10-3	93

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-140c-4jm.D
Acq On : 12 Oct 2019 14:08
Operator :
Sample :
Misc :
ALS Vial : 4 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			PHENANTHRENECARBOXYLIC ACID, 1,2,3 ,4,4A,4B,5,6,10,10A-DECAHYDRO- $$ 1-PHENANTHRENECARBOXYLIC ACID, 1,2 ,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1, 4A-DIMETHYL-7-(1-METHYLETHYL)-, [1 R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A .ALPHA.)]-			
			Abietic acid $$ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid	513344	000514-10-3	70
60	37.361	0.24	D:\DATABASE\DEMO.L			
			ABIETA-7,13-DIEN-18-OIC ACID $$ 1- PHENANTHRENECARBOXYLIC ACID, 1,2,3 ,4,4A,4B,5,6,10,10A-DECAHYDRO- $$ 1-PHENANTHRENECARBOXYLIC ACID, 1,2 ,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1, 4A-DIMETHYL-7-(1-METHYLETHYL)-, [1 R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A .ALPHA.)]-	168419	000514-10-3	93
			ABIETA-7,13-DIEN-18-OIC ACID $$ 1- PHENANTHRENECARBOXYLIC ACID, 1,2,3 ,4,4A,4B,5,6,10,10A-DECAHYDRO- $$ 1-PHENANTHRENECARBOXYLIC ACID, 1,2 ,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1, 4A-DIMETHYL-7-(1-METHYLETHYL)-, [1 R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A .ALPHA.)]-	168420	000514-10-3	89
			Palustric acid $$ Podocarpa-8,13-d ien-15-oic acid, 13-isopropyl- $$ 1-Phenanthrenecarboxylic acid, 1,2 ,3,4,4a,5,6,9,10,10a-decahydro-1,4 a-dimethyl-7-(1-methylethyl)-, (1R -(1.alpha.,4a.beta.,10a.alpha.))- $$ 8,13-Abietadien-18-oic acid	513439	001945-53-5	83
61	37.437	0.19	D:\DATABASE\DEMO.L			
			ABIETA-7,13-DIEN-18-OIC ACID $$ 1- PHENANTHRENECARBOXYLIC ACID, 1,2,3 ,4,4A,4B,5,6,10,10A-DECAHYDRO- $$ 1-PHENANTHRENECARBOXYLIC ACID, 1,2 ,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1, 4A-DIMETHYL-7-(1-METHYLETHYL)-, [1 R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A .ALPHA.)]-	168419	000514-10-3	93
			ABIETA-7,13-DIEN-18-OIC ACID $$ 1- PHENANTHRENECARBOXYLIC ACID, 1,2,3 ,4,4A,4B,5,6,10,10A-DECAHYDRO- $$ 1-PHENANTHRENECARBOXYLIC ACID, 1,2 ,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1, 4A-DIMETHYL-7-(1-METHYLETHYL)-, [1 R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A .ALPHA.)]-	168420	000514-10-3	70
			Abietic acid $$ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10,	513344	000514-10-3	64

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-140c-4jm.D
Acq On : 12 Oct 2019 14:08
Operator :
Sample :
Misc :
ALS Vial : 4 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autointl.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid			
62	37.507	0.20	D:\DATABASE\DEMO.L			
			ABIETA-7,13-DIEN-18-OIC ACID $$ 1- PHENANTHRENECARBOXYLIC ACID, 1,2,3 ,4,4A,4B,5,6,10,10A-DECAHYDRO- $$ 1-PHENANTHRENECARBOXYLIC ACID, 1,2 ,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1, 4A-DIMETHYL-7-(1-METHYLETHYL)-, [1 R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A .ALPHA.)]-	168419	000514-10-3	90
			Abietic acid $$ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid	513344	000514-10-3	78
			Abietic acid $$ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid	513378	000514-10-3	78
63	37.707	3.44	D:\DATABASE\DEMO.L			
			Abietic acid $$ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid	513378	000514-10-3	99
			Abietic acid $$ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid	513347	000514-10-3	93
			2,7-PHENANTHRENEDIOL, 9,10-DIHYDRO -3,4,6-TRIMETHOXY- $$ 2,7-DIHYDROX Y-3,4,6-TRIMETHOXY-9,10-DIHYDROPHE NANTRENE	513565	039499-93-9	90
64	38.485	0.05	D:\DATABASE\DEMO.L			
			Abietic acid $$ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid	513378	000514-10-3	92
			Abietic acid $$ 1-Phenanthrenecarb	513347	000514-10-3	91

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsen-140c-4jm.D
Acq On : 12 Oct 2019 14:08
Operator :
Sample :
Misc :
ALS Vial : 4 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid			
			.beta.-Pimaric acid $$ .delta.6,8(14)-Abietadienoic acid $$ l-Pimari c acid $$ l-Sapietic acid	513374	000079-54-9	70
65	38.831	0.11	D:\DATABASE\DEMO.L			
			Abietic acid $$ l-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid	513344	000514-10-3	87
			Abietic acid $$ l-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid	513347	000514-10-3	78
			Abietic acid $$ l-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid	513378	000514-10-3	66
66	39.014	0.20	D:\DATABASE\DEMO.L			
			4-Androsten-6.beta.-ol-3,17-dione	513437	999513-45-0	44
			Abietic acid $$ l-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid	513378	000514-10-3	42
			6-Hydroxy-7-isopropyl-1,4a-dimethy 1-1,2,3,4,4a,9,10,10a-octahydro-1- phenanthrenemethanol, (1.alpha., 4 a.beta., 10a.alpha)- $$ Abieta-8,1 1,13-triene-12,18-diol #	513428	022595-48-8	38

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-160c-1jm.D
Acq On : 10 Oct 2019 11:23
Operator :
Sample :
Misc :
ALS Vial : 2 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

%#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	1.962	5.31	D:\DATABASE\DEMO.L			
			Methyl Alcohol $$ Methanol $$ Carb inol $$ Methyl hydroxide	5073	000067-56-1	2
			METHANOL $$ HYDROXYMETHANE $$ ALCO HOL, METHYL $$ ALCOOL METHYLIQUE	5075	000067-56-1	2
			Methyl Alcohol $$ Methanol $$ Carb inol $$ Methyl hydroxide	5072	000067-56-1	2
2	2.135	0.13	D:\DATABASE\DEMO.L			
			Pentane, 2,4-dimethyl- $$ 2,4-Dime thylpentane	18750	000108-08-7	91
			PENTANE, 2,4-DIMETHYL- $$ 2,4-DIME THYLPENTANE $$ PENTANE, 2,4-DIMETH YL	19002	000108-08-7	80
			PENTANE, 2,4-DIMETHYL- $$ 2,4-DIME THYLPENTANE $$ PENTANE, 2,4-DIMETH YL	18833	000108-08-7	80
3	2.205	11.63	D:\DATABASE\DEMO.L			
			Hexane, 3-methyl- $$ 2-Ethylpentan e $$ 3-Methylhexane	18743	000589-34-4	68
			HEXANE, 3-METHYL- $$ 3-METHYLHEXAN E $$ 2-ETHYLPENTANE $$ HEXANE, 3-M ETHYL	18992	000589-34-4	64
			HEXANE, 3-METHYL- $$ 3-METHYLHEXAN E $$ 2-ETHYLPENTANE $$ HEXANE, 3-M ETHYL	18994	000589-34-4	64
4	2.243	4.41	D:\DATABASE\DEMO.L			
			Cyclopentane, 1,3-dimethyl- $$ 1,3 -Dimethylcyclopentane	101343	002453-00-1	91
			Cyclopentane, 1,3-dimethyl-, cis- $$ cis-1,3-Dimethylcyclopentane $$ 1,3-Dimethylcyclopentane cis $$ 1 ,3-Dimethylcyclopentane #	62231	002532-58-3	91
			1,3-DIMETHYLCYCLOPENTANE $$ CYCLOP ENTANE, 1,3-DIMETHYL-, CIS- $$ 1,3 -DIMETHYLCYCLOPENTANE (CIS) $$ 1,3 -DIMETHYLCYCLOPENTANE CIS	62286	002532-58-3	91
5	2.335	6.72	D:\DATABASE\DEMO.L			
			CYCLOHEXANE, METHYL- $$ METHYLCYCL OHEXANE $$ 1-METHYLCYCLOHEXANE $$ CYCLOHEXANE, METHYL	141469	000108-87-2	96
			CYCLOHEXANE, METHYL- $$ METHYLCYCL OHEXANE $$ 1-METHYLCYCLOHEXANE $$ CYCLOHEXANE, METHYL	141470	000108-87-2	95
			Cyclohexane, methyl- $$ Cyclohexyl methane $$ Hexahydrotoluene $$ Met hylcyclohexane	141386	000108-87-2	94
6	2.421	67.95	D:\DATABASE\DEMO.L			
			Toluene $$ Benzene, methyl $$ Meth acide $$ Methylbenzene	158580	000108-88-3	91
			BENZENE, METHYL- $$ METHYLBENZENE $$ TOLUENE $$ ANTISAL 1A	158622	000108-88-3	91
			Toluene $$ Benzene, methyl $$ Meth acide $$ Methylbenzene	158581	000108-88-3	87

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Data Path : F:\DATA MS\daa\
Data File : WLM-10prsen-160c-1jm.D
Acq On    : 10 Oct 2019  11:23
Operator  :
Sample    :
Misc      :
ALS Vial  : 2   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autointl.e

#     RT  Area%          Library/ID                    Ref#     CAS#   Qual
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7   2.745  0.84 D:\DATABASE\DEMO.L
               ETHYLCYCLOHEXANE $$ ETHYLCYCLOHEXA  54425 001678-91-7 70
               Cyclohexane, ethyl- $$ Ethylcycloh 141506 001678-91-7 70
               exane
               Cyclohexane, ethyl- $$ Ethylcycloh 141508 001678-91-7 70
               exane

8  33.499  0.09 D:\DATABASE\DEMO.L
               KAURA-5,16-DIEN-18-OL $$ KAURA-5,1 492904 023837-99-2 72
               6-DIEN-18(OR 19)-OL $$ KAURA-5,16-
               DIEN-19-OL
               PHENANTHRENE, 7-ETHENYL-1,2,3,4,4A 481161 018319-61-4 59
               ,5,6,7,8,9,10,10A-DODECAHYDRO-1,1,
               4A,7-TETRAMETHYL-, [4AS-(4A.ALPHA.
               ,7.ALPHA.,10A.BETA.)]- $$ PIMARA-8
               (9),15-DIENE $$ PODOCARP-8-ENE, 13
               .ALPHA.-METHYL-13-VINYL-
               Kaura-5,16-dien-18(or 19)-ol $$ Ka 492860 023837-99-2 55
               ura-5,16-dien-18-ol #

9  35.476  0.63 D:\DATABASE\DEMO.L
               PHENOL, 5-[2-(3-HYDROXY-4-METHOXYP 513563 111394-45-7 83
               HENYL)ETHENYL]-2,3-DIMETHOXY-, (Z)
               - $$ 2,3-DIMETHOXY-5-[2-(3-HYDROXY
               -4-METHOXYPHENYL)ETHENYL]PHENOL (Z
               ) $$ COMBRETASTATIN A3
               Xanthen-9-one, 1-hydroxy-3,5,8-tri 504583 049599-09-9 56
               methoxy- $$ 5,8-Dimethylbellidifol
               in $$ 1-Hydroxy-3,5,8-trimethoxyxa
               nthen-9-one $$ 1-Hydroxy-3,5,8-tri
               methoxy-9H-xanthen-9-one #
               1-[1-(4-METHYLTHIO)HEXYLIDENE]-4-P 504561 113035-73-7 52
               HENYLCYCLOHEXANE

0  35.751  0.14 D:\DATABASE\DEMO.L
               DEHYDROABIETIC ACID                464556 000000-00-0 97
               METHYL ABIETA-8,11,13-TRIEN-18-OAT 464550 001235-74-1 94
               E $$ 1-PHENANTHRENECARBOXYLIC ACID
               , 1,2,3,4,4A,9,10,10A-OCTAHYDRO-1,
               4A-DIMETHYL-7-(1-METHYLETHYL)-, ME
               THYL ESTER, [1R-(1.ALPHA.,4A.BETA.
               ,10A.ALPHA.)]- $$ DEHYDROABIETIC A
               CID METHYL ESTER $$ METHYL DEHYDRO
               ABIETATE
               1-Phenanthrenecarboxylic acid, 1,2 464538 001235-74-1 94
               ,3,4,4a,9,10,10a-octahydro-1,4a-di
               methyl-7-(1-methylethyl)-, methyl
               ester, [1R-(1.alpha.,4a.beta.,10a.
               alpha.)]- $$ Podocarpa-8,11,13-tri
               en-15-oic acid, 13-isopropyl-, met
               hyl ester $$ Methyl dehydroabietat

1  36.092  0.17 D:\DATABASE\DEMO.L
               Phenol, 2,4-bis(1-phenylethyl)- $$ 504578 002769-94-0 68
                2,4-Bis(1-phenylethyl)phenol #
               3-((1-Amino-2-naphthyl)methylene)- 504402 999504-41-4 44
               2-benzofuran-1(3H)-one peak 1
               PIMARA-8(14),15-DIEN-18-OIC ACID $ 258698 000127-27-5 43
               $ 1-PHENANTHRENECARBOXYLIC ACID, 7
```

```
Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-160c-1jm.D
Acq On    : 10 Oct 2019  11:23
Operator  :
Sample    :
Misc      :
ALS Vial  : 2   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L              Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#     RT  Area%          Library/ID                  Ref#     CAS#   Qual
                  -ETHENYL-1,2,3,4,4A,4B,5,6,7,9,10,
                  10A-DODECAHYDRO-1,4A,7-TRIMETHYL-,
                   [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,
                  7.BETA.,10A.ALPHA.)]- $$ (+)-PIMAR
                  IC ACID $$ .ALPHA.-PIMARIC ACID

12  36.383  0.05 D:\DATABASE\DEMO.L
                  METHYL ABIETA-7,13-DIEN-18-OATE $$ 258918 000127-25-3 95
                   1-PHENANTHRENECARBOXYLIC ACID, 1,
                  2,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1
                  ,4A-DIMETHYL-7-(1-METHYLETHYL)-, M
                  ETHYL ESTER, [1R-(1.ALPHA.,4A.BETA
                  .,4B.ALPHA.,10A.ALPHA.)]- $$ ABALY
                  N $$ ABIETIC ACID METHYL ESTER
                  Methyl abietate $$ 1-Phenanthrenec 258889 000127-25-3 95
                  arboxylic acid, 1,2,3,4,4a,4b,5,6,
                  10,10a-decahydro-1,4a-dimethyl-7-(
                  1-methylethyl)-, methyl ester, [1R
                  -(1.alpha.,4a.beta.,4b.alpha.,10a.
                  alpha.)]- $$ Podocarpa-7,13-dien-1
                  5-oic acid, 13-isopropyl-, methyl
                  ester $$ Abalyn
                  METHYL ABIETA-7,13-DIEN-18-OATE $$ 480551 000127-25-3 93
                   1-PHENANTHRENECARBOXYLIC ACID, 1,
                  2,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1
                  ,4A-DIMETHYL-7-(1-METHYLETHYL)-, M
                  ETHYL ESTER, [1R-(1.ALPHA.,4A.BETA
                  .,4B.ALPHA.,10A.ALPHA.)]- $$ ABALY
                  N $$ ABIETIC ACID METHYL ESTER

13  36.589  0.13 D:\DATABASE\DEMO.L
                  KAUR-16-EN-18-OIC ACID $$ KAUR-16- 168418 020316-84-1 87
                  EN-18-OIC ACID, (4.BETA.)- $$ (-)-
                  KAURNENOIC ACID $$ (4-BETA)-KAUR-1
                  6-EN-18-OIC ACID
                  Phenol, 2,4-bis(1-phenylethyl)- $$ 504578 002769-94-0 83
                   2,4-Bis(1-phenylethyl)phenol #
                  Androst-5-en-17-ol, 4,4-dimethyl-  513436 999513-44-9 51

14  36.756  0.03 D:\DATABASE\DEMO.L
                  (7-ISOPROPYL-1,4-DIMETHYL-2-AZULEN 513663 039665-56-0 80
                  YL)(PHENYL)METHANONE $$ METHANONE,
                   [1,4-DIMETHYL-7-(1-METHYLETHYL)-2
                  -AZULENYL]PHENYL- $$ 2-BENZOYLGUAI
                  AZULENE
                  Methanone, [1,4-dimethyl-7-(1-meth 513367 039665-56-0 80
                  ylethyl)-2-azulenyl]phenyl- $$ 2-B
                  enzoylguaiazulene $$ (7-Isopropyl-
                  1,4-dimethyl-2-azulenyl)(phenyl)me
                  thanone #
                  Palustric acid $$ Podocarpa-8,13-d 513439 001945-53-5 64
                  ien-15-oic acid, 13-isopropyl- $$
                  1-Phenanthrenecarboxylic acid, 1,2
                  ,3,4,4a,5,6,9,10,10a-decahydro-1,4
                  a-dimethyl-7-(1-methylethyl)-, (1R
                  -(1.alpha.,4a.beta.,10a.alpha.))-
                  $$ 8,13-Abietadien-18-oic acid

15  36.950  0.06 D:\DATABASE\DEMO.L
```

Library Search Report

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-160c-1jm.D
Acq On : 10 Oct 2019 11:23
Operator :
Sample :
Misc :
ALS Vial : 2 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

?k#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			ABIETA-8,11,13-TRIEN-18-OIC ACID $ $ PODOCARPA-8,11,13-TRIEN-15-SAEURE, 13-ISOPROPYL-	503106	999503-11-8	95
			1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1R-(1.alpha.,4a.beta.,10a.alpha.)]- $$ Podocarpa-8,11,13-trien-15-oic acid, 13-isopropyl- $$ Abieta-8,11,13-trien-18-oic acid $$ Abietic acid, dehydro-	503093	001740-19-8	95
			1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,9,10,10A-OCTAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL)-, [1R-(1.ALPHA.,4A.BETA.,10A.ALPHA.)]- $$ (-)-DEHYDROABIETIC ACID $$ 1,2,3,4,4A,9,10,10A-OCTAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL)-1-PHENANTHRENECARBOXYLIC ACID	503110	001740-19-8	95
16	37.015	0.14	D:\DATABASE\DEMO.L ABIETA-8,11,13-TRIEN-18-OIC ACID $ $ PODOCARPA-8,11,13-TRIEN-15-SAEURE, 13-ISOPROPYL-	503106	999503-11-8	78
			1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1R-(1.alpha.,4a.beta.,10a.alpha.)]- $$ Podocarpa-8,11,13-trien-15-oic acid, 13-isopropyl- $$ Abieta-8,11,13-trien-18-oic acid $$ Abietic acid, dehydro-	503081	001740-19-8	56
			ABIETA-8,11,13-TRIEN-18-OIC ACID $ $ 1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,9,10,10A-OCTAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL)-, [1S-(1.ALPHA.,4A.ALPHA.,10A.BETA.)]- $$ 13-ISOPROPYLPODOCARPA-8,11,13-TRIEN-16-OIC ACID $$ 4-EPIABIETIC ACID, DEHYDRO-	503112	005155-70-4	53
17	37.669	1.48	D:\DATABASE\DEMO.L Abietic acid $$ 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,4b,5,6,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1R-(1.alpha.,4a.beta.,4b.alpha.,10a.alpha.)]- $$ Podocarpa-7,13-dien-15-oic acid, 13-isopropyl- $$ L-abietic acid	513378	000514-10-3	99
			Abietic acid $$ 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,4b,5,6,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1R-(1.alpha.,4a.beta.,4b.alpha.,10a.alpha.)]- $$ Podocarpa-7,13-dien-15-oic acid, 13-isopropyl- $$ L-abietic acid	513344	000514-10-3	96
			Abietic acid $$ 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,4b,5,6,10,10a-decahydro-1,4a-dimethyl-7-(1-m	513347	000514-10-3	94

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-160c-1jm.D
Acq On : 10 Oct 2019 11:23
Operator :
Sample :
Misc :
ALS Vial : 2 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid			
18	38.830	0.08	D:\DATABASE\DEMO.L 1,4-DIHYDRO-9-ISOPROPYLIDENE-5,6,7 ,8-TETRAMETHOXY-1,4-METHANONAPHTHA LENE	513581	000000-00-0	64
			Benzofuran-2-one, 4-amino-2,3-dihy dro-3,3-dimethyl-	380133	999380-13-7	25
			8-Chloro-2-methylquinoline $$ 8-Ch loroquinaldine $$ Quinaldine, 8-ch loro- $$ Quinoline, 8-chloro-2-met hyl-	380142	003033-82-7	18

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-160c-2jmu.D
Acq On : 9 Oct 2019 21:16
Operator :
Sample :
Misc :
ALS Vial : 4 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

k#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	1.994	0.08	D:\DATABASE\DEMO.L			
			ETHANOL $$ HYDROXYETHANE $$ 1-HYDR OXYETHANE $$ ABSOLUTE ALCOHOL	5097	000064-17-5	86
			ETHANOL $$ HYDROXYETHANE $$ 1-HYDR OXYETHANE $$ ABSOLUTE ALCOHOL	5099	000064-17-5	86
			ETHANOL $$ HYDROXYETHANE $$ 1-HYDR OXYETHANE $$ ABSOLUTE ALCOHOL	5093	000064-17-5	78
2	2.135	0.04	D:\DATABASE\DEMO.L			
			Pentane, 2,4-dimethyl- $$ 2,4-Dime thylpentane	18750	000108-08-7	87
			Pentane, 2,4-dimethyl- $$ 2,4-Dime thylpentane	18799	000108-08-7	86
			PENTANE, 2,4-DIMETHYL- $$ 2,4-DIME THYLPENTANE $$ PENTANE, 2,4-DIMETH YL	19001	000108-08-7	86
3	2.205	7.70	D:\DATABASE\DEMO.L			
			Hexane, 3-methyl- $$ 2-Ethylpentan e $$ 3-Methylhexane	18811	000589-34-4	91
			HEXANE, 3-METHYL- $$ 3-METHYLHEXAN E $$ 2-ETHYLPENTANE $$ HEXANE, 3-M ETHYL	18994	000589-34-4	87
			HEXANE, 3-METHYL- $$ 3-METHYLHEXAN E $$ 2-ETHYLPENTANE $$ HEXANE, 3-M ETHYL	18824	000589-34-4	74
4	2.243	3.27	D:\DATABASE\DEMO.L			
			Cyclopentane, 1,3-dimethyl- $$ 1,3 -Dimethylcyclopentane	101343	002453-00-1	94
			1,3-DIMETHYLCYCLOPENTANE $$ CYCLOP ENTANE, 1,3-DIMETHYL-, CIS- $$ 1,3 -DIMETHYLCYCLOPENTANE (CIS) $$ 1,3 -DIMETHYLCYCLOPENTANE CIS	62286	002532-58-3	91
			Cyclopentane, 1,3-dimethyl-, cis- $$ cis-1,3-Dimethylcyclopentane $$ 1,3-Dimethylcyclopentane cis $$ 1 ,3-Dimethylcyclopentane #	62231	002532-58-3	91
5	2.335	6.35	D:\DATABASE\DEMO.L			
			CYCLOHEXANE, METHYL- $$ METHYLCYCL OHEXANE $$ 1-METHYLCYCLOHEXANE $$ CYCLOHEXANE, METHYL	141469	000108-87-2	96
			CYCLOHEXANE, METHYL- $$ METHYLCYCL OHEXANE $$ 1-METHYLCYCLOHEXANE $$ CYCLOHEXANE, METHYL	141470	000108-87-2	95
			Cyclohexane, methyl- $$ Cyclohexyl methane $$ Hexahydrotoluene $$ Met hylcyclohexane	141386	000108-87-2	94
6	2.421	73.40	D:\DATABASE\DEMO.L			
			BENZENE, METHYL- $$ METHYLBENZENE $$ TOLUENE $$ ANTISAL 1A	158622	000108-88-3	91
			Toluene $$ Benzene, methyl $$ Meth acide $$ Methylbenzene	158580	000108-88-3	91
			METHYLBENZENE $$ BENZENE,-METHYL	158608	000108-88-3	90
7	2.745	1.19	D:\DATABASE\DEMO.L			
			CYCLOHEXANE, ETHYL- $$ ETHYLCYCLOH	141561	001678-91-7	93

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Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-160c-2jmu.D
Acq On    :  9 Oct 2019  21:16
Operator  :
Sample    :
Misc      :
ALS Vial  : 4   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e

%#     RT  Area%          Library/ID                    Ref#     CAS#   Qual
                  EXANE $$ ETHYL CYCLOHEXANE $$ ETHY
                  LCYCLOHEXAN
                  Cyclohexane, ethyl- $$ Ethylcycloh 141506 001678-91-7 93
                  exane
                  CYCLOHEXANE, ETHYL- $$ ETHYLCYCLOH 141564 001678-91-7 81
                  EXANE $$ ETHYL CYCLOHEXANE $$ ETHY
                  LCYCLOHEXAN

 8  17.320  0.06 D:\DATABASE\DEMO.L
                  2H-2,4a-Methanonaphthalene, 1,3,4, 350641 001135-66-6 99
                  5,6,7-hexahydro-1,1,5,5-tetramethy
                  l-, (2S)- $$ 2H-2,4a-Methanonaphth
                  alene, 1,3,4,5,6,7-hexahydro-1,1,5
                  ,5-tetramethyl-, (2S,4aR)-(-)- $$
                  Isolongifolene $$ (-)-Isolongifoli
                  ne
                  2H-2,4a-Methanonaphthalene, 1,3,4, 350640 001135-66-6 99
                  5,6,7-hexahydro-1,1,5,5-tetramethy
                  l-, (2S)- $$ 2H-2,4a-Methanonaphth
                  alene, 1,3,4,5,6,7-hexahydro-1,1,5
                  ,5-tetramethyl-, (2S,4aR)-(-)- $$
                  Isolongifolene $$ (-)-Isolongifoli
                  ne
                  2H-2,4A-METHANONAPHTHALENE, 1,3,4, 350804 001135-66-6 99
                  5,6,7-HEXAHYDRO-1,1,5,5-TETRAMETHY
                  L-, (2S)- $$ (-)-ISOLONGIFOLENE $$
                   (-)-ISOLONGIPOLINE $$ (2S)-1,3,4,
                  5,6,7-HEXAHYDRO-1,1,5,5-TETRAMETHY
                  L-2H-2,4A-METHANONAPHTHALENE

 9  30.306  0.06 D:\DATABASE\DEMO.L
                  PIMARA-8,15-DIENE $$ PHENANTHRENE, 481165 055255-56-6 94
                   7-ETHENYL-1,2,3,4,4A,5,6,7,8,9,10
                  ,10A-DODECAHYDRO-1,1,4A,7-TETRAMET
                  HYL- $$ 7.ALPHA.-ETHENYL-1,1,4A,7.
                  BETA.-TETRAMETHYL-1,2,3,4,4A,5,6,7
                  ,8,9,10,10A-DODECAHYDROPHENANTHREN
                  Phenanthrene, 7-ethenyl-1,2,3,4,4a 481092 055255-56-6 94
                  ,5,6,7,8,9,10,10a-dodecahydro-1,1,
                  4a,7-tetramethyl- $$ Pimara-8,15-d
                  iene #
                  ENT-PIMARA-8,15-DIENE              481166 021561-92-2 91

10  33.493  0.24 D:\DATABASE\DEMO.L
                  (+)1A7,4A,9,10,10A-DODECAHYDRO-1,4 481209 000000-00-0 53
                  A,7-TRIMETHYL-7-VINYL-1-PHENANTHRE
                  NCARBALDEHYDSHYL 4,AZC.BETA.THIOME
                  THYL](12-YL2ETHYLTHIOYLENC1ETHYLDE
                  THYL3-YLAPHTHC]TAOXM.BETA.ANO6, [U
                  CHOALFPAL[YL9
                  1,2-BIS(4-ETHOXYPHENYL)DIAZENE 1-O 223740 004792-83-0 46
                  XIDE $$ 4, 4'-BIS(ETHOXY)AZOXYBENZ
                  ENE $$ 4,4'-AZOXYDIPHENETOLE $$ 4,
                  4'-AZOXYPHENETOLE
                  PREGN-7-ENE, (5.ALPHA.)- $$ 5.ALPH 492909 063518-70-7 45
                  A.-PREGN-7-ENE

11  33.790  0.04 D:\DATABASE\DEMO.L
                  Diazene, bis(4-ethoxyphenyl)-, 1-o 223735 004792-83-0 44
```

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsen-160c-2jmu.D
Acq On : 9 Oct 2019 21:16
Operator :
Sample :
Misc :
ALS Vial : 4 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autointl.e

%#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			xide $$ Azoxybenzene, 4,4'-diethoxy- $$ p,p'-Azoxyphenetole $$ 4,4'-Azoxydiphenetole			
			1,2-BIS(4-ETHOXYPHENYL)DIAZENE 1-OXIDE $$ 4, 4'-BIS(ETHOXY)AZOXYBENZENE $$ 4,4'-AZOXYDIPHENETOLE $$ 4, 4'-AZOXYPHENETOLE	223740	004792-83-0	44
			RETINOL $$ (ALL-E)-3,7-DIMETHYL-9-(2,6,6-TRIMETHYL-1-CYCLOHEXEN-1-YL)-2,4,6,8-NONATETRAEN-1-OL $$ .ALPHA.LIN $$ .ALPHA.STEROL	13722	000068-26-8	42
12	33.866	0.11	D:\DATABASE\DEMO.L			
			10,13-DIMETHYL-4,5,6,7,8,9,10,11,12,13,14,15-DODECAHYDRO-1H-CYCLOPENTA[A]PHENANTHRENE $$ ANDROSTA-2,16-DIENE	466180	999466-18-8	95
			1-Methyl-10,18-bisnorabieta-8,11,13-triene	466158	999466-16-6	94
			4-(N-METHYLAMINO)-6,7-(1,2,3,4-TETRAHYDRO-1,1,4,4-TETRAMETHYLBENZO)INDOLE	466219	000000-00-0	83
13	34.309	0.06	D:\DATABASE\DEMO.L			
			1-Phenanthrenecarboxylic acid, 7-ethenyl-1,2,3,4,4a,5,6,7,8,9,10,10a-dodecahydro-1,4a,7-trimethyl-, methyl ester, [1R-(1.alpha.,4a.beta.,7.beta.,10a.alpha.)]- $$ Podocarp-8-en-15-oic acid, 13.alpha.-methyl-13-vinyl-, methyl ester	466507	003582-26-1	55
			3,3,4,5,5,8-HEXAMETHYL-3,5,6,7-TETRAHYDRO-S-INDACEN-1(2H)-ONE $$ S-INDACEN-1(2H)-ONE, 3,5,6,7-TETRAHYDRO-3,3,4,5,5,8-HEXAMETHYL- $$ 3,3,4,5,5,8-HEXAMETHYL-1-S-HYDRINDACENONE	466221	038754-94-8	46
			4b,8-Dimethyl-2-isopropylphenanthrene, 4b,5,6,7,8,8a,9,10-octahydro-	466159	999466-16-7	46
14	34.541	0.10	D:\DATABASE\DEMO.L			
			1,2,4-TRIAZOLO(3,4-C)(1,2,4)-BENZOTRIAZIN-1(5H)-ONE	282352	000000-00-0	53
			Phenanthrene, 7-ethenyl-1,2,3,4,4a,5,6,7,8,9,10,10a-dodecahydro-1,1,4a,7-tetramethyl- $$ Pimara-8,15-diene #	481092	055255-56-6	46
			1,1,4A-TRIMETHYL-6-METHYLENE-5-(3-METHYLENE-4-PENTENYL)DECAHYDRONAPHTHALENE $$ NAPHTHALENE, DECAHYDRO-1,1,4A-TRIMETHYL-6-METHYLENE-5-(3-METHYLENE-4-PENTENYL)-, [4AS-(4A.ALPHA.,5.ALPHA.,8A.BETA.)]- $$ LABDA-8(20),13(16),14-TRIENE $$ SCLARE	481157	000511-02-4	42
15	35.400	0.03	D:\DATABASE\DEMO.L			
			KAUR-16-EN-18-OIC ACID, 6,7-DIHYDROXY-, .GAMMA.-LACTONE, (4.ALPHA.,6.ALPHA.,7.ALPHA.)- $$ 7.ALPHA.-HYD	229294	015959-13-4	50

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-160c-2jmu.D
Acq On : 9 Oct 2019 21:16
Operator :
Sample :
Misc :
ALS Vial : 4 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

k#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			ROXYKAURENOLIDE $$ 7ALPHA-HYDROXYK AURENOLIDE $$ KAUR-16-EN-18-OIC AC ID, 6,7-DIHYDROXY-, GAMMA-LACTONE, (4ALPHA,6ALPHA,7ALPHA)-			
			2-(ACETYLAMINO)PHENYL ACETATE $$ A CETIC ACID 2-ACETYLAMINO-PHENYL ES TER	227934	999227-93-7	47
			p-Heptyloxyaniline $$ 4-n-Heptylox yaniline	228109	039905-44-7	47
16	35.503	1.61	D:\DATABASE\DEMO.L			
			O-HYDROGEN PERDEUTERIO HEXADECANOI C ACID	504545	039756-30-4	90
			Phenol, 2,4-bis(1-phenylethyl)- $$ 2,4-Bis(1-phenylethyl)phenol #	504578	002769-94-0	55
			Xanthen-9-one, 1-hydroxy-3,5,8-tri methoxy- $$ 5,8-Dimethylbellidifol in $$ 1-Hydroxy-3,5,8-trimethoxyxa nthen-9-one $$ 1-Hydroxy-3,5,8-tri methoxy-9H-xanthen-9-one #	504583	049599-09-9	55
17	35.757	0.32	D:\DATABASE\DEMO.L			
			DEHYDROABIETIC ACID	464556	000000-00-0	97
			METHYL ABIETA-8,11,13-TRIEN-18-OAT E $$ 1-PHENANTHRENECARBOXYLIC ACID , 1,2,3,4,4A,9,10,10A-OCTAHYDRO-1, 4A-DIMETHYL-7-(1-METHYLETHYL)-, ME THYL ESTER, [1R-(1.ALPHA.,4A.BETA. ,10A.ALPHA.)]- $$ DEHYDROABIETIC A CID METHYL ESTER $$ METHYL DEHYDRO ABIETATE	464549	001235-74-1	95
			METHYL ABIETA-8,11,13-TRIEN-18-OAT E $$ 1-PHENANTHRENECARBOXYLIC ACID , 1,2,3,4,4A,9,10,10A-OCTAHYDRO-1, 4A-DIMETHYL-7-(1-METHYLETHYL)-, ME THYL ESTER, [1R-(1.ALPHA.,4A.BETA. ,10A.ALPHA.)]- $$ DEHYDROABIETIC A CID METHYL ESTER $$ METHYL DEHYDRO ABIETATE	464550	001235-74-1	94
18	35.930	0.06	D:\DATABASE\DEMO.L			
			PHENOL, 5-[2-(3-HYDROXY-4-METHOXYP HENYL)ETHENYL]-2,3-DIMETHOXY-, (Z) - $$ 2,3-DIMETHOXY-5-[2-(3-HYDROXY -4-METHOXYPHENYL)ETHENYL]PHENOL (Z) $$ COMBRETASTATIN A3	513563	111394-45-7	80
			Androst-5-en-17-ol, 4,4-dimethyl-	513436	999513-44-9	46
			PIMARA-8(14),15-DIEN-18-OIC ACID $ $ 1-PHENANTHRENECARBOXYLIC ACID, 7 -ETHENYL-1,2,3,4,4A,4B,5,6,7,9,10, 10A-DODECAHYDRO-1,4A,7-TRIMETHYL-, [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA., 7.BETA.,10A.ALPHA.)]- $$ (+)-PIMAR IC ACID $$ .ALPHA.-PIMARIC ACID	504608	000127-27-5	35
19	36.027	0.06	D:\DATABASE\DEMO.L			
			4,4"-DIMETHYL-1,1':3',1'-TERPHENYL -2'-CARBOXYLIC ACID	513657	000000-00-0	55
			Pimaric acid $$ 1-Phenanthrenecarb	466434	000127-27-5	42

```
Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-160c-2jmu.D
Acq On    :  9 Oct 2019  21:16
Operator  :
Sample    :
Misc      :
ALS Vial  : 4   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e
```

t#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			oxylic acid, 7-ethenyl-1,2,3,4,4a, 4b,5,6,7,9,10,10a-dodecahydro-1,4a ,7-trimethyl-, [1R-(1.alpha.,4a.be ta.,4b.alpha.,7.beta.,10a.alpha.)] - $$ Podocarp-8(14)-en-15-oic acid , 13.alpha.-methyl-13-vinyl- $$ D- pimaric acid			
			ABIETA-7,13-DIEN-18-OIC ACID $$ 1- PHENANTHRENECARBOXYLIC ACID, 1,2,3 ,4,4A,4B,5,6,10,10A-DECAHYDRO- $$ 1-PHENANTHRENECARBOXYLIC ACID, 1,2 ,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1, 4A-DIMETHYL-7-(1-METHYLETHYL)-, [1 R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A .ALPHA.)]-	168419	000514-10-3	41
20	36.102	0.19	D:\DATABASE\DEMO.L			
			PHENOL, 5-[2-(3-HYDROXY-4-METHOXYP HENYL)ETHENYL]-2,3-DIMETHOXY-, (Z) - $$ 2,3-DIMETHOXY-5-[2-(3-HYDROXY -4-METHOXYPHENYL)ETHENYL]PHENOL (Z) $$ COMBRETASTATIN A3	513563	111394-45-7	90
			Androst-5-en-17-ol, 4,4-dimethyl-	513436	999513-44-9	50
			Abietic acid $$ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid	513378	000514-10-3	38
21	36.383	0.15	D:\DATABASE\DEMO.L			
			Methyl abietate $$ 1-Phenanthrenec arboxylic acid, 1,2,3,4,4a,4b,5,6, 10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, methyl ester, [1R -(1.alpha.,4a.beta.,4b.alpha.,10a. alpha.)]- $$ Podocarpa-7,13-dien-1 5-oic acid, 13-isopropyl-, methyl ester $$ Abalyn	258889	000127-25-3	99
			METHYL ABIETA-7,13-DIEN-18-OATE $$ 1-PHENANTHRENECARBOXYLIC ACID, 1, 2,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1 ,4A-DIMETHYL-7-(1-METHYLETHYL)-, M ETHYL ESTER, [1R-(1.ALPHA.,4A.BETA .,4B.ALPHA.,10A.ALPHA.)]- $$ ABALY N $$ ABIETIC ACID METHYL ESTER	258918	000127-25-3	99
			METHYL ABIETA-7,13-DIEN-18-OATE $$ 1-PHENANTHRENECARBOXYLIC ACID, 1, 2,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1 ,4A-DIMETHYL-7-(1-METHYLETHYL)-, M ETHYL ESTER, [1R-(1.ALPHA.,4A.BETA .,4B.ALPHA.,10A.ALPHA.)]- $$ ABALY N $$ ABIETIC ACID METHYL ESTER	480551	000127-25-3	95
22	36.508	0.02	D:\DATABASE\DEMO.L			
			Phenol, 2,4-bis(1-phenylethyl)- $$ 2,4-Bis(1-phenylethyl)phenol #	504578	002769-94-0	83
			Pimaric acid $$ 1-Phenanthrenecarb	466434	000127-27-5	55

```
Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-160c-2jmu.D
Acq On    :  9 Oct 2019  21:16
Operator  :
Sample    :
Misc      :
ALS Vial  : 4   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e

#     RT  Area%          Library/ID                    Ref#     CAS#   Qual
                                                      ------------------------
              oxylic acid, 7-ethenyl-1,2,3,4,4a,
              4b,5,6,7,9,10,10a-dodecahydro-1,4a
              ,7-trimethyl-, [1R-(1.alpha.,4a.be
              ta.,4b.alpha.,7.beta.,10a.alpha.)]
              - $$ Podocarp-8(14)-en-15-oic acid
              , 13.alpha.-methyl-13-vinyl- $$ D-
              pimaric acid
              PINE ROSIN MIXTURE                  504612 000000-00-0 51

3  36.605  0.25 D:\DATABASE\DEMO.L
              KAUR-16-EN-18-OIC ACID $$ KAUR-16-  168418 020316-84-1 87
              EN-18-OIC ACID, (4.BETA.)- $$ (-)-
              KAURNENOIC ACID $$ (4-BETA)-KAUR-1
              6-EN-18-OIC ACID
              Phenol, 2,4-bis(1-phenylethyl)- $$  504578 002769-94-0 80
               2,4-Bis(1-phenylethyl)phenol #
              Androst-5-en-17-ol, 4,4-dimethyl-   513436 999513-44-9 66

4  36.761  0.11 D:\DATABASE\DEMO.L
              Palustric acid $$ Podocarpa-8,13-d  513439 001945-53-5 64
              ien-15-oic acid, 13-isopropyl- $$
              1-Phenanthrenecarboxylic acid, 1,2
              ,3,4,4a,5,6,9,10,10a-decahydro-1,4
              a-dimethyl-7-(1-methylethyl)-, (1R
              -(1.alpha.,4a.beta.,10a.alpha.))-
              $$ 8,13-Abietadien-18-oic acid
              Phenol, 2,4-bis(1-phenylethyl)- $$  504578 002769-94-0 60
               2,4-Bis(1-phenylethyl)phenol #
              Abietic acid $$ 1-Phenanthrenecarb  513344 000514-10-3 49
              oxylic acid, 1,2,3,4,4a,4b,5,6,10,
              10a-decahydro-1,4a-dimethyl-7-(1-m
              ethylethyl)-, [1R-(1.alpha.,4a.bet
              a.,4b.alpha.,10a.alpha.)]- $$ Podo
              carpa-7,13-dien-15-oic acid, 13-is
              opropyl- $$ L-abietic acid

5  36.864  0.01 D:\DATABASE\DEMO.L
              1H-NAPHTHO[2,3-C]PYRAN-5,10-DIONE,  513558 084018-43-9 91
               3,4-DIHYDRO-7,9-DIMETHOXY-1,3-DIM
              ETHYL-, CIS-(.+-.)- $$ (+,-)-CIS-7
              ,9-DIMETHOXY-1,3-DIMETHYL-3,4,5,10
              -TETRAHYDRONAPHTHO[2,3-C]PYRAN-5,1
              0-DIONE
              Androst-5-en-17-ol, 4,4-dimethyl-   513436 999513-44-9 83
              KAUR-16-EN-18-OIC ACID $$ KAUR-16-  168418 020316-84-1 70
              EN-18-OIC ACID, (4.BETA.)- $$ (-)-
              KAURNENOIC ACID $$ (4-BETA)-KAUR-1
              6-EN-18-OIC ACID

6  36.983  0.29 D:\DATABASE\DEMO.L
              ABIETA-8,11,13-TRIEN-18-OIC ACID $  503106 999503-11-8 97
              $ PODOCARPA-8,11,13-TRIEN-15-SARUR
              E, 13-ISOPROPYL-
              1-Phenanthrenecarboxylic acid, 1,2  503093 001740-19-8 94
              ,3,4,4a,9,10,10a-octahydro-1,4a-di
              methyl-7-(1-methylethyl)-, [1R-(1.
              alpha.,4a.beta.,10a.alpha.)]- $$ P
              odocarpa-8,11,13-trien-15-oic acid
              , 13-isopropyl- $$ Abieta-8,11,13-
```

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Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-160c-2jmu.D
Acq On    :  9 Oct 2019  21:16
Operator  :
Sample    :
Misc      :
ALS Vial  : 4   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autointl.e
```

#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			trien-18-oic acid $$ Abietic acid, dehydro-			
			1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,9,10,10A-OCTAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL)-, [1R-(1.ALPHA.,4A.BETA.,10A.ALPHA.)]- $$ (-)-DEHYDROABIETIC ACID $$ 1,2,3,4,4A,9,10,10A-OCTAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL)-1-PHENANTHRENECARBOXYLIC ACID	503110	001740-19-8	86
7	37.042	0.42	D:\DATABASE\DEMO.L			
			1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1R-(1.alpha.,4a.beta.,10a.alpha.)]- $$ Podocarpa-8,11,13-trien-15-oic acid, 13-isopropyl- $$ Abieta-8,11,13-trien-18-oic acid $$ Abietic acid, dehydro-	503093	001740-19-8	89
			1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,9,10,10A-OCTAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL)-, [1R-(1.ALPHA.,4A.BETA.,10A.ALPHA.)]- $$ (-)-DEHYDROABIETIC ACID $$ 1,2,3,4,4A,9,10,10A-OCTAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL)-1-PHENANTHRENECARBOXYLIC ACID	503110	001740-19-8	83
			1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1R-(1.alpha.,4a.beta.,10a.alpha.)]- $$ Podocarpa-8,11,13-trien-15-oic acid, 13-isopropyl- $$ Abieta-8,11,13-trien-18-oic acid $$ Abietic acid, dehydro-	503081	001740-19-8	70
8	37.275	0.15	D:\DATABASE\DEMO.L			
			ABIETA-7,13-DIEN-18-OIC ACID $$ 1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,4B,5,6,10,10A-DECAHYDRO- $$ 1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL)-, [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A.ALPHA.)]-	168420	000514-10-3	86
			Abietic acid $$ 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,4b,5,6,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1R-(1.alpha.,4a.beta.,4b.alpha.,10a.alpha.)]- $$ Podocarpa-7,13-dien-15-oic acid, 13-isopropyl- $$ L-abietic acid	513378	000514-10-3	70
			Abietic acid $$ 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,4b,5,6,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1R-(1.alpha.,4a.beta.,4b.alpha.,10a.alpha.)]- $$ Podocarpa-7,13-dien-15-oic acid, 13-is	513344	000514-10-3	66

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-160c-2jmu.D
Acq On : 9 Oct 2019 21:16
Operator :
Sample :
Misc :
ALS Vial : 4 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			opropyl- $$ L-abietic acid			
29	37.734	3.12	D:\DATABASE\DEMO.L			
			Abietic acid $$ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid	513378	000514-10-3	99
			Abietic acid $$ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid	513344	000514-10-3	93
			Abietic acid $$ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid	513347	000514-10-3	90
30	38.825	0.26	D:\DATABASE\DEMO.L			
			Silane, tributylchloro- $$ Tributy lchlorosilane $$ Chlorotributylsil ane	380665	000995-45-9	25
			3-Bromomethyl-2-hydroxy-6-isopropy 1-2,4,6-cycloheptatrien-1-one	380835	999380-83-9	25
			SILANE, TRIBUTYLCHLORO- $$ CHLOROT RIBUTYLSILANE $$ TRIBUTYLCHLOROSIL ANE	380678	000995-45-9	25
31	39.019	0.27	D:\DATABASE\DEMO.L			
			Abietic acid $$ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid	513347	000514-10-3	59
			Abietic acid $$ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid	513378	000514-10-3	46
			Thiazolidin-4-one, 3-(2-furfuryl)- 5-(2-pyridylmethylene)-2-thioxo- $ $ (5E)-3-(2-Furylmethyl)-5-(2-pyri dinylmethylene)-2-thioxo-1,3-thiaz olidin-4-one #	294155	307343-71-1	38

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Data Path : F:\DATA MS\daa\
Data File : WLM-10prsen-160c-3jmu.D
Acq On    :  9 Oct 2019  17:59
Operator  :
Sample    :
Misc      :
ALS Vial  : 3   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#     RT  Area%          Library/ID                  Ref#     CAS#   Qual
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  1   2.000  0.09 D:\DATABASE\DEMO.L
                  ETHANOL $$ HYDROXYETHANE $$ 1-HYDR   5102 000064-17-5 86
                  OXYETHANE $$ ABSOLUTE ALCOHOL
                  ETHANOL $$ HYDROXYETHANE $$ 1-HYDR   5099 000064-17-5 86
                  OXYETHANE $$ ABSOLUTE ALCOHOL
                  ETHANOL $$ HYDROXYETHANE $$ 1-HYDR   5090 000064-17-5 78
                  OXYETHANE $$ 100C.NPA

  2   2.140  0.07 D:\DATABASE\DEMO.L
                  Pentane, 2,4-dimethyl- $$ 2,4-Dime  18750 000108-08-7 91
                  thylpentane
                  Pentane, 2,4-dimethyl- $$ 2,4-Dime  18753 000108-08-7 91
                  thylpentane
                  PENTANE, 2,4-DIMETHYL- $$ 2,4-DIME  19001 000108-08-7 90
                  THYLPENTANE $$ PENTANE, 2,4-DIMETH
                  YL

  3   2.205  9.59 D:\DATABASE\DEMO.L
                  Hexane, 3-methyl- $$ 2-Ethylpentan  18743 000589-34-4 68
                  e $$ 3-Methylhexane
                  HEXANE, 3-METHYL- $$ 3-METHYLHEXAN  18994 000589-34-4 64
                  E $$ 2-ETHYLPENTANE $$ HEXANE, 3-M
                  ETHYL
                  HEPTANE $$ ALIPHATIC HYDROCARBON $  18986 000142-82-5 62
                  $ DIPROPYL METHANE $$ DIPROPYLMETH
                  ANE

  4   2.243  3.88 D:\DATABASE\DEMO.L
                  1,3-DIMETHYLCYCLOPENTANE $$ CYCLOP  62286 002532-58-3 91
                  ENTANE, 1,3-DIMETHYL-, CIS- $$ 1,3
                  -DIMETHYLCYCLOPENTANE (CIS) $$ 1,3
                  -DIMETHYLCYCLOPENTANE CIS
                  Cyclopentane, 1,3-dimethyl-, cis-   62231 002532-58-3 91
                  $$ cis-1,3-Dimethylcyclopentane $$
                   1,3-Dimethylcyclopentane cis $$ 1
                  ,3-Dimethylcyclopentane #
                  Cyclopentane, 1,3-dimethyl- $$ 1,3 101343 002453-00-1 91
                  -Dimethylcyclopentane

  5   2.335  6.78 D:\DATABASE\DEMO.L
                  CYCLOHEXANE, METHYL- $$ METHYLCYCL 141469 000108-87-2 96
                  OHEXANE $$ 1-METHYLCYCLOHEXANE $$
                  CYCLOHEXANE, METHYL
                  CYCLOHEXANE, METHYL- $$ METHYLCYCL 141467 000108-87-2 95
                  OHEXANE $$ 1-METHYLCYCLOHEXANE $$
                  CYCLOHEXANE, METHYL
                  CYCLOHEXANE, METHYL- $$ METHYLCYCL 141470 000108-87-2 95
                  OHEXANE $$ 1-METHYLCYCLOHEXANE $$
                  CYCLOHEXANE, METHYL

  6   2.421 72.51 D:\DATABASE\DEMO.L
                  Toluene $$ Benzene, methyl $$ Meth 158580 000108-88-3 91
                  acide $$ Methylbenzene
                  BENZENE, METHYL- $$ METHYLBENZENE  158622 000108-88-3 91
                  $$ TOLUENE $$ ANTISAL 1A
                  Toluene $$ Benzene, methyl $$ Meth 158579 000108-88-3 90
                  acide $$ Methylbenzene

  7   2.751  1.07 D:\DATABASE\DEMO.L
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Data Path : F:\DATA MS\daa\
Data File : WLM-10prsen-160c-3jmu.D
Acq On    :  9 Oct 2019  17:59
Operator  :
Sample    :
Misc      :
ALS Vial  : 3   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autointl.e

ak#     RT  Area%          Library/ID                  Ref#     CAS#   Qual
                Cyclohexane, ethyl- $$ Ethylcycloh 141506 001678-91-7 93
                exane
                CYCLOHEXANE, ETHYL- $$ ETHYLCYCLOH 141561 001678-91-7 93
                EXANE $$ ETHYL CYCLOHEXANE $$ ETHY
                LCYCLOHEXAN
                Cyclohexane, ethyl- $$ Ethylcycloh 141508 001678-91-7 93
                exane

 8  33.499  0.18 D:\DATABASE\DEMO.L
                KAURA-5,16-DIEN-18-OL $$ KAURA-5,1 492904 023837-99-2 72
                6-DIEN-18(OR 19)-OL $$ KAURA-5,16-
                DIEN-19-OL
                Kaura-5,16-dien-18(or 19)-ol $$ Ka 492860 023837-99-2 53
                ura-5,16-dien-18-ol #
                PHENANTHRENE, 7-ETHENYL-1,2,3,4,4A 481161 018319-61-4 51
                ,5,6,7,8,9,10,10A-DODECAHYDRO-1,1,
                4A,7-TETRAMETHYL-, [4AS-(4A.ALPHA.
                ,7.ALPHA.,10A.BETA.)]- $$ PIMARA-8
                (9),15-DIENE $$ PODOCARP-8-ENE, 13
                .ALPHA.-METHYL-13-VINYL-

 9  33.871  0.08 D:\DATABASE\DEMO.L
                10,13-DIMETHYL-4,5,6,7,8,9,10,11,1 466180 999466-18-8 96
                2,13,14,15-DODECAHYDRO-1H-CYCLOPEN
                TA[A]PHENANTHRENE $$ ANDROSTA-2,16
                -DIENE
                1-Methyl-10,18-bisnorabieta-8,11,1 466158 999466-16-6 94
                3-triene
                3,7-DI-TERT-BUTYL-1-NAPHTHOL       466222 000000-00-0 80

10  34.314  0.05 D:\DATABASE\DEMO.L
                1-Phenanthrenecarboxylic acid, 7-e 466507 003582-26-1 64
                thenyl-1,2,3,4,4a,5,6,7,8,9,10,10a
                -dodecahydro-1,4a,7-trimethyl-, me
                thyl ester, [1R-(1.alpha.,4a.beta.
                ,7.beta.,10a.alpha.)]- $$ Podocarp
                -8-en-15-oic acid, 13.alpha.-methy
                l-13-vinyl-, methyl ester
                METHYL PIMARA-8,15-DIEN-18-OATE $$ 466513 003582-26-1 55
                 1-PHENANTHRENECARBOXYLIC ACID, 7-
                ETHENYL-1,2,3,4,4A,5,6,7,8,9,10,10
                A-DODECAHYDRO-1,4A,7-TRIMETHYL-, M
                ETHYL ESTER, [1R-(1.ALPHA.,4A.BETA
                .,7.BETA.,10A.ALPHA.)]- $$ METHYL
                8,15-PIMARADIEN-18-OATE
                METHYL PIMARA-8,15-DIEN-18-OATE $$ 466512 019907-21-2 42
                 1-PHENANTHRENECARBOXYLIC ACID, 7-
                ETHENYL-1,2,3,4,4A,5,6,7,8,9,10,10
                A-DODECAHYDRO-1,4A,7-TRIMETHYL-, M
                ETHYL ESTER, [1R-(1.ALPHA.,4A.BETA
                .,7.ALPHA.,10A.ALPHA.)]- $$ METHYL
                 8,15-ISOPIMARADIEN-18-OATE

11  35.497  1.42 D:\DATABASE\DEMO.L
                1-[1-(4-METHYLTHIO)HEXYLIDENE]-4-P 504561 113035-73-7 58
                HENYLCYCLOHEXANE
                O-HYDROGEN PERDEUTERIO HEXADECANOI 504545 039756-30-4 56
                C ACID
                Xanthen-9-one, 1-hydroxy-3,5,8-tri 504583 049599-09-9 48
```

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Data Path : F:\DATA MS\daa\
Data File : WLM-10prsen-160c-3jmu.D
Acq On    :  9 Oct 2019  17:59
Operator  :
Sample    :
Misc      :
ALS Vial  : 3   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e
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%#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			methoxy- §§ 5,8-Dimethylbellidifolin §§ 1-Hydroxy-3,5,8-trimethoxyxanthan-9-one §§ 1-Hydroxy-3,5,8-trimethoxy-9H-xanthen-9-one #			
12	35.757	0.29	D:\DATABASE\DEMO.L			
			DEHYDROABIETIC ACID	464556	000000-00-0	97
			1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methylethyl)-, methyl ester, [1R-(1.alpha.,4a.beta.,10a.alpha.)]- §§ Podocarpa-8,11,13-trien-15-oic acid, 13-isopropyl-, methyl ester §§ Methyl dehydroabietat	464536	001235-74-1	93
			METHYL ABIETA-8,11,13-TRIEN-18-OATE §§ 1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,9,10,10A-OCTAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL)-, METHYL ESTER, [1R-(1.ALPHA.,4A.BETA.,10A.ALPHA.)]- §§ DEHYDROABIETIC ACID METHYL ESTER §§ METHYL DEHYDROABIETATE	464550	001235-74-1	93
13	35.908	0.04	D:\DATABASE\DEMO.L			
			Pimaric acid §§ 1-Phenanthrenecarboxylic acid, 7-ethenyl-1,2,3,4,4a,4b,5,6,7,9,10,10a-dodecahydro-1,4a,7-trimethyl-, [1R-(1.alpha.,4a.beta.,4b.alpha.,7.beta.,10a.alpha.)]- §§ Podocarp-8(14)-en-15-oic acid, 13.alpha.-methyl-13-vinyl- §§ D-pimaric acid	466434	000127-27-5	70
			PHENOL, 5-[2-(3-HYDROXY-4-METHOXYPHENYL)ETHENYL]-2,3-DIMETHOXY-, (Z)- §§ 2,3-DIMETHOXY-5-[2-(3-HYDROXY-4-METHOXYPHENYL)ETHENYL]PHENOL (Z) §§ COMBRETASTATIN A3	513563	111394-45-7	64
			KAUR-16-EN-18-OIC ACID §§ KAUR-16-EN-18-OIC ACID, (4.BETA.)- §§ (-)-KAURNENOIC ACID §§ (4-BETA)-KAUR-16-EN-18-OIC ACID	168418	020316-84-1	38
14	36.113	0.11	D:\DATABASE\DEMO.L			
			1H-NAPHTHO[2,3-C]PYRAN-5,10-DIONE, 3,4-DIHYDRO-7,9-DIMETHOXY-1,3-DIMETHYL-, CIS-(.+-.)- §§ (+,-)-CIS-7,9-DIMETHOXY-1,3-DIMETHYL-3,4,5,10-TETRAHYDRONAPHTHO[2,3-C]PYRAN-5,10-DIONE	513558	084018-43-9	83
			Palustric acid §§ Podocarpa-8,13-dien-15-oic acid, 13-isopropyl- §§ 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,5,6,9,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, (1R-(1.alpha.,4a.beta.,10a.alpha.))- §§ 8,13-Abietadien-18-oic acid	513439	001945-53-5	52
			1-PHENANTHRENECARBOXYLIC ACID, 7-ETHENYL-1,2,3,4,4A,4B,5,6,7,8,10,10A-DODECAHYDRO-1,4A,7-TRIMETHYL-, [	466436	005835-26-7	51

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-160c-3jmu.D
Acq On : 9 Oct 2019 17:59
Operator :
Sample :
Misc :
ALS Vial : 3 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autointl.e

%#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,7.ALPHA.,10A.ALPHA.)]- §§ ISOPIMARIC ACID §§ PODOCARP-7-EN-15-OIC ACID, 13.BETA.-METHYL-13-VINYL-			
15	36.383	0.09	D:\DATABASE\DEMO.L			
			Methyl abietate §§ 1-Phenanthrenec arboxylic acid, 1,2,3,4,4a,4b,5,6,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, methyl ester, [1R-(1.alpha.,4a.beta.,4b.alpha.,10a.alpha.)]- §§ Podocarpa-7,13-dien-15-oic acid, 13-isopropyl-, methyl ester §§ Abalyn	258889	000127-25-3	95
			METHYL ABIETA-7,13-DIEN-18-OATE §§ 1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL)-, METHYL ESTER, [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A.ALPHA.)]- §§ ABALYN §§ ABIETIC ACID METHYL ESTER	258918	000127-25-3	95
			METHYL ABIETA-7,13-DIEN-18-OATE §§ 1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL)-, METHYL ESTER, [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A.ALPHA.)]- §§ ABALYN §§ ABIETIC ACID METHYL ESTER	480551	000127-25-3	94
16	36.610	0.14	D:\DATABASE\DEMO.L			
			Phenol, 2,4-bis(1-phenylethyl)- §§ 2,4-Bis(1-phenylethyl)phenol #	504578	002769-94-0	94
			KAUR-16-EN-18-OIC ACID §§ KAUR-16-EN-18-OIC ACID, (4.BETA.)- §§ (-)-KAURNENOIC ACID §§ (4-BETA)-KAUR-16-EN-18-OIC ACID	168418	020316-84-1	78
			Abietic acid §§ 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,4b,5,6,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1R-(1.alpha.,4a.beta.,4b.alpha.,10a.alpha.)]- §§ Podocarpa-7,13-dien-15-oic acid, 13-isopropyl- §§ L-abietic acid	513378	000514-10-3	78
17	36.761	0.11	D:\DATABASE\DEMO.L			
			Palustric acid §§ Podocarpa-8,13-dien-15-oic acid, 13-isopropyl- §§ 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,5,6,9,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, (1R-(1.alpha.,4a.beta.,10a.alpha.))- §§ 8,13-Abietadien-18-oic acid	513439	001945-53-5	70
			1-PHENANTHRENECARBOXYLIC ACID, 7-ETHENYL-1,2,3,4,4A,4B,5,6,7,8,10,10A-DODECAHYDRO-1,4A,7-TRIMETHYL-, [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,7.ALPHA.,10A.ALPHA.)]- §§ ISOPIMARIC ACID §§ PODOCARP-7-EN-15-OIC ACID, 13.BETA.-METHYL-13-VINYL-	466436	005835-26-7	64

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Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-160c-3jmu.D
Acq On    :  9 Oct 2019  17:59
Operator  :
Sample    :
Misc      :
ALS Vial  : 3   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autointl.e

%#     RT  Area%          Library/ID                    Ref#     CAS#   Qual

                Abietic acid §§ 1-Phenanthrenecarb 513344 000514-10-3 58
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid

18  37.037  0.70 D:\DATABASE\DEMO.L
                ABIETA-7,13-DIEN-18-OIC ACID §§ 1- 168419 000514-10-3 70
                PHENANTHRENECARBOXYLIC ACID, 1,2,3
                ,4,4A,4B,5,6,10,10A-DECAHYDRO- §§
                1-PHENANTHRENECARBOXYLIC ACID, 1,2
                ,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,
                4A-DIMETHYL-7-(1-METHYLETHYL)-, [1
                R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A
                .ALPHA.)]-
                Abietic acid §§ 1-Phenanthrenecarb 513344 000514-10-3 55
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid
                1-PHENANTHRENECARBOXYLIC ACID, 7-E 466436 005835-26-7 42
                THENYL-1,2,3,4,4A,4B,5,6,7,8,10,10
                A-DODECAHYDRO-1,4A,7-TRIMETHYL-, [
                1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,7.
                ALPHA.,10A.ALPHA.)]- §§ ISOPIMARIC
                 ACID §§ PODOCARP-7-EN-15-OIC ACID
                , 13.BETA.-METHYL-13-VINYL-

19  37.264  0.22 D:\DATABASE\DEMO.L
                ABIETA-7,13-DIEN-18-OIC ACID §§ 1- 168420 000514-10-3 83
                PHENANTHRENECARBOXYLIC ACID, 1,2,3
                ,4,4A,4B,5,6,10,10A-DECAHYDRO- §§
                1-PHENANTHRENECARBOXYLIC ACID, 1,2
                ,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,
                4A-DIMETHYL-7-(1-METHYLETHYL)-, [1
                R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A
                .ALPHA.)]-
                Abietic acid §§ 1-Phenanthrenecarb 513344 000514-10-3 70
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid
                5-N-PROPYL-5-[(2-METHOXY-2-CYCLOPE 513631 000000-00-0 64
                NTENYL)ETHENYL]-2-N-PROPYL-2-CYCLO
                PENTENE-1,4-DIONE

20  37.404  0.04 D:\DATABASE\DEMO.L
                Abietic acid §§ 1-Phenanthrenecarb 513344 000514-10-3 78
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
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Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-160c-3jmu.D
Acq On : 9 Oct 2019 17:59
Operator :
Sample :
Misc :
ALS Vial : 3 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autointl.e

%#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			opropyl- §§ L-abietic acid			
			ABIETA-7,13-DIEN-18-OIC ACID §§ 1-	168420	000514-10-3	78
			PHENANTHRENECARBOXYLIC ACID, 1,2,3			
			,4,4A,4B,5,6,10,10A-DECAHYDRO- §§			
			1-PHENANTHRENECARBOXYLIC ACID, 1,2			
			,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,			
			4A-DIMETHYL-7-(1-METHYLETHYL)-, [1			
			R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A			
			.ALPHA.)]-			
			Abietic acid §§ 1-Phenanthrenecarb	513378	000514-10-3	60
			oxylic acid, 1,2,3,4,4a,4b,5,6,10,			
			10a-decahydro-1,4a-dimathyl-7-(1-m			
			ethylethyl)-, [1R-(1.alpha.,4a.bet			
			a.,4b.alpha.,10a.alpha.)]- §§ Podo			
			carpa-7,13-dien-15-oic acid, 13-is			
			opropyl- §§ L-abietic acid			
21	37.712	2.24	D:\DATABASE\DEMO.L			
			Abietic acid §§ 1-Phenanthrenecarb	513378	000514-10-3	99
			oxylic acid, 1,2,3,4,4a,4b,5,6,10,			
			10a-decahydro-1,4a-dimathyl-7-(1-m			
			ethylethyl)-, [1R-(1.alpha.,4a.bet			
			a.,4b.alpha.,10a.alpha.)]- §§ Podo			
			carpa-7,13-dien-15-oic acid, 13-is			
			opropyl- §§ L-abietic acid			
			Abietic acid §§ 1-Phenanthrenecarb	513344	000514-10-3	95
			oxylic acid, 1,2,3,4,4a,4b,5,6,10,			
			10a-decahydro-1,4a-dimathyl-7-(1-m			
			ethylethyl)-, [1R-(1.alpha.,4a.bet			
			a.,4b.alpha.,10a.alpha.)]- §§ Podo			
			carpa-7,13-dien-15-oic acid, 13-is			
			opropyl- §§ L-abietic acid			
			Abietic acid §§ 1-Phenanthrenecarb	513347	000514-10-3	94
			oxylic acid, 1,2,3,4,4a,4b,5,6,10,			
			10a-decahydro-1,4a-dimathyl-7-(1-m			
			ethylethyl)-, [1R-(1.alpha.,4a.bet			
			a.,4b.alpha.,10a.alpha.)]- §§ Podo			
			carpa-7,13-dien-15-oic acid, 13-is			
			opropyl- §§ L-abietic acid			
22	38.825	0.15	D:\DATABASE\DEMO.L			
			1,4-DIHYDRO-9-ISOPROPYLIDENE-5,6,7	513581	000000-00-0	90
			,8-TETRAMETHOXY-1,4-METHANONAPHTHA			
			LENE			
			Abietic acid §§ 1-Phenanthrenecarb	513378	000514-10-3	56
			oxylic acid, 1,2,3,4,4a,4b,5,6,10,			
			10a-decahydro-1,4a-dimathyl-7-(1-m			
			ethylethyl)-, [1R-(1.alpha.,4a.bet			
			a.,4b.alpha.,10a.alpha.)]- §§ Podo			
			carpa-7,13-dien-15-oic acid, 13-is			
			opropyl- §§ L-abietic acid			
			Abietic acid §§ 1-Phenanthrenecarb	513347	000514-10-3	45
			oxylic acid, 1,2,3,4,4a,4b,5,6,10,			
			10a-decahydro-1,4a-dimathyl-7-(1-m			
			ethylethyl)-, [1R-(1.alpha.,4a.bet			
			a.,4b.alpha.,10a.alpha.)]- §§ Podo			
			carpa-7,13-dien-15-oic acid, 13-is			
			opropyl- §§ L-abietic acid			

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-160c-3jmu.D
Acq On : 9 Oct 2019 17:59
Operator :
Sample :
Misc :
ALS Vial : 3 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
23	39.014	0.14	D:\DATABASE\DEMO.L			
			Abietic acid §§ 1-Phenanthrenecarb	513378	000514-10-3	89
			oxylic acid, 1,2,3,4,4a,4b,5,6,10,			
			10a-decahydro-1,4a-dimethyl-7-(1-m			
			ethylethyl)-, [1R-(1.alpha.,4a.bet			
			a.,4b.alpha.,10a.alpha.)]- §§ Podo			
			carpa-7,13-dien-15-oic acid, 13-is			
			opropyl- §§ L-abietic acid			
			Palustric acid §§ Podocarpa-8,13-d	513439	001945-53-5	83
			ien-15-oic acid, 13-isopropyl- §§			
			1-Phenanthrenecarboxylic acid, 1,2			
			,3,4,4a,5,6,9,10,10a-decahydro-1,4			
			a-dimethyl-7-(1-methylethyl)-, (1R			
			-(1.alpha.,4a.beta.,10a.alpha.))-			
			§§ 8,13-Abietadien-18-oic acid			
			Abietic acid §§ 1-Phenanthrenecarb	513347	000514-10-3	78
			oxylic acid, 1,2,3,4,4a,4b,5,6,10,			
			10a-decahydro-1,4a-dimethyl-7-(1-m			
			ethylethyl)-, [1R-(1.alpha.,4a.bet			
			a.,4b.alpha.,10a.alpha.)]- §§ Podo			
			carpa-7,13-dien-15-oic acid, 13-is			
			opropyl- §§ L-abietic acid			

Data Path : F:\DATA MS\daa\
Data File : WLM-10pssen-160c-4jm.D
Acq On : 12 Oct 2019 11:41
Operator :
Sample :
Misc :
ALS Vial : 1 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	1.962	6.13	D:\DATABASE\DEMO.L			
			Methyl Alcohol $$ Methanol $$ Carb inol $$ Methyl hydroxide	5073	000067-56-1	2
			METHANOL $$ HYDROXYMETHANE $$ ALCO HOL, METHYL $$ ALCOOL METHYLIQUE	5075	000067-56-1	2
			Methyl Alcohol $$ Methanol $$ Carb inol $$ Methyl hydroxide	5072	000067-56-1	2
2	2.065	0.01	D:\DATABASE\DEMO.L			
			DECANE-3,4-D2	22506	019165-57-2	39
			FORMIC ACID, PROPYL ESTER $$ PROPY L FORMATE $$ FORMIATE DE PROPYLE $ $ HCOOCH2CH2CH3	5244	000110-74-7	33
			HEXANE, 3-METHYL- $$ 3-METHYLHEXAN E $$ 2-ETHYLPENTANE $$ HEXANE, 3-M ETHYL	18994	000589-34-4	23
3	2.135	0.16	D:\DATABASE\DEMO.L			
			Pentane, 2,4-dimethyl- $$ 2,4-Dime thylpentane	18753	000108-08-7	91
			Pentane, 2,4-dimethyl- $$ 2,4-Dime thylpentane	18750	000108-08-7	87
			PENTANE, 2,2-DIMETHYL- $$ 2,2-DIME THYLPENTANE	65647	000590-35-2	64
4	2.205	11.78	D:\DATABASE\DEMO.L			
			HEXANE, 3-METHYL- $$ 3-METHYLHEXAN E $$ 2-ETHYLPENTANE $$ HEXANE, 3-M ETHYL	18994	000589-34-4	83
			Hexane, 3-methyl- $$ 2-Ethylpentan e $$ 3-Methylhexane	18811	000589-34-4	80
			Hexane, 3-methyl- $$ 2-Ethylpentan e $$ 3-Methylhexane	18754	000589-34-4	64
5	2.243	4.56	D:\DATABASE\DEMO.L			
			Cyclopentane, 1,3-dimethyl-, cis- $$ cis-1,3-Dimethylcyclopentane $$ 1,3-Dimethylcyclopentane cis $$ 1 ,3-Dimethylcyclopentane #	62231	002532-58-3	91
			1,3-DIMETHYLCYCLOPENTANE $$ CYCLOP ENTANE, 1,3-DIMETHYL-, CIS- $$ 1,3 -DIMETHYLCYCLOPENTANE (CIS) $$ 1,3 -DIMETHYLCYCLOPENTANE CIS	62286	002532-58-3	91
			Cyclopentane, 1,3-dimethyl- $$ 1,3 -Dimethylcyclopentane	101343	002453-00-1	91
6	2.335	6.74	D:\DATABASE\DEMO.L			
			CYCLOHEXANE, METHYL- $$ METHYLCYCL OHEXANE $$ 1-METHYLCYCLOHEXANE $$ CYCLOHEXANE, METHYL	141469	000108-87-2	96
			CYCLOHEXANE, METHYL- $$ METHYLCYCL OHEXANE $$ 1-METHYLCYCLOHEXANE $$ CYCLOHEXANE, METHYL	141470	000108-87-2	95
			Cyclohexane, methyl- $$ Cyclohexyl methane $$ Hexahydrotoluene $$ Met hylcyclohexane	141386	000108-87-2	94
7	2.421	60.91	D:\DATABASE\DEMO.L			
			Toluene $$ Benzene, methyl $$ Meth	158579	000108-88-3	91

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Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-160c-4jm.D
Acq On    : 12 Oct 2019  11:41
Operator  :
Sample    :
Misc      :
ALS Vial  : 1   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e
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k#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			acide §§ Methylbenzene			
			BENZENE, METHYL- §§ METHYLBENZENE §§ TOLUENE §§ ANTISAL 1A	158622	000108-88-3	91
			Toluene §§ Benzene, methyl §§ Meth acide §§ Methylbenzene	158580	000108-88-3	91
8	2.745	1.06	D:\DATABASE\DEMO.L			
			Cyclohexane, ethyl- §§ Ethylcycloh exane	141506	001678-91-7	93
			CYCLOHEXANE, ETHYL- §§ ETHYLCYCLOH EXANE §§ ETHYL CYCLOHEXANE §§ ETHY LCYCLOHEXAN	141561	001678-91-7	93
			CYCLOHEXANE, ETHYL- §§ ETHYLCYCLOH EXANE §§ ETHYL CYCLOHEXANE §§ ETHY LCYCLOHEXAN	141562	001678-91-7	76
9	2.875	0.38	D:\DATABASE\DEMO.L			
			Toluene §§ Benzene, methyl §§ Meth acide §§ Methylbenzene	158586	000108-88-3	93
			BENZENE, METHYL- §§ METHYLBENZENE §§ TOLUENE §§ ANTISAL 1A	158623	000108-88-3	90
			METHYLFULVENE	158616	000000-00-0	90
10	17.320	0.03	D:\DATABASE\DEMO.L			
			2H-2,4A-METHANONAPHTHALENE, 1,3,4, 5,6,7-HEXAHYDRO-1,1,5,5-TETRAMETHY L-, (2S)- §§ (-)-ISOLONGIFOLENE §§ (-)-ISOLONGIFOLINE §§ (2S)-1,3,4, 5,6,7-HEXAHYDRO-1,1,5,5-TETRAMETHY L-2H-2,4A-METHANONAPHTHALENE	350804	001135-66-6	98
			2H-2,4a-Methanonaphthalene, 1,3,4, 5,6,7-hexahydro-1,1,5,5-tetramethy l-, (2S)- §§ 2H-2,4a-Methanonaphth alene, 1,3,4,5,6,7-hexahydro-1,1,5 ,5-tetramethyl-, (2S,4aR)-(-)- §§ Isolongifolene §§ (-)-Isolongifoli ne	350641	001135-66-6	98
			2H-2,4A-METHANONAPHTHALENE, 1,3,4, 5,6,7-HEXAHYDRO-1,1,5,5-TETRAMETHY L-, (2S)- §§ (-)-ISOLONGIFOLENE §§ (-)-ISOLONGIFOLINE §§ (2S)-1,3,4, 5,6,7-HEXAHYDRO-1,1,5,5-TETRAMETHY L-2H-2,4A-METHANONAPHTHALENE	350800	001135-66-6	98
11	17.714	0.01	D:\DATABASE\DEMO.L			
			2,2,3,3,4,4,5,5-OCTAFLUORO-N-(3-ME THOXYPHENYL)PENTANAMIDE §§ PENTANA MIDE, 2,2,3,3,4,4,5,5-OCTAFLUORO-N -(3-METHOXYPHENYL)-	7474	339166-43-7	37
			2-METHOXY-4-(METHOXYMETHYL)-6-METH YLNICOTINONITRILE §§ PYRIDINE-3-CA RBONITRILE, 2,4-DIMETHOXY-6-METHYL	7347	063644-84-8	9
			1,3-OXATHIOL-1-IUM, 4-HYDROXY-2-[(1-METHYLETHYL)THIO]-5-(TRIFLUOROAC ETYL)-, HYDROXIDE, INNER SALT §§ 2 -ISOPROPYLTHIO-5-TRIFLUORACETYL-1, 3-OXATHIOLYIUM-4-OLAT	7423	096088-83-4	9
12	28.605	0.01	D:\DATABASE\DEMO.L			

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Sample :
Misc :
ALS Vial : 1 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			4-(METHOXYMETHYL)-6-METHYL-2-PHENO XYNICOTINONITRILE §§ PYRIDINE-3-CA RBONITRILE, 4-METHOXYMETHYL-6-METH YL-2-PHENOXY-	7413	332057-36-0	16
			3-(3-OXO-3H-BENZO[F]CHROMEN-2-YL)- 2,4(1H,3H)-QUINOLINEDIONE §§ 4-HYD ROXY-3-(2-OXO-2H-1-OXA-3-PHENANTHR YL)-2(1H)-QUINOLINONE	7476	999007-47-7	9
			4-BROMO-N-[(6-METHYL-2-PYRIDYL)AMI NOMETHYL]PHTHALIMIDE §§ 5-BROMO-2- {[(6-METHYL-2-PYRIDINYL)AMINO]METH YL}-1H-ISOINDOLE-1,3(2H)-DIONE	7473	999007-47-4	9
13	30.301	0.03	D:\DATABASE\DEMO.L			
			ENT-PIMARA-8,15-DIENE	481166	021561-92-2	91
			4H,8H-BENZO[1,2-B:3,4-B']DIPYRAN-4 -ONE, 5-METHOXY-2,8,8-TRIMETHYL- § § 5-METHOXY-2,8,8-TRIMETHYL-4H,8H- BENZO[1,2-B:3,4-B']DIPYRAN-4-ONE § § 5-O-METHYLALLOPTAEROXYLIN §§ ALL OPTAEROXYLIN METHYL ETHER	481134	035930-31-5	78
			PIMARA-8,15-DIENE §§ PHENANTHRENE, 7-ETHENYL-1,2,3,4,4A,5,6,7,8,9,10 ,10A-DODECAHYDRO-1,1,4A,7-TETRAMET HYL- §§ 7.ALPHA.-ETHENYL-1,1,4A,7. BETA.-TETRAMETHYL-1,2,3,4,4A,5,6,7 ,8,9,10,10A-DODECAHYDROPHENANTHREN	481165	055255-56-6	74
14	30.717	0.01	D:\DATABASE\DEMO.L			
			4-(METHOXYMETHYL)-6-METHYL-2-PHENO XYNICOTINONITRILE §§ PYRIDINE-3-CA RBONITRILE, 4-METHOXYMETHYL-6-METH YL-2-PHENOXY-	7413	332057-36-0	22
			4-BROMO-N-[(6-METHYL-2-PYRIDYL)AMI NOMETHYL]PHTHALIMIDE §§ 5-BROMO-2- {[(6-METHYL-2-PYRIDINYL)AMINO]METH YL}-1H-ISOINDOLE-1,3(2H)-DIONE	7473	999007-47-4	10
			9-(4-HYDROXYPHENYL)-3,3,6,6-TETRAM ETHYL-3,4,6,7,8A,9-HEXAHYDRO-1,8(2 H,5H)-ACRIDINEDIONE	7482	999007-48-3	9
15	31.219	0.00	D:\DATABASE\DEMO.L			
			4-(METHOXYMETHYL)-6-METHYL-2-PHENO XYNICOTINONITRILE §§ PYRIDINE-3-CA RBONITRILE, 4-METHOXYMETHYL-6-METH YL-2-PHENOXY-	7413	332057-36-0	10
			2-METHOXY-4-(METHOXYMETHYL)-6-METH YLNICOTINONITRILE §§ PYRIDINE-3-CA RBONITRILE, 2,4-DIMETHOXY-6-METHYL	7347	063644-84-8	9
			3-(3-OXO-3H-BENZO[F]CHROMEN-2-YL)- 2,4(1H,3H)-QUINOLINEDIONE §§ 4-HYD ROXY-3-(2-OXO-2H-1-OXA-3-PHENANTHR YL)-2(1H)-QUINOLINONE	7476	999007-47-7	9
16	31.262	0.00	D:\DATABASE\DEMO.L			
			4-(METHOXYMETHYL)-6-METHYL-2-PHENO XYNICOTINONITRILE §§ PYRIDINE-3-CA RBONITRILE, 4-METHOXYMETHYL-6-METH YL-2-PHENOXY-	7413	332057-36-0	16

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Data Path : F:\DATA MS\daa\
Data File : WLM-10prsen-160c-4jm.D
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Sample    :
Misc      :
ALS Vial  : 1   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autointl.e

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                3-(3-OXO-3H-BENZO[F]CHROMEN-2-YL)-   7476 999007-47-7  9
                2,4(1H,3H)-QUINOLINEDIONE §§ 4-HYD
                ROXY-3-(2-OXO-2H-1-OXA-3-PHENANTHR
                YL)-2(1H)-QUINOLINONE
                4-BROMO-N-[(6-METHYL-2-PYRIDYL)AMI   7473 999007-47-4  9
                NOMETHYL]PHTHALIMIDE §§ 5-BROMO-2-
                {[(6-METHYL-2-PYRIDINYL)AMINO]METH
                YL}-1H-ISOINDOLE-1,3(2H)-DIONE

17  31.700  0.03 D:\DATABASE\DEMO.L
                6-ETHYL-2-METHYL-4,6-DIHYDRO-2H-[1   7414 334023-40-4 27
                ,4]OXAZINO[3,2-C]QUINOLINE-3,5-DIO
                NE §§ 6-ETHYL-2-METHYL-2H-1-OXA-4,
                6-PHENANTHROLINE-3,5(4H,6H)-DIONE
                §§ 6-ETHYL-2-METHYL-6,10B-DIHYDRO-
                2H-[1,4]OXAZINO[3,2-C]QUINOLINE-3,
                5-DIONE
                2-METHOXY-4-(METHOXYMETHYL)-6-METH   7347 063644-84-8 14
                YLNICOTINONITRILE §§ PYRIDINE-3-CA
                RBONITRILE, 2,4-DIMETHOXY-6-METHYL
                1-Tetradecanamine §§ Tetradecylami   4817 002016-42-4 10
                ne §§ Armeen 14 §§ Myristylamine

18  31.830  0.01 D:\DATABASE\DEMO.L
                4-(METHOXYMETHYL)-6-METHYL-2-PHENO   7413 332057-36-0 25
                XYNICOTINONITRILE §§ PYRIDINE-3-CA
                RBONITRILE, 4-METHOXYMETHYL-6-METH
                YL-2-PHENOXY-
                3-(3-OXO-3H-BENZO[F]CHROMEN-2-YL)-   7476 999007-47-7 10
                2,4(1H,3H)-QUINOLINEDIONE §§ 4-HYD
                ROXY-3-(2-OXO-2H-1-OXA-3-PHENANTHR
                YL)-2(1H)-QUINOLINONE
                2,2'-(1,4-Piperazinediyl)bis[N-(4-   7524 293766-05-9  9
                methoxyphenyl)succinimide]

19  31.986  0.02 D:\DATABASE\DEMO.L
                6-ETHYL-2-METHYL-4,6-DIHYDRO-2H-[1   7414 334023-40-4 25
                ,4]OXAZINO[3,2-C]QUINOLINE-3,5-DIO
                NE §§ 6-ETHYL-2-METHYL-2H-1-OXA-4,
                6-PHENANTHROLINE-3,5(4H,6H)-DIONE
                §§ 6-ETHYL-2-METHYL-6,10B-DIHYDRO-
                2H-[1,4]OXAZINO[3,2-C]QUINOLINE-3,
                5-DIONE
                2,2'-(1,4-Piperazinediyl)bis[N-(4-   7524 293766-05-9  9
                methoxyphenyl)succinimide]
                2,2'-(1,4-PIPERAZINEDIYL)BIS[N-(4-   7525 293766-05-9  9
                METHOXYPHENYL)SUCCINIMIDE]

20  32.105  0.02 D:\DATABASE\DEMO.L
                3-Methyl-1-phenyl-2-azafluorene §§ 480961 062578-39-6 47
                 3-Methyl-1-phenyl-9H-indeno[2,1-c
                ]pyridine #
                3-METHYL-3-PHENYL-3H-NAPHTHO[2,3-B 481155 000000-00-0 47
                ]PYRAN
                Benzenamine, 4-methoxy-3-tricyclo[ 480906 999480-91-8 46
                3.3.1.1(3,7)]dec-1-yl-

21  32.305  0.01 D:\DATABASE\DEMO.L
                4-(METHOXYMETHYL)-6-METHYL-2-PHENO   7413 332057-36-0 25
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Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-160c-4jm.D
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Sample :
Misc :
ALS Vial : 1 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			XYNICOTINONITRILE §§ PYRIDINE-3-CARBONITRILE, 4-METHOXYMETHYL-6-METHYL-2-PHENOXY-			
			1-Dodecanamine §§ Dodecylamine §§ n-Dodecylamine §§ Alamine 4	4652	000124-22-1	9
			1-DODECANAMINE §§ 1-AMINODODECANE §§ 1-DODECYLAMINE §§ ALAMINE 4	4661	000124-22-1	9
22	32.391	0.02	D:\DATABASE\DEMO.L			
			1-PHENYL-3-METHYL-4-(2-PROP-2-YL)-5-ACETOXYPYRAZOLE	419699	000000-00-0	38
			1-PHENYL-2-ACETYL-3-METHYL-5-(PROP-2-YL)-2,5-DIHYDROPYRAZOLE-5-ONE	419698	000000-00-0	38
			5-Trifluoromethyl-3-methylthiazolidine-2-thione §§ 3-Methyl-5-(trifluoromethyl)-1,3-thiazolidine-2-thione #	419133	186791-22-0	35
23	32.608	0.00	D:\DATABASE\DEMO.L			
			4-(METHOXYMETHYL)-6-METHYL-2-PHENOXYNICOTINONITRILE §§ PYRIDINE-3-CARBONITRILE, 4-METHOXYMETHYL-6-METHYL-2-PHENOXY-	7413	332057-36-0	16
			1,12-DODECANEDIAMINE §§ DODECANE-1,12-DIAMINE §§ 1, 12-DIAMINODODECANE §§ 1, 12-DODECANEDIAMINE	4754	002783-17-7	9
			1,12-DODECANEDIAMINE §§ DODECANE-1,12-DIAMINE	4751	999004-75-2	9
24	32.780	0.01	D:\DATABASE\DEMO.L			
			1-Hexadecanamine §§ Hexadecylamine §§ n-Cetylamine §§ n-Hexadecylamine	4902	000143-27-1	38
			2-METHOXY-4-(METHOXYMETHYL)-6-METHYLNICOTINONITRILE §§ PYRIDINE-3-CARBONITRILE, 2,4-DIMETHOXY-6-METHYL	7347	063644-84-8	16
			4-(METHOXYMETHYL)-6-METHYL-2-PHENOXYNICOTINONITRILE §§ PYRIDINE-3-CARBONITRILE, 4-METHOXYMETHYL-6-METHYL-2-PHENOXY-	7413	332057-36-0	12
25	32.975	0.00	D:\DATABASE\DEMO.L			
			2-METHOXY-4-(METHOXYMETHYL)-6-METHYLNICOTINONITRILE §§ PYRIDINE-3-CARBONITRILE, 2,4-DIMETHOXY-6-METHYL	7347	063644-84-8	12
			Taurolidine §§ 2H-1,2,4-Thiadiazine, 4,4'-methylenebis[tetrahydro-, 1,1,1',1'-tetraoxide §§ 4,4'-Methylenebis(tetrahydro-1,2,4-thiadiazine 1,1-dioxide) §§ Taurolin	4983	019388-87-5	9
			D.G.E.B.A.	454	000000-00-0	9
26	33.375	0.01	D:\DATABASE\DEMO.L			
			6-ETHYL-2-METHYL-4,6-DIHYDRO-2H-[1,4]OXAZINO[3,2-C]QUINOLINE-3,5-DIONE §§ 6-ETHYL-2-METHYL-2H-1-OXA-4,6-PHENANTHROLINE-3,5(4H,6H)-DIONE §§ 6-ETHYL-2-METHYL-6,10B-DIHYDRO-	7414	334023-40-4	20

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  Data Path : F:\DATA MS\daa\
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  Unknown Spectrum:   Apex
  Integration Events: ChemStation Integrator - autointl.e

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                5-DIONE
                4-(METHOXYMETHYL)-6-METHYL-2-PHENO   7413 332057-36-0 12
                XYNICOTINONITRILE §§ PYRIDINE-3-CA
                RBONITRILE, 4-METHOXYMETHYL-6-METH
                YL-2-PHENOXY-
                Taurolidine §§ 2H-1,2,4-Thiadiazin   4983 019388-87-5 10
                e, 4,4'-methylenebis[tetrahydro-,
                1,1,1',1'-tetraoxide §§ 4,4'-Methy
                lenebis(tetrahydro-1,2,4-thiadiazi
                ne 1,1-dioxide) §§ Taurolin

 27  33.499  0.11 D:\DATABASE\DEMO.L
                Diazene, bis(4-ethoxyphenyl)-, 1-o 223735 004792-83-0 46
                xide §§ Azoxybenzene, 4,4'-diethox
                y- §§ p,p'-Azoxyphenetole §§ 4,4'-
                Azoxydiphenetole
                1,2-BIS(4-ETHOXYPHENYL)DIAZENE 1-O 223740 004792-83-0 46
                XIDE §§ 4, 4'-BIS(ETHOXY)AZOXYBENZ
                ENE §§ 4,4'-AZOXYDIPHENETOLE §§ 4,
                4'-AZOXYPHENETOLE
                14-ISOPROPYL-3,7,11-TRIMETHYL-1,3, 181371 001898-13-1 45
                6,10-CYCLOTETRADECATETRAENE §§ 1,3
                ,6,10-CYCLOTETRADECATETRAENE, 3,7,
                11-TRIMETHYL-14-(1-METHYLETHYL)-,
                [S-(E,Z,E,E)]- §§ (+)-CEMBRENE §§
                (+)-THUMBERGEN

 28  33.693  0.01 D:\DATABASE\DEMO.L
                2-METHOXY-4-(METHOXYMETHYL)-6-METH   7347 063644-84-8 14
                YLNICOTINONITRILE §§ PYRIDINE-3-CA
                RBONITRILE, 2,4-DIMETHOXY-6-METHYL
                Taurolidine §§ 2H-1,2,4-Thiadiazin   4983 019388-87-5 10
                e, 4,4'-methylenebis[tetrahydro-,
                1,1,1',1'-tetraoxide §§ 4,4'-Methy
                lenebis(tetrahydro-1,2,4-thiadiazi
                ne 1,1-dioxide) §§ Taurolin
                2,2'-(1,4-Piperazinediyl)bis[N-(4-   7524 293766-05-9 10
                methoxyphenyl)succinimide]

 29  33.791  0.02 D:\DATABASE\DEMO.L
                7-BENZYLOXY-2-HYDROXY-2H-[1,4]BENZ 166364 000000-00-0 27
                OXAZIN-3(4H)-ONE
                3-Phenylpropionic acid, 2,7-dimeth 167176 999167-17-9 10
                yloct-7-en-5-yn-4-yl ester
                9-Benzyladenine N(1)-oxide §§ 9-Be 164412 004261-16-9 10
                nzyl-1-oxido-9H-purin-6-ylamine #

 30  33.861  0.07 D:\DATABASE\DEMO.L
                1-Methyl-10,18-bisnorabieta-8,11,1 466158 999466-16-6 94
                3-triene
                3,3,4,5,5,8-HEXAMETHYL-3,5,6,7-TET 466221 038754-94-8 91
                RAHYDRO-9-INDACEN-1(2H)-ONE §§ 9-I
                NDACEN-1(2H)-ONE, 3,5,6,7-TETRAHYD
                RO-3,3,4,5,5,8-HEXAMETHYL- §§ 3,3,
                4,5,5,8-HEXAMETHYL-1-9-HYDRINDACEN
                ONE
                s-Indacen-1(2H)-one, 3,5,6,7-tetra 466171 038754-94-8 91
                hydro-3,3,4,5,5,8-hexamethyl- §§ 3
                ,3,4,5,5,8-Hexamethyl-3,5,6,7-tetr
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  Sample    :
  Misc      :
  ALS Vial  : 1   Sample Multiplier: 1

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  Unknown Spectrum:   Apex
  Integration Events: ChemStation Integrator - autoint1.e

Pk#     RT  Area%          Library/ID                    Ref#     CAS#   Qual
                ahydro-8-indacen-1(2H)-one #

 31  34.136  0.01 D:\DATABASE\DEMO.L
                No matches found

 32  34.190  0.00 D:\DATABASE\DEMO.L
                3-HYDROXY-4-METHOXY-2,3,6A,9A-TETR   7461 052819-96-2  6
                AHYDROCYCLOPENTA[C]FURO[3',2':4,5]
                FURO[2,3-H]CHROMENE-1,11-DIONE §§
                CYCLOPENTA[C]FURO[3',2':4,5]FURO[2
                ,3-H][1]BENZOPYRAN-1,11-DIONE, 2,3
                ,6A,9A-TETRAHYDRO-3-HYDROXY-4-METH
                OXY-, [3S-(3.ALPHA.,6A.ALPHA.,9A.A
                LPHA.)]-

 33  34.212  0.00 D:\DATABASE\DEMO.L
                2-METHOXY-4-(METHOXYMETHYL)-6-METH   7347 063644-84-8 22
                YLNICOTINONITRILE §§ PYRIDINE-3-CA
                RBONITRILE, 2,4-DIMETHOXY-6-METHYL
                1-Hexadecanamine §§ Hexadecylamine   4902 000143-27-1 10
                 §§ n-Cetylamine §§ n-Hexadecylami
                ne
                Carbamic acid, (2-chloroethylidene   3171 005336-13-0  9
                )bis-, diethyl ester §§ Carbamic a
                cid, (2-chloroethylidene)di-, diet
                hyl ester

 34  34.315  0.05 D:\DATABASE\DEMO.L
                1-Phenanthrenecarboxylic acid, 7-e 466507 003582-26-1 86
                thenyl-1,2,3,4,4a,5,6,7,8,9,10,10a
                -dodecahydro-1,4a,7-trimethyl-, me
                thyl ester, [1R-(1.alpha.,4a.beta.
                ,7.beta.,10a.alpha.)]- §§ Podocarp
                -8-en-15-oic acid, 13.alpha.-methy
                l-13-vinyl-, methyl ester
                METHYL PIMARA-8,15-DIEN-18-OATE §§ 466513 003582-26-1 86
                 1-PHENANTHRENECARBOXYLIC ACID, 7-
                ETHENYL-1,2,3,4,4A,5,6,7,8,9,10,10
                A-DODECAHYDRO-1,4A,7-TRIMETHYL-, M
                ETHYL ESTER, [1R-(1.ALPHA.,4A.BETA
                .,7.BETA.,10A.ALPHA.)]- §§ METHYL
                8,15-PIMARADIEN-18-OATE
                METHYL PIMARA-7,15-DIEN-18-OATE §§ 466517 001686-62-0 55
                 1-PHENANTHRENECARBOXYLIC ACID, 7-
                ETHENYL-1,2,3,4,4A,4B,5,6,7,8,10,1
                0A-DODECAHYDRO-1,4A,7-TRIMETHYL-,
                METHYL ESTER, [1R-(1.ALPHA.,4A.BET
                A.,4B.ALPHA.,7.ALPHA.,10A.ALPHA.)]
                - §§ ISOPIMARATE §§ ISOPIMARIC ACI
                D, METHYL ESTER

 35  34.536  0.06 D:\DATABASE\DEMO.L
                KAUR-16-EN-18-OIC ACID §§ KAUR-16- 168418 020316-84-1 45
                EN-18-OIC ACID, (4.BETA.)- §§ (-)-
                KAURENOIC ACID §§ (4-BETA)-KAUR-1
                6-EN-18-OIC ACID
                ABIETA-7,13-DIEN-18-OIC ACID §§ 1- 168420 000514-10-3 25
                PHENANTHRENECARBOXYLIC ACID, 1,2,3
                ,4,4A,4B,5,6,10,10A-DECAHYDRO- §§
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Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-160c-4jm.D
Acq On : 12 Oct 2019 11:41
Operator :
Sample :
Misc :
ALS Vial : 1 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL)-, [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A.ALPHA.)]-			
			4H-[1,2,4]Triazole-3-thiol, 4-benzyl-5-furan-2-yl-	165414	999165-41-7	14
36	34.676	0.00	D:\DATABASE\DEMO.L			
			2H-3,9A-METHANO-1-BENZOXEPIN, OCTAHYDRO-2,2,5A,9-TETRAMETHYL-, [3R-(3.ALPHA.,5A.ALPHA.,9.ALPHA.,9A.ALPHA.)]- §§ .BETA.-AGAROFURAN, DIHYDRO- §§ .BETA.-DIHYDROAGAROFURAN §§ 2H-3,9A-METHANO-1-BENZOXEPIN, OCTAHYDRO-2,2,5A,9-TETRAMETHYL-	3110	005956-09-2	10
			Ethyl 2-((diethoxyphosphoryl)oxy)-3,3,3-trifluoropropanoate	3375	999003-37-6	2
37	34.790	0.03	D:\DATABASE\DEMO.L			
			2H-3,9A-METHANO-1-BENZOXEPIN, OCTAHYDRO-2,2,5A,9-TETRAMETHYL-, [3R-(3.ALPHA.,5A.ALPHA.,9.ALPHA.,9A.ALPHA.)]- §§ .BETA.-AGAROFURAN, DIHYDRO- §§ .BETA.-DIHYDROAGAROFURAN §§ 2H-3,9A-METHANO-1-BENZOXEPIN, OCTAHYDRO-2,2,5A,9-TETRAMETHYL-	3110	005956-09-2	8
			Diethyl 3-chloro-2-hydroxypropylmalonate	3235	999003-23-6	4
			DIETHYL 2-(3-CHLORO-2-HYDROXYPROPYL)MALONATE §§ DIETHYL 3-CHLORO-2-HYDROXYPROPYLMALONATE	3236	999003-23-7	4
38	34.925	0.03	D:\DATABASE\DEMO.L			
			KAUR-16-EN-18-OIC ACID §§ KAUR-16-EN-18-OIC ACID, (4.BETA.)- §§ (-)-KAURNENOIC ACID §§ (4-BETA)-KAUR-16-EN-18-OIC ACID	168418	020316-84-1	14
			ABIETA-7,13-DIEN-18-OIC ACID §§ 1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,4B,5,6,10,10A-DECAHYDRO- §§ 1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL)-, [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A.ALPHA.)]-	168419	000514-10-3	11
			1-benzylindole	162408	999162-41-1	10
39	35.028	0.04	D:\DATABASE\DEMO.L			
			4,5-Bis-dimethoxymethyl-octanedioic acid, dimethyl ester	124248	999124-25-1	53
			1-Cyclopentanecarboxylic acid, 3-hydroxy-5-(1-hydroxy-2,2-dimethoxyethyl)-, methyl ester, (1'S,3R,5R)-(+-)-	123361	999123-36-4	53
			2-Cyclohexyldimethylsilyloxy-pentadecane	124366	999124-36-9	53
40	35.136	0.03	D:\DATABASE\DEMO.L			

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Data File : WLM-10prsan-160c-4jm.D
Acq On : 12 Oct 2019 11:41
Operator :
Sample :
Misc :
ALS Vial : 1 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			BUTYL 2-(METHYLAMINO)BENZOATE §§ ANTHRANILIC ACID, N-METHYL-, BUTYL ESTER §§ N-BUTYL O-METHYLAMINOBENZOATE	209256	015236-34-7	18
			3-(2-PHENYLETHYL)BENZONITRILE §§ BENZONITRILE, M-PHENETHYL- §§ 1-(3-CYANOPHENYL)-2-PHENYLETHANE §§ M-CYANO-1,2-DIPHENYLETHANE	162420	034176-91-5	14
			N-Benzoylglycine ethyl ester §§ Benzoic amide, N-(ethoxycarbonyl)methyl- §§ Ethyl (benzoylamino)acetate #	209238	001499-53-2	14
41	35.184	0.01	D:\DATABASE\DEMO.L			
			1,5,11-CYCLOTETRADECATRIENE-1-CARBOXYLIC ACID, 11-(HYDROXYMETHYL)-8-[1-(HYDROXYMETHYL)ETHENYL]-5-METHYL-, (Z,Z,E)- §§ 9-METHYL-1-HYDROXYMETHYL-5-HYDROXYCARBONYL-12-(1-HYDROXYMETHYL)-ETHENYL-CYCLOTETRADECA-1,5,9-TRI-ENE	170254	099486-51-8	9
			BENZENE, HEXADECYL- §§ 1-PHENYLHEXADECANE §§ HEXADECYLBENZENE §§ HEXADECANE, 1(OR 16)-PHENYL-	168424	001459-09-2	9
			2(5H)-Furanone, 3-(2-benzyl-2-propenyl)-4-methyl-5-phenyl-	168490	999168-49-3	9
42	35.211	0.01	D:\DATABASE\DEMO.L			
			KAUR-16-EN-18-OIC ACID §§ KAUR-16-EN-18-OIC ACID, (4.BETA.)- §§ (-)-KAURNENOIC ACID §§ (4-BETA)-KAUR-16-EN-18-OIC ACID	168418	020316-84-1	12
			1H-Pyrazole-1-acetamide, 4-iodo-N-(phenylmethyl)-	170579	999170-58-2	12
			N-(4-Isopropylbenzyl)-3-phenylpropionamide §§ N-(4-Isopropylbenzyl)-3-phenylpropanamide #	166995	300862-83-3	11
43	35.314	0.02	D:\DATABASE\DEMO.L			
			bis[(2Z)-Hex-2-en-1-yloxy](dimethyl)silane	123429	999123-43-2	45
			KAUR-16-EN-18-OIC ACID §§ KAUR-16-EN-18-OIC ACID, (4.BETA.)- §§ (-)-KAURNENOIC ACID §§ (4-BETA)-KAUR-16-EN-18-OIC ACID	168418	020316-84-1	35
			N-(2-(3,4-BIS[(TRIMETHYLSILYL)OXY]PHENYL)-2-[(TRIMETHYLSILYL)OXY]ETHYL)(TRIMETHYL)-N-(TRIMETHYLSILYL)SILANAMINE §§ NOREPINEPHRINE, N,N,O,O',O"-PENTAKIS(TRIMETHYLSILYL)- §§ NOREPINEPHRINE-PENTATMS	7530	056114-59-1	22
44	35.395	0.04	D:\DATABASE\DEMO.L			
			2,5-DIMETHYLBICYCLO[3.3.0]OCT-6-EN-8-ONE	227241	000000-00-0	38
			1a,2,5,5-Tetramethyl-cis-1a,4a,5,6,7,8-hexahydro-gamma-chromene	227946	999227-94-9	38
			1,3,4-Thiadiazol-2-amine, 5-[[(4-fluorophenyl)methyl]thio]-	228627	999228-63-0	35

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-160c-4jm.D
Acq On : 12 Oct 2019 11:41
Operator :
Sample :
Misc :
ALS Vial : 1 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

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45	35.492	1.11	D:\DATABASE\DEMO.L			
			Xanthen-9-one, 1-hydroxy-3,5,8-tri methoxy- $$ 5,8-Dimethylbellidifol in $$ 1-Hydroxy-3,5,8-trimethoxyxa nthen-9-one $$ 1-Hydroxy-3,5,8-tri methoxy-9H-xanthen-9-one #	504583	049599-09-9	50
			Androst-5-en-17-ol, 4,4-dimethyl-	513436	999513-44-9	46
			ROSIN ACIDS	504611	000000-00-0	41
46	35.665	0.08	D:\DATABASE\DEMO.L			
			Androst-5-en-17-ol, 4,4-dimethyl-	513436	999513-44-9	83
			1-Hydroxy-3,7,8-trimethoxyxanthen- 9-one $$ 8-Hydroxy-1,2,6-trimethox y-9H-xanthen-9-one #	504580	020882-69-3	43
			2-ACETYL-4,9-DIMETHOXY-7-METHYL-5H -FURO[3,2-G][1]-BENZOPYRAN-5-ONE	513538	092611-83-1	38
47	35.762	0.24	D:\DATABASE\DEMO.L			
			DEHYDROABIETIC ACID	464556	000000-00-0	97
			1-Phenanthrenecarboxylic acid, 1,2 ,3,4,4a,9,10,10a-octahydro-1,4a-di methyl-7-(1-methylethyl)-, methyl ester, [1R-(1.alpha.,4a.beta.,10a. alpha.)]- $$ Podocarpa-8,11,13-tri en-15-oic acid, 13-isopropyl-, met hyl ester $$ Methyl dehydroabietat	464538	001235-74-1	96
			METHYL ABIETA-8,11,13-TRIEN-18-OAT E $$ 1-PHENANTHRENECARBOXYLIC ACID , 1,2,3,4,4A,9,10,10A-OCTAHYDRO-1, 4A-DIMETHYL-7-(1-METHYLETHYL)-, ME THYL ESTER, [1R-(1.ALPHA.,4A.BETA. ,10A.ALPHA.)]- $$ DEHYDROABIETIC A CID METHYL ESTER $$ METHYL DEHYDRO ABIETATE	464550	001235-74-1	96
48	35.908	0.07	D:\DATABASE\DEMO.L			
			BENZ[A]ANTHRACENONE	513655	099707-96-7	64
			KAUR-16-EN-18-OIC ACID $$ KAUR-16- EN-18-OIC ACID, (4.BETA.)- $$ (-)- KAURNENOIC ACID $$ (4-BETA)-KAUR-1 6-EN-18-OIC ACID	168418	020316-84-1	47
			Palustric acid $$ Podocarpa-8,13-d ien-15-oic acid, 13-isopropyl- $$ 1-Phenanthrenecarboxylic acid, 1,2 ,3,4,4a,5,6,9,10,10a-decahydro-1,4 a-dimethyl-7-(1-methylethyl)-, (1R -(1.alpha.,4a.beta.,10a.alpha.))- $$ 8,13-Abietadien-18-oic acid	513439	001945-53-5	41
49	35.930	0.06	D:\DATABASE\DEMO.L			
			Pimaric acid $$ 1-Phenanthrenecarb oxylic acid, 7-ethenyl-1,2,3,4,4a, 4b,5,6,7,9,10,10a-dodecahydro-1,4a ,7-trimethyl-, [1R-(1.alpha.,4a.be ta.,4b.alpha.,7.beta.,10a.alpha.)] - $$ Podocarp-8(14)-en-15-oic acid , 13.alpha.-methyl-13-vinyl- $$ D- pimaric acid	466434	000127-27-5	70

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 Data Path : F:\DATA MS\daa\
 Data File : WLM-10prsan-160c-4jm.D
 Acq On    : 12 Oct 2019  11:41
 Operator  :
 Sample    :
 Misc      :
 ALS Vial  : 1   Sample Multiplier: 1

 Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

 Unknown Spectrum:   Apex
 Integration Events: ChemStation Integrator - autointl.e

%#     RT  Area%          Library/ID                   Ref#     CAS#   Qual
                Palustric acid §§ Podocarpa-8,13-d 513439 001945-53-5 55
                ien-15-oic acid, 13-isopropyl- §§
                1-Phenanthrenecarboxylic acid, 1,2
                ,3,4,4a,5,6,9,10,10a-decahydro-1,4
                a-dimethyl-7-(1-methylethyl)-, (1R
                -(1.alpha.,4a.beta.,10a.alpha.))-
                §§ 8,13-Abietadien-18-oic acid
                KAUR-16-EN-18-OIC ACID §§ KAUR-16- 168418 020316-84-1 55
                EN-18-OIC ACID, (4.BETA.)- §§ (-)-
                KAURNENOIC ACID §§ (4-BETA)-KAUR-1
                6-EN-18-OIC ACID

50  36.016  0.08 D:\DATABASE\DEMO.L
                Androst-5-en-17-ol, 4,4-dimethyl-  513436 999513-44-9 53
                1-Hydroxy-3,7,8-trimethoxyxanthen- 504580 020882-69-3 46
                9-one §§ 8-Hydroxy-1,2,6-trimethox
                y-9H-xanthen-9-one #
                KAUR-16-EN-18-OIC ACID §§ KAUR-16- 168418 020316-84-1 45
                EN-18-OIC ACID, (4.BETA.)- §§ (-)-
                KAURNENOIC ACID §§ (4-BETA)-KAUR-1
                6-EN-18-OIC ACID

51  36.097  0.16 D:\DATABASE\DEMO.L
                1H-NAPHTHO[2,3-C]PYRAN-5,10-DIONE, 513558 084018-43-9 74
                 3,4-DIHYDRO-7,9-DIMETHOXY-1,3-DIM
                ETHYL-, CIS-(.+-.)- §§ (+,-)-CIS-7
                ,9-DIMETHOXY-1,3-DIMETHYL-3,4,5,10
                -TETRAHYDRONAPHTHO[2,3-C]PYRAN-5,1
                0-DIONE
                2-ACETYL-4,9-DIMETHOXY-7-METHYL-5H 513538 092611-83-1 46
                -FURO[3,2-G][1]-BENZOPYRAN-5-ONE
                KAUR-16-EN-18-OIC ACID §§ KAUR-16- 168418 020316-84-1 45
                EN-18-OIC ACID, (4.BETA.)- §§ (-)-
                KAURNENOIC ACID §§ (4-BETA)-KAUR-1
                6-EN-18-OIC ACID

52  36.194  0.05 D:\DATABASE\DEMO.L
                Abietic acid §§ 1-Phenanthrenecarb 513378 000514-10-3 59
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid
                2-(DIPHENYLMETHYLENE)OCTAHYDRO-4H- 513666 082432-11-9 56
                INDEN-4-ONE §§ BICYCLO[4.3.0]NONAN
                -2-ONE, 8-(DIPHENYLMETHYLENE)- §§
                BICYCLO[4.3.0]NONANE-2-ONE, 8-DIPH
                ENYLMETHYLENE-
                Bicyclo[4.3.0]nonan-2-one, 8-(diph 513389 082432-11-9 56
                enylmethylene)- §§ 2-(Diphenylmeth
                ylene)octahydro-4H-indan-4-one #

53  36.254  0.07 D:\DATABASE\DEMO.L
                Androst-5-en-17-ol, 4,4-dimethyl-  513436 999513-44-9 81
                Palustric acid §§ Podocarpa-8,13-d 513439 001945-53-5 50
                ien-15-oic acid, 13-isopropyl- §§
                1-Phenanthrenecarboxylic acid, 1,2
                ,3,4,4a,5,6,9,10,10a-decahydro-1,4
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Data File : WLM-10prsen-160c-4jm.D
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Operator  :
Sample    :
Misc      :
ALS Vial  : 1   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e

#     RT  Area%          Library/ID                    Ref#     CAS#   Qual
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              a-dimethyl-7-(1-methylethyl)-, (1R
              -(1.alpha.,4a.beta.,10a.alpha.))-
              §§ 8,13-Abietadien-18-oic acid
              1-Hydroxy-3,7,8-trimethoxyxanthen- 504580 020882-69-3 41
              9-one §§ 8-Hydroxy-1,2,6-trimethox
              y-9H-xanthen-9-one #

4  36.389  0.19 D:\DATABASE\DEMO.L
              Methyl abietate §§ 1-Phenanthrenec 258889 000127-25-3 97
              arboxylic acid, 1,2,3,4,4a,4b,5,6,
              10,10a-decahydro-1,4a-dimethyl-7-(
              1-methylethyl)-, methyl ester, [1R
              -(1.alpha.,4a.beta.,4b.alpha.,10a.
              alpha.)]- §§ Podocarpa-7,13-dien-1
              5-oic acid, 13-isopropyl-, methyl
              ester §§ Abalyn
              METHYL ABIETA-7,13-DIEN-18-OATE §§ 258918 000127-25-3 97
               1-PHENANTHRENECARBOXYLIC ACID, 1,
              2,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1
              ,4A-DIMETHYL-7-(1-METHYLETHYL)-, M
              ETHYL ESTER, [1R-(1.ALPHA.,4A.BETA
              .,4B.ALPHA.,10A.ALPHA.)]- §§ ABALY
              N §§ ABIETIC ACID METHYL ESTER
              METHYL ABIETA-7,13-DIEN-18-OATE §§ 480551 000127-25-3 95
               1-PHENANTHRENECARBOXYLIC ACID, 1,
              2,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1
              ,4A-DIMETHYL-7-(1-METHYLETHYL)-, M
              ETHYL ESTER, [1R-(1.ALPHA.,4A.BETA
              .,4B.ALPHA.,10A.ALPHA.)]- §§ ABALY
              N §§ ABIETIC ACID METHYL ESTER

5  36.513  0.11 D:\DATABASE\DEMO.L
              1H-NAPHTHO[2,3-C]PYRAN-5,10-DIONE, 513558 084018-43-9 90
               3,4-DIHYDRO-7,9-DIMETHOXY-1,3-DIM
              ETHYL-, CIS-(.+-.)- §§ (+,-)-CIS-7
              ,9-DIMETHOXY-1,3-DIMETHYL-3,4,5,10
              -TETRAHYDRONAPHTHO[2,3-C]PYRAN-5,1
              0-DIONE
              KAUR-16-EN-18-OIC ACID §§ KAUR-16- 168418 020316-84-1 64
              EN-18-OIC ACID, (4.BETA.)- §§ (-)-
              KAURNENOIC ACID §§ (4-BETA)-KAUR-1
              6-EN-18-OIC ACID
              Androst-5-en-17-ol, 4,4-dimethyl-  513436 999513-44-9 55

6  36.610  0.27 D:\DATABASE\DEMO.L
              O-HYDROGEN PERDEUTERIO HEXADECANOI 504545 039756-30-4 90
              C ACID
              KAUR-16-EN-18-OIC ACID §§ KAUR-16- 168418 020316-84-1 90
              EN-18-OIC ACID, (4.BETA.)- §§ (-)-
              KAURNENOIC ACID §§ (4-BETA)-KAUR-1
              6-EN-18-OIC ACID
              Palustric acid §§ Podocarpa-8,13-d 513439 001945-53-5 78
              ien-15-oic acid, 13-isopropyl- §§
              1-Phenanthrenecarboxylic acid, 1,2
              ,3,4,4a,5,6,9,10,10a-decahydro-1,4
              a-dimethyl-7-(1-methylethyl)-, (1R
              -(1.alpha.,4a.beta.,10a.alpha.))-
              §§ 8,13-Abietadien-18-oic acid
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Sample    :
Misc      :
ALS Vial  : 1   Sample Multiplier: 1

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Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e

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57  36.751  0.35 D:\DATABASE\DEMO.L
                 Abietic acid §§ 1-Phenanthrenecarb 513344 000514-10-3 64
                 oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                 10a-decahydro-1,4a-dimethyl-7-(1-m
                 ethylethyl)-, [1R-(1.alpha.,4a.bet
                 a.,4b.alpha.,10a.alpha.)]- §§ Podo
                 carpa-7,13-dien-15-oic acid, 13-is
                 opropyl- §§ L-abietic acid
                 KAUR-16-EN-18-OIC ACID §§ KAUR-16- 168418 020316-84-1 64
                 EN-18-OIC ACID, (4.BETA.)- §§ (-)-
                 KAURNENOIC ACID §§ (4-BETA)-KAUR-1
                 6-EN-18-OIC ACID
                 Methanone, [1,4-dimethyl-7-(1-meth 513367 039665-56-0 55
                 ylethyl)-2-azulenyl]phenyl- §§ 2-B
                 enzoylguaiazulene §§ (7-Isopropyl-
                 1,4-dimethyl-2-azulenyl)(phenyl)me
                 thanone #

58  36.972  0.35 D:\DATABASE\DEMO.L
                 1-Phenanthrenecarboxylic acid, 1,2 503081 001740-19-8 96
                 ,3,4,4a,9,10,10a-octahydro-1,4a-di
                 methyl-7-(1-methylethyl)-, [1R-(1.
                 alpha.,4a.beta.,10a.alpha.)]- §§ P
                 odocarpa-8,11,13-trien-15-oic acid
                 , 13-isopropyl- §§ Abieta-8,11,13-
                 trien-18-oic acid §§ Abietic acid,
                  dehydro-
                 1-Phenanthrenecarboxylic acid, 1,2 503093 001740-19-8 95
                 ,3,4,4a,9,10,10a-octahydro-1,4a-di
                 methyl-7-(1-methylethyl)-, [1R-(1.
                 alpha.,4a.beta.,10a.alpha.)]- §§ P
                 odocarpa-8,11,13-trien-15-oic acid
                 , 13-isopropyl- §§ Abieta-8,11,13-
                 trien-18-oic acid §§ Abietic acid,
                  dehydro-
                 1-PHENANTHRENECARBOXYLIC ACID, 1,2 503110 001740-19-8 95
                 ,3,4,4A,9,10,10A-OCTAHYDRO-1,4A-DI
                 METHYL-7-(1-METHYLETHYL)-, [1R-(1.
                 ALPHA.,4A.BETA.,10A.ALPHA.)]- §§ (
                 -)-DEHYDROABIETIC ACID §§ 1,2,3,4,
                 4A,9,10,10A-OCTAHYDRO-1,4A-DIMETHY
                 L-7-(1-METHYLETHYL)-1-PHENANTHRENE
                 CARBOXYLIC ACID

59  37.032  0.67 D:\DATABASE\DEMO.L
                 1-Phenanthrenecarboxylic acid, 1,2 503081 001740-19-8 80
                 ,3,4,4a,9,10,10a-octahydro-1,4a-di
                 methyl-7-(1-methylethyl)-, [1R-(1.
                 alpha.,4a.beta.,10a.alpha.)]- §§ P
                 odocarpa-8,11,13-trien-15-oic acid
                 , 13-isopropyl- §§ Abieta-8,11,13-
                 trien-18-oic acid §§ Abietic acid,
                  dehydro-
                 1-Phenanthrenecarboxylic acid, 1,2 503093 001740-19-8 60
                 ,3,4,4a,9,10,10a-octahydro-1,4a-di
                 methyl-7-(1-methylethyl)-, [1R-(1.
                 alpha.,4a.beta.,10a.alpha.)]- §§ P
                 odocarpa-8,11,13-trien-15-oic acid
                 , 13-isopropyl- §§ Abieta-8,11,13-
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Data Path : D:\DATA 03\DEM\
Data File : WLM-10prsen-160c-4jm.D
Acq On : 12 Oct 2019 11:41
Operator :
Sample :
Misc :
ALS Vial : 1 Sample Multiplier: 1

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Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			trien-18-oic acid §§ Abietic acid, dehydro-			
			1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,9,10,10A-OCTAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL)-, [1R-(1.ALPHA.,4A.BETA.,10A.ALPHA.)]- §§ (-)-DEHYDROABIETIC ACID §§ 1,2,3,4,4A,9,10,10A-OCTAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL)-1-PHENANTHRENECARBOXYLIC ACID	503110	001740-19-8	60
60	37.237	0.69	D:\DATABASE\DEMO.L			
			ABIETA-7,13-DIEN-18-OIC ACID §§ 1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,4B,5,6,10,10A-DECAHYDRO- §§ 1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL)-, [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A.ALPHA.)]-	168419	000514-10-3	87
			1H-2,10A-ETHANOPHENANTHRENE, KAUR-16-EN-18-OIC ACID DERIV. §§ KAUR-16-EN-18-OIC ACID §§ KAUR-16-EN-18-OIC ACID, (4.ALPHA.)- §§ (-)-ENT-KAUR-16-EN-19-OIC ACID	513651	006730-83-2	64
			Abietic acid §§ 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,4b,5,6,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1R-(1.alpha.,4a.beta.,4b.alpha.,10a.alpha.)]- §§ Podocarpa-7,13-dien-15-oic acid, 13-isopropyl- §§ L-abietic acid	513344	000514-10-3	64
61	37.464	0.14	D:\DATABASE\DEMO.L			
			ABIETA-7,13-DIEN-18-OIC ACID §§ 1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,4B,5,6,10,10A-DECAHYDRO- §§ 1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL)-, [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A.ALPHA.)]-	168420	000514-10-3	89
			1H-2,10A-ETHANOPHENANTHRENE, KAUR-16-EN-18-OIC ACID DERIV. §§ KAUR-16-EN-18-OIC ACID §§ KAUR-16-EN-18-OIC ACID, (4.ALPHA.)- §§ (-)-ENT-KAUR-16-EN-19-OIC ACID	513651	006730-83-2	64
			ABIETA-7,13-DIEN-18-OIC ACID §§ 1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,4B,5,6,10,10A-DECAHYDRO- §§ 1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL)-, [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A.ALPHA.)]-	168419	000514-10-3	60
62	37.685	2.34	D:\DATABASE\DEMO.L			
			Abietic acid §§ 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,4b,5,6,10,	513378	000514-10-3	99

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-160c-4jm.D
Acq On : 12 Oct 2019 11:41
Operator :
Sample :
Misc :
ALS Vial : 1 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid			
			Abietic acid $$ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid	513344	000514-10-3	94
			Abietic acid $$ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid	513347	000514-10-3	93
63	38.506	0.12	D:\DATABASE\DEMO.L			
			Abietic acid $$ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid	513378	000514-10-3	92
			Abietic acid $$ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid	513347	000514-10-3	78
			.beta.-Pimaric acid $$ .delta.6,8(14)-Abietadienoic acid $$ l-Pimari c acid $$ l-Sapietic acid	513374	000079-54-9	76
64	38.755	0.04	D:\DATABASE\DEMO.L			
			Abietic acid $$ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid	513378	000514-10-3	90
			Abietic acid $$ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid	513347	000514-10-3	64
			1H-2,10A-ETHANOPHENANTHRENE, KAUR- 16-EN-18-OIC ACID DERIV. $$ KAUR-1 6-EN-18-OIC ACID $$ KAUR-16-EN-18- OIC ACID, (4.ALPHA.)- $$ (-)-ENT-K AUR-16-EN-19-OIC ACID	513651	006730-83-2	60

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Data Path : F:\DATA MS\daa\
Data File : WLM-10prsen-160c-4jm.D
Acq On    : 12 Oct 2019  11:41
Operator  :
Sample    :
Misc      :
ALS Vial  : 1   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e

#     RT  Area%          Library/ID                  Ref#     CAS#   Qual
-------------------------------------------------------------------------

5  38.831  0.14 D:\DATABASE\DEMO.L
                Abietic acid §§ 1-Phenanthrenecarb 513344 000514-10-3 53
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid
                1,4-BENZENEDICARBOXYLIC ACID, DIET 380622 000636-09-9 38
                HYL ESTER §§ DIETHYL ESTER OF 1,4-
                BENZENEDICARBOXYLIC ACID §§ DIETHY
                L P-PHTHALATE §§ DIETHYL TEREPHTHA
                LATE
                Naphthalene, 1,2,3,4-tetrahydro-6- 380125 019353-86-7 25
                nitro- §§ 6-Nitrotetralin §§ 6-Nit
                ro-1,2,3,4-tetrahydronaphthalene #

6  39.014  0.19 D:\DATABASE\DEMO.L
                Abietic acid §§ 1-Phenanthrenecarb 513347 000514-10-3 50
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid
                Abietic acid §§ 1-Phenanthrenecarb 513378 000514-10-3 44
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid
                CYCLOTETRADECA[B]FURAN-7(4H)-ONE,  294174 070701-53-0 25
                2,5,6,8,9,12,13,15A-OCTAHYDRO-3,6,
                10,14-TETRAMETHYL- §§ (3Z,10E,14E)
                -6,7-EPOXY-3,6,10,14-TETRAMETHYL-2
                ,4,5,6,7,8,9,12,13,15A-DECAHYDROCY
                CLOTETRADECA(B)FURAN
```

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsen-180c-ljm.D
Acq On : 10 Oct 2019 12:12
Operator :
Sample :
Misc :
ALS Vial : 3 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	1.962	4.47	D:\DATABASE\DEMO.L			
			Methyl Alcohol $$ Methanol $$ Carb inol $$ Methyl hydroxide	5073	000067-56-1	2
			METHANOL $$ HYDROXYMETHANE $$ ALCO HOL, METHYL $$ ALCOOL METHYLIQUE	5075	000067-56-1	2
			Methyl Alcohol $$ Methanol $$ Carb inol $$ Methyl hydroxide	5072	000067-56-1	2
2	2.135	0.13	D:\DATABASE\DEMO.L			
			Pentane, 2,4-dimethyl- $$ 2,4-Dime thylpentane	18750	000108-08-7	87
			PENTANE, 2,4-DIMETHYL- $$ 2,4-DIME THYLPENTANE $$ PENTANE, 2,4-DIMETH YL	19002	000108-08-7	80
			PENTANE, 2,4-DIMETHYL- $$ 2,4-DIME THYLPENTANE $$ PENTANE, 2,4-DIMETH YL	18833	000108-08-7	80
3	2.205	11.57	D:\DATABASE\DEMO.L			
			Hexane, 3-methyl- $$ 2-Ethylpentan e $$ 3-Methylhexane	18811	000589-34-4	83
			HEXANE, 3-METHYL- $$ 3-METHYLHEXAN E $$ 2-ETHYLPENTANE $$ HEXANE, 3-M ETHYL	18994	000589-34-4	81
			PENTANE, 2,3-DIMETHYL- $$ 2,3-DIME THYLPENTANE $$ 3, 4-DIMETHYLPENTAN E $$ 3,4-DIMETHYLPENTANE	62374	000565-59-3	68
4	2.243	4.47	D:\DATABASE\DEMO.L			
			1,3-DIMETHYLCYCLOPENTANE $$ CYCLOP ENTANE, 1,3-DIMETHYL-, CIS- $$ 1,3 -DIMETHYLCYCLOPENTANE (CIS) $$ 1,3 -DIMETHYLCYCLOPENTANE CIS	62286	002532-58-3	91
			Cyclopentane, 1,3-dimethyl-, cis- $$ cis-1,3-Dimethylcyclopentane $$ 1,3-Dimethylcyclopentane cis $$ 1 ,3-Dimethylcyclopentane #	62231	002532-58-3	91
			Cyclopentane, 1,3-dimethyl- $$ 1,3 -Dimethylcyclopentane	101343	002453-00-1	91
5	2.334	6.89	D:\DATABASE\DEMO.L			
			CYCLOHEXANE, METHYL- $$ METHYLCYCL OHEXANE $$ 1-METHYLCYCLOHEXANE $$ CYCLOHEXANE, METHYL	141469	000108-87-2	96
			CYCLOHEXANE, METHYL- $$ METHYLCYCL OHEXANE $$ 1-METHYLCYCLOHEXANE $$ CYCLOHEXANE, METHYL	141470	000108-87-2	95
			Cyclohexane, methyl- $$ Cyclohexyl methane $$ Hexahydrotoluene $$ Met hylcyclohexane	141386	000108-87-2	94
6	2.421	68.41	D:\DATABASE\DEMO.L			
			Toluene $$ Benzene, methyl $$ Meth acide $$ Methylbenzene	158580	000108-88-3	91
			BENZENE, METHYL- $$ METHYLBENZENE $$ TOLUENE $$ ANTISAL 1A	158622	000108-88-3	91
			BENZENE, METHYL- $$ METHYLBENZENE $$ TOLUENE $$ ANTISAL 1A	158625	000108-88-3	90

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Data Path : P:\DATA MS\data\
Data File : WLM-10pesen-180c-1jm.D
Acq On    : 10 Oct 2019  12:12
Operator  :
Sample    :
Misc      :
ALS Vial  : 3   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autointl.e

#     RT  Area%          Library/ID                   Ref#     CAS#   Qual
_____________________________________________________________________________

7   2.745  0.88 D:\DATABASE\DEMO.L
                CYCLOHEXANE, ETHYL- §§ ETHYLCYCLOH  54538 001678-91-7 70
                EXANE §§ ETHYL CYCLOHEXANE §§ ETHY
                LCYCLOHEXAN
                ETHYLCYCLOHEXANE §§ ETHYLCYCLOHEXA  54425 001678-91-7 70
                CYCLOHEXANE, ETHYL- §§ ETHYLCYCLOH 141558 001678-91-7 70
                EXANE §§ ETHYL CYCLOHEXANE §§ ETHY
                LCYCLOHEXAN

8  34.541  0.13 D:\DATABASE\DEMO.L
                Pentacyclo[7.5.0.0(2,8).0(5,14).0( 132851 079772-15-9 48
                7,11)]tetradecane
                PENTACYCLO[7.5.0.0(2,8).0(5,14).0( 132860 079772-15-9 48
                7,11)]TETRADECANE
                Phenanthrene, 7-ethenyl-1,2,3,4,4a 481092 055255-56-6 30
                ,5,6,7,8,9,10,10a-dodecahydro-1,1,
                4a,7-tetramethyl- §§ Pimara-8,15-d
                iene #

9  35.465  0.09 D:\DATABASE\DEMO.L
                Pimaric acid §§ 1-Phenanthrenecarb 466434 000127-27-5 64
                oxylic acid, 7-ethenyl-1,2,3,4,4a,
                4b,5,6,7,9,10,10a-dodecahydro-1,4a
                ,7-trimethyl-, [1R-(1.alpha.,4a.be
                ta.,4b.alpha.,7.beta.,10a.alpha.)]
                - §§ Podocarp-8(14)-en-15-oic acid
                , 13.alpha.-methyl-13-vinyl- §§ D-
                pimaric acid
                KAUR-16-EN-18-OIC ACID §§ KAUR-16- 168418 020316-84-1 46
                EN-18-OIC ACID, (4.BETA.)- §§ (-)-
                KAURNENOIC ACID §§ (4-BETA)-KAUR-1
                6-EN-18-OIC ACID
                Chromium, carbonyl-(.eta.-4-1,3-bu 398828 999398-83-2 38
                tadiene)(.eta.-5-pentamethylcyclop
                entadienyl)-

0  35.756  0.06 D:\DATABASE\DEMO.L
                DEHYDROABIETIC ACID                 464556 000000-00-0 97
                1-Phenanthrenecarboxylic acid, 1,2 464538 001235-74-1 95
                ,3,4,4a,9,10,10a-octahydro-1,4a-di
                methyl-7-(1-methylethyl)-, methyl
                ester, [1R-(1.alpha.,4a.beta.,10a.
                alpha.)]- §§ Podocarpa-8,11,13-tri
                en-15-oic acid, 13-isopropyl-, met
                hyl ester §§ Methyl dehydroabietat
                METHYL ABIETA-8,11,13-TRIEN-18-OAT 464550 001235-74-1 95
                E §§ 1-PHENANTHRENECARBOXYLIC ACID
                , 1,2,3,4,4A,9,10,10A-OCTAHYDRO-1,
                4A-DIMETHYL-7-(1-METHYLETHYL)-, ME
                THYL ESTER, [1R-(1.ALPHA.,4A.BETA.
                ,10A.ALPHA.)]- §§ DEHYDROABIETIC A
                CID METHYL ESTER §§ METHYL DEHYDRO
                ABIETATE

1  36.091  0.14 D:\DATABASE\DEMO.L
                INDOLIZINO[1,2-B]QUINOLIN-9(11H)-O 504762 054318-62-6 93
                NE, 8-[(FORMYLOXY)METHYL]-7-(1-OXO
                PROPYL)- §§ 8-FORMYLOXYMETHYL-7-(1
                -OXOPROPYL)INDOLIZINO)1,2-B)QUINOL
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Data Path : F:\DATA MS\daa\
Data File : WLM-10prsen-180c-ljm.D
Acq On    : 10 Oct 2019  12:12
Operator  :
Sample    :
Misc      :
ALS Vial  : 3   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e

k#     RT  Area%          Library/ID                    Ref#     CAS#   Qual
                IN-9(11H)-ONE
                PIMARA-8(14),15-DIEN-18-OIC ACID § 504608 000127-27-5 80
                § 1-PHENANTHRENECARBOXYLIC ACID, 7
                -ETHENYL-1,2,3,4,4A,4B,5,6,7,9,10,
                10A-DODECAHYDRO-1,4A,7-TRIMETHYL-,
                 [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,
                7.BETA.,10A.ALPHA.)]- §§ (+)-PIMAR
                IC ACID §§ .ALPHA.-PIMARIC ACID
                Xanthan-9-one, 1-hydroxy-3,5,8-tri 504583 049599-09-9 64
                methoxy- §§ 5,8-Dimethylbellidifol
                in §§ 1-Hydroxy-3,5,8-trimethoxyxa
                nthan-9-one §§ 1-Hydroxy-3,5,8-tri
                methoxy-9H-xanthen-9-one #

12  36.383  0.06 D:\DATABASE\DEMO.L
                METHYL ABIETA-7,13-DIEN-18-OATE §§ 480551 000127-25-3 99
                 1-PHENANTHRENECARBOXYLIC ACID, 1,
                2,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1
                ,4A-DIMETHYL-7-(1-METHYLETHYL)-, M
                ETHYL ESTER, [1R-(1.ALPHA.,4A.BETA
                .,4B.ALPHA.,10A.ALPHA.)]- §§ ABALY
                N §§ ABIETIC ACID METHYL ESTER
                METHYL ABIETA-7,13-DIEN-18-OATE §§ 258918 000127-25-3 96
                 1-PHENANTHRENECARBOXYLIC ACID, 1,
                2,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1
                ,4A-DIMETHYL-7-(1-METHYLETHYL)-, M
                ETHYL ESTER, [1R-(1.ALPHA.,4A.BETA
                .,4B.ALPHA.,10A.ALPHA.)]- §§ ABALY
                N §§ ABIETIC ACID METHYL ESTER
                Methyl abietate §§ 1-Phenanthrenec 258889 000127-25-3 96
                arboxylic acid, 1,2,3,4,4a,4b,5,6,
                10,10a-decahydro-1,4a-dimethyl-7-(
                1-methylethyl)-, methyl ester, [1R
                -(1.alpha.,4a.beta.,4b.alpha.,10a.
                alpha.)]- §§ Podocarpa-7,13-dien-1
                5-oic acid, 13-isopropyl-, methyl
                ester §§ Abalyn

13  36.594  0.45 D:\DATABASE\DEMO.L
                KAUR-16-EN-18-OIC ACID §§ KAUR-16- 168418 020316-84-1 87
                EN-18-OIC ACID, (4.BETA.)- §§ (-)-
                KAURMENOIC ACID §§ (4-BETA)-KAUR-1
                6-EN-18-OIC ACID
                Phenol, 2,4-bis(1-phenylethyl)- §§ 504578 002769-94-0 86
                 2,4-Bis(1-phenylethyl)phenol #
                4-Androsten-6.beta.-ol-3,17-dione  513437 999513-45-0 80

14  36.945  0.22 D:\DATABASE\DEMO.L
                1-Phenanthrenecarboxylic acid, 1,2 503093 001740-19-8 83
                ,3,4,4a,9,10,10a-octahydro-1,4a-di
                methyl-7-(1-methylethyl)-, [1R-(1.
                alpha.,4a.beta.,10a.alpha.)]- §§ P
                odocarpa-8,11,13-trien-15-oic acid
                , 13-isopropyl- §§ Abieta-8,11,13-
                trien-18-oic acid §§ Abietic acid,
                 dehydro-
                1-PHENANTHRENECARBOXYLIC ACID, 1,2 503110 001740-19-8 83
                ,3,4,4A,9,10,10A-OCTAHYDRO-1,4A-DI
                METHYL-7-(1-METHYLETHYL)-, [1R-(1.
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Data Path : F:\DATA MS\daa\
Data File : WLM-10prsen-180c-1jm.D
Acq On : 10 Oct 2019 12:12
Operator :
Sample :
Misc :
ALS Vial : 3 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autointl.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			ALPHA.,4A.BETA.,10A.ALPHA.)]- §§ (-)-DEHYDROABIETIC ACID §§ 1,2,3,4, 4A,9,10,10A-OCTAHYDRO-1,4A-DIMETHY L-7-(1-METHYLETHYL)-1-PHENANTHRENE CARBOXYLIC ACID			
			1-Phenanthrenecarboxylic acid, 1,2 ,3,4,4a,9,10,10a-octahydro-1,4a-di methyl-7-(1-methylethyl)-, [1R-(1. alpha.,4a.beta.,10a.alpha.)]- §§ P odocarpa-8,11,13-trien-15-oic acid , 13-isopropyl- §§ Abieta-8,11,13- trien-18-oic acid §§ Abietic acid, dehydro-	503082	001740-19-8	59
15	37.150	0.00	D:\DATABASE\DEMO.L			
			ABIETA-8,11,13-TRIEN-18-OIC ACID § § 1-PHENANTHRENECARBOXYLIC ACID, 1 ,2,3,4,4A,9,10,10A-OCTAHYDRO-1,4A- DIMETHYL-7-(1-METHYLETHYL)-, [1S-(1.ALPHA.,4A.ALPHA.,10A.BETA.)]- §§ 13-ISOPROPYLPODOCARPA-8,11,13-TRI EN-16-OIC ACID §§ 4-EPIABIETIC ACI D, DEHYDRO-	503112	005155-70-4	91
			1-Phenanthrenecarboxylic acid, 1,2 ,3,4,4a,9,10,10a-octahydro-1,4a-di methyl-7-(1-methylethyl)-, [1S-(1. alpha.,4a.alpha.,10a.beta.)]- §§ P odocarpa-8,11,13-trien-16-oic acid , 13-isopropyl- §§ Callitrisic aci d §§ 4-Epiabietic acid, dehydro-	503094	005155-70-4	91
			ABIETA-7,13-DIEN-18-OIC ACID §§ 1- PHENANTHRENECARBOXYLIC ACID, 1,2,3 ,4,4A,4B,5,6,10,10A-DECAHYDRO- §§ 1-PHENANTHRENECARBOXYLIC ACID, 1,2 ,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1, 4A-DIMETHYL-7-(1-METHYLETHYL)-, [1 R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A .ALPHA.)]-	168419	000514-10-3	83
16	37.220	0.00	D:\DATABASE\DEMO.L			
			ABIETA-7,13-DIEN-18-OIC ACID §§ 1- PHENANTHRENECARBOXYLIC ACID, 1,2,3 ,4,4A,4B,5,6,10,10A-DECAHYDRO- §§ 1-PHENANTHRENECARBOXYLIC ACID, 1,2 ,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1, 4A-DIMETHYL-7-(1-METHYLETHYL)-, [1 R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A .ALPHA.)]-	168420	000514-10-3	78
			Abietic acid §§ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- §§ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- §§ L-abietic acid	513378	000514-10-3	60
			Palustric acid §§ Podocarpa-8,13-d ien-15-oic acid, 13-isopropyl- §§ 1-Phenanthrenecarboxylic acid, 1,2 ,3,4,4a,5,6,9,10,10a-decahydro-1,4	513439	001945-53-5	58

```
Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-180c-1jm.D
Acq On    : 10 Oct 2019  12:12
Operator  :
Sample    :
Misc      :
ALS Vial  : 3   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autointl.e

#     RT  Area%          Library/ID                  Ref#     CAS#   Qual
_____________________________________________________________________

              a-dimethyl-7-(1-methylethyl)-, (1R
              -(1.alpha.,4a.beta.,10a.alpha.))-
              §§ 8,13-Abietadien-18-oic acid

7  37.690  2.05 D:\DATABASE\DEMO.L
              Abietic acid §§ 1-Phenanthrenecarb 513378 000514-10-3 99
              oxylic acid, 1,2,3,4,4a,4b,5,6,10,
              10a-decahydro-1,4a-dimethyl-7-(1-m
              ethylethyl)-, [1R-(1.alpha.,4a.bet
              a.,4b.alpha.,10a.alpha.)]- §§ Podo
              carpa-7,13-dien-15-oic acid, 13-is
              opropyl- §§ L-abietic acid
              Abietic acid §§ 1-Phenanthrenecarb 513344 000514-10-3 96
              oxylic acid, 1,2,3,4,4a,4b,5,6,10,
              10a-decahydro-1,4a-dimethyl-7-(1-m
              ethylethyl)-, [1R-(1.alpha.,4a.bet
              a.,4b.alpha.,10a.alpha.)]- §§ Podo
              carpa-7,13-dien-15-oic acid, 13-is
              opropyl- §§ L-abietic acid
              Abietic acid §§ 1-Phenanthrenecarb 513347 000514-10-3 90
              oxylic acid, 1,2,3,4,4a,4b,5,6,10,
              10a-decahydro-1,4a-dimethyl-7-(1-m
              ethylethyl)-, [1R-(1.alpha.,4a.bet
              a.,4b.alpha.,10a.alpha.)]- §§ Podo
              carpa-7,13-dien-15-oic acid, 13-is
              opropyl- §§ L-abietic acid
```

```
ata Path : F:\DATA MS\daa\
ata File : WLM-10pr2en-180c-2jm.D
cq On    : 12 Oct 2019   8:00
perator  :
ample    :
isc      :
LS Vial  : 1   Sample Multiplier: 1

earch Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

nknown Spectrum:   Apex
ntegration Events: ChemStation Integrator - autointl.e

     RT  Area%          Library/ID                    Ref#     CAS#   Qual
   1.962  6.63 D:\DATABASE\DEMO.L
            Methyl Alcohol $$ Methanol $$ Carb   5073 000067-56-1  2
            inol $$ Methyl hydroxide
            METHANOL $$ HYDROXYMETHANE $$ ALCO   5075 000067-56-1  2
            HOL, METHYL $$ ALCOOL METHYLIQUE
            Methyl Alcohol $$ Methanol $$ Carb   5072 000067-56-1  2
            inol $$ Methyl hydroxide

   2.070  0.02 D:\DATABASE\DEMO.L
            Decyl trifluoroacetate $$ Decyl 2,  32006 000333-88-0 42
            2,2-trifluoroacetate $$ 1-Decanol,
             trifluoroacetate $$ Acetic acid,
            trifluoro-, decyl ester
            2-BUTANOL $$ 2-HYDROXYBUTANE $$ BU   5194 000078-92-2 38
            TAN-2-OL $$ (1)-BUTAN-2-OL
            2-ETHOXYETHANOL $$ ETHYLGLYCOL       5272 999005-27-3 33

   2.135  0.18 D:\DATABASE\DEMO.L
            Pentane, 2,4-dimethyl- $$ 2,4-Dime  18753 000108-08-7 91
            thylpentane
            Pentane, 2,4-dimethyl- $$ 2,4-Dime  18750 000108-08-7 87
            thylpentane
            PENTANE, 2,4-DIMETHYL- $$ 2,4-DIME  19001 000108-08-7 83
            THYLPENTANE $$ PENTANE, 2,4-DIMETH
            YL

   2.200 12.59 D:\DATABASE\DEMO.L
            HEXANE, 3-METHYL- $$ 3-METHYLHEXAN  18994 000589-34-4 64
            E $$ 2-ETHYLPENTANE $$ HEXANE, 3-M
            ETHYL
            Hexane, 3-methyl- $$ 2-Ethylpentan  18743 000589-34-4 62
            e $$ 3-Methylhexane
            HEPTANE $$ ALIPHATIC HYDROCARBON $   18986 000142-82-5 58
            $ DIPROPYL METHANE $$ DIPROPYLMETH
            ANE

   2.243  4.83 D:\DATABASE\DEMO.L
            Cyclopentane, 1,3-dimethyl- $$ 1,3 101343 002453-00-1 91
            -Dimethylcyclopentane
            1,3-DIMETHYLCYCLOPENTANE $$ CYCLOP  62286 002532-58-3 91
            ENTANE, 1,3-DIMETHYL-, CIS- $$ 1,3
            -DIMETHYLCYCLOPENTANE (CIS) $$ 1,3
            -DIMETHYLCYCLOPENTANE CIS
            Cyclopentane, 1,3-dimethyl-, cis-   62231 002532-58-3 91
            $$ cis-1,3-Dimethylcyclopentane $$
             1,3-Dimethylcyclopentane cis $$ 1
            ,3-Dimethylcyclopentane #

   2.335  7.14 D:\DATABASE\DEMO.L
            CYCLOHEXANE, METHYL- $$ METHYLCYCL 141469 000108-87-2 96
            OHEXANE $$ 1-METHYLCYCLOHEXANE $$
            CYCLOHEXANE, METHYL
            CYCLOHEXANE, METHYL- $$ METHYLCYCL 141467 000108-87-2 95
            OHEXANE $$ 1-METHYLCYCLOHEXANE $$
            CYCLOHEXANE, METHYL
            CYCLOHEXANE, METHYL- $$ METHYLCYCL 141470 000108-87-2 95
            OHEXANE $$ 1-METHYLCYCLOHEXANE $$
            CYCLOHEXANE, METHYL
```

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Data Path : F:\DATA MS\daa\
Data File : WLM-10prsen-180c-2jm.D
Acq On    : 12 Oct 2019    8:00
Operator  :
Sample    :
Misc      :
ALS Vial  : 1   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#     RT  Area%          Library/ID                  Ref#     CAS#   Qual
-----------------------------------------------------------------------------
 7   2.421 58.68 D:\DATABASE\DEMO.L
                 Toluene $$ Benzene, methyl $$ Meth 158580 000108-88-3 91
                 acide $$ Methylbenzene
                 BENZENE, METHYL- $$ METHYLBENZENE  158625 000108-88-3 90
                 $$ TOLUENE $$ ANTISAL 1A
                 BENZENE, METHYL- $$ METHYLBENZENE  158622 000108-88-3 87
                 $$ TOLUENE $$ ANTISAL 1A

 8   2.745  1.07 D:\DATABASE\DEMO.L
                 Cyclohexane, ethyl- $$ Ethylcycloh 141508 001678-91-7 93
                 exane
                 CYCLOHEXANE, ETHYL- $$ ETHYLCYCLOH 141562 001678-91-7 81
                 EXANE $$ ETHYL CYCLOHEXANE $$ ETHY
                 LCYCLOHEXAN
                 CYCLOHEXANE, ETHYL- $$ ETHYLCYCLOH 141528 001678-91-7 81
                 EXANE $$ ETHYL CYCLOHEXANE $$ ETHY
                 LCYCLOHEXAN

 9   2.859  0.51 D:\DATABASE\DEMO.L
                 1,3,5-Cycloheptatriene $$ Tropilid 158600 000544-25-2 87
                 ene $$ Cyclohepta-1,3,5-triene $$
                 Cycloheptatriene
                 1,3,5-CYCLOHEPTATRIENE $$ CYCLOHEP 158637 000544-25-2 83
                 TA-1,3,5-TRIENE $$ CYCLOHEPTATRIEN
                 E $$ CYCLOHEPTATRIENE [UN2603] [FL
                 AMMABLE LIQUID]
                 1,3,5-CYCLOHEPTATRIENE $$ CYCLOHEP 158604 000544-25-2 80
                 TA-1,3,5-TRIENE $$ CYCLOHEPTATRIEN
                 E $$ CYCLOHEPTATRIENE [UN2603] [FL
                 AMMABLE LIQUID]

10  17.304  0.03 D:\DATABASE\DEMO.L
                 2H-2,4a-Methanonaphthalene, 1,3,4, 350641 001135-66-6 98
                 5,6,7-hexahydro-1,1,5,5-tetramethy
                 l-, (2S)- $$ 2H-2,4a-Methanonahth
                 alene, 1,3,4,5,6,7-hexahydro-1,1,5
                 ,5-tetramethyl-, (2S,4aR)-(-)- $$
                 Isolongifolene $$ (-)-Isolongifoli
                 ne
                 2H-2,4A-METHANONAPHTHALENE, 1,3,4, 350804 001135-66-6 97
                 5,6,7-HEXAHYDRO-1,1,5,5-TETRAMETHY
                 L-, (2S)- $$ (-)-ISOLONGIFOLENE $$
                  (-)-ISOLONGIFOLINE $$ (2S)-1,3,4,
                 5,6,7-HEXAHYDRO-1,1,5,5-TETRAMETHY
                 L-2H-2,4A-METHANONAPHTHALENE
                 2H-2,4A-METHANONAPHTHALENE, 1,3,4, 350805 001135-66-6 96
                 5,6,7-HEXAHYDRO-1,1,5,5-TETRAMETHY
                 L-, (2S)- $$ (-)-ISOLONGIFOLENE $$
                  (-)-ISOLONGIFOLINE $$ (2S)-1,3,4,
                 5,6,7-HEXAHYDRO-1,1,5,5-TETRAMETHY
                 L-2H-2,4A-METHANONAPHTHALENE

11  17.693  0.01 D:\DATABASE\DEMO.L
                 2-METHOXY-4-(METHOXYMETHYL)-6-METH   7347 063644-84-8 12
                 YLNICOTINONITRILE $$ PYRIDINE-3-CA
                 RBONITRILE, 2,4-DIMETHOXY-6-METHYL
                 3-(3-OXO-3H-BENZO[F]CHROMEN-2-YL)-   7476 999007-47-7  9
                 2,4(1H,3H)-QUINOLINEDIONE $$ 4-HYD
                 ROXY-3-(2-OXO-2H-1-OXA-3-PHENANTHR
```

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Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-180c-2jm.D
Acq On    : 12 Oct 2019    8:00
Operator  :
Sample    :
Misc      :
ALS Vial  : 1   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e

k#     RT  Area%          Library/ID                    Ref#     CAS#   Qual
                YL)-2(1H)-QUINOLINONE
                2,2,3,3,4,4,5,5-OCTAFLUORO-N-(3-ME   7474 339166-43-7  9
                THOXYPHENYL)PENTANAMIDE §§ PENTANA
                MIDE, 2,2,3,3,4,4,5,5-OCTAFLUORO-N
                -(3-METHOXYPHENYL)-

12  28.599  0.00 D:\DATABASE\DEMO.L
                4-(METHOXYMETHYL)-6-METHYL-2-PHENO   7413 332057-36-0 38
                XYNICOTINONITRILE §§ PYRIDINE-3-CA
                RBONITRILE, 4-METHOXYMETHYL-6-METH
                YL-2-PHENOXY-
                1-Dodecanamine §§ Dodecylamine §§    4652 000124-22-1  9
                n-Dodecylamine §§ Alamine 4
                1-DODECANAMINE §§ 1-AMINODODECANE    4661 000124-22-1  9
                §§ 1-DODECYLAMINE §§ ALAMINE 4

13  28.934  0.00 D:\DATABASE\DEMO.L
                4-(METHOXYMETHYL)-6-METHYL-2-PHENO   7413 332057-36-0 22
                XYNICOTINONITRILE §§ PYRIDINE-3-CA
                RBONITRILE, 4-METHOXYMETHYL-6-METH
                YL-2-PHENOXY-
                2-METHOXY-4-(METHOXYMETHYL)-6-METH   7347 063644-84-8 12
                YLNICOTINONITRILE §§ PYRIDINE-3-CA
                RBONITRILE, 2,4-DIMETHOXY-6-METHYL
                4-BROMO-N-[(6-METHYL-2-PYRIDYL)AMI   7473 999007-47-4 12
                NOMETHYL]PHTHALIMIDE §§ 5-BROMO-2-
                {[(6-METHYL-2-PYRIDINYL)AMINO]METH
                YL}-1H-ISOINDOLE-1,3(2H)-DIONE

14  30.301  0.03 D:\DATABASE\DEMO.L
                PIMARA-8,15-DIENE §§ PHENANTHRENE,  481165 055255-56-6 93
                 7-ETHENYL-1,2,3,4,4A,5,6,7,8,9,10
                ,10A-DODECAHYDRO-1,1,4A,7-TETRAMET
                HYL- §§ 7.ALPHA.-ETHENYL-1,1,4A,7.
                BETA.-TETRAMETHYL-1,2,3,4,4A,5,6,7
                ,8,9,10,10A-DODECAHYDROPHENANTHREN
                Phenanthrene, 7-ethenyl-1,2,3,4,4a  481092 055255-56-6 93
                ,5,6,7,8,9,10,10a-dodecahydro-1,1,
                4a,7-tetramethyl- §§ Pimara-8,15-d
                iene #
                4H,8H-BENZO[1,2-B:3,4-B']DIPYRAN-4  481134 035930-31-5 83
                -ONE, 5-METHOXY-2,8,8-TRIMETHYL- §
                § 5-METHOXY-2,8,8-TRIMETHYL-4H,8H-
                BENZO[1,2-B:3,4-B']DIPYRAN-4-ONE §
                § 5-O-METHYLALLOPTAEROXYLIN §§ ALL
                OPTAEROXYLIN METHYL ETHER

15  30.711  0.01 D:\DATABASE\DEMO.L
                4-(METHOXYMETHYL)-6-METHYL-2-PHENO   7413 332057-36-0 10
                XYNICOTINONITRILE §§ PYRIDINE-3-CA
                RBONITRILE, 4-METHOXYMETHYL-6-METH
                YL-2-PHENOXY-
                4-BROMO-N-[(6-METHYL-2-PYRIDYL)AMI   7473 999007-47-4  9
                NOMETHYL]PHTHALIMIDE §§ 5-BROMO-2-
                {[(6-METHYL-2-PYRIDINYL)AMINO]METH
                YL}-1H-ISOINDOLE-1,3(2H)-DIONE
                9-(4-HYDROXYPHENYL)-3,3,6,6-TETRAM   7482 999007-48-3  9
                ETHYL-3,4,6,7,8A,9-HEXAHYDRO-1,8(2
                H,5H)-ACRIDINEDIONE
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ata Path : F:\DATA MS\daa\
ata File : WLM-10green-180c-2jm.D
cq On    : 12 Oct 2019    8:00
perator  :
ample    :
isc      :
LS Vial  : 1   Sample Multiplier: 1

earch Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

nknown Spectrum:   Apex
ntegration Events: ChemStation Integrator - autointl.e
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RT	Area%	Library/ID	Ref#	CAS#	Qual
31.252	0.01	D:\DATABASE\DEMO.L			
		4-(METHOXYMETHYL)-6-METHYL-2-PHENOXYNICOTINONITRILE §§ PYRIDINE-3-CARBONITRILE, 4-METHOXYMETHYL-6-METHYL-2-PHENOXY-	7413	332057-36-0	27
		Ethanediamide, N-allyl-N'-(2,5-dimethylphenyl)-	7392	331864-72-3	25
		1-DODECANAMINE §§ 1-AMINODODECANE §§ 1-DODECYLAMINE §§ ALAMINE 4	4661	000124-22-1	12
31.273	0.00	D:\DATABASE\DEMO.L			
		4-(METHOXYMETHYL)-6-METHYL-2-PHENOXYNICOTINONITRILE §§ PYRIDINE-3-CARBONITRILE, 4-METHOXYMETHYL-6-METHYL-2-PHENOXY-	7413	332057-36-0	10
		1-DODECANAMINE §§ 1-AMINODODECANE §§ 1-DODECYLAMINE §§ ALAMINE 4	4661	000124-22-1	9
		1-Dodecanamine §§ Dodecylamine §§ n-Dodecylamine §§ Alamine 4	4652	000124-22-1	9
31.700	0.02	D:\DATABASE\DEMO.L			
		6-ETHYL-2-METHYL-4,6-DIHYDRO-2H-[1,4]OXAZINO[3,2-C]QUINOLINE-3,5-DIONE §§ 6-ETHYL-2-METHYL-2H-1-OXA-4,6-PHENANTHROLINE-3,5(4H,6H)-DIONE §§ 6-ETHYL-2-METHYL-6,10B-DIHYDRO-2H-[1,4]OXAZINO[3,2-C]QUINOLINE-3,5-DIONE	7414	334023-40-4	27
		9-(4-HYDROXYPHENYL)-3,3,6,6-TETRAMETHYL-3,4,6,7,8A,9-HEXAHYDRO-1,8(2H,5H)-ACRIDINEDIONE	7482	999007-48-3	10
		1,3-OXATHIOL-1-IUM, 4-HYDROXY-2-[(1-METHYLETHYL)THIO]-5-(TRIFLUOROACETYL)-, HYDROXIDE, INNER SALT §§ 2-ISOPROPYLTHIO-5-TRIFLUORACETYL-1,3-OXATHIOLYIUM-4-OLAT	7423	096088-83-4	10
31.824	0.01	D:\DATABASE\DEMO.L			
		Norfluoxatine §§ 3-Phenyl-3-[4-(trifluoromethyl)phenoxy]-1-propanamine #	4995	056161-73-0	1
31.986	0.01	D:\DATABASE\DEMO.L			
		4-(METHOXYMETHYL)-6-METHYL-2-PHENOXYNICOTINONITRILE §§ PYRIDINE-3-CARBONITRILE, 4-METHOXYMETHYL-6-METHYL-2-PHENOXY-	7413	332057-36-0	27
		4-BROMO-N-[(6-METHYL-2-PYRIDYL)AMINOMETHYL]PHTHALIMIDE §§ 5-BROMO-2-{[(6-METHYL-2-PYRIDINYL)AMINO]METHYL}-1H-ISOINDOLE-1,3(2H)-DIONE	7473	999007-47-4	16
		2-METHOXY-4-(METHOXYMETHYL)-6-METHYLNICOTINONITRILE §§ PYRIDINE-3-CARBONITRILE, 2,4-DIMETHOXY-6-METHYL	7347	063644-84-8	12
32.067	0.02	D:\DATABASE\DEMO.L			
		9-(4-HYDROXYPHENYL)-3,3,6,6-TETRAMETHYL-3,4,6,7,8A,9-HEXAHYDRO-1,8(2	7482	999007-48-3	25

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Data Path : F:\DATA MS\data\
Data File : WLM-10pesen-180c-2jm.D
Acq On    : 12 Oct 2019    8:00
Operator  :
Sample    :
Misc      :
ALS Vial  : 1   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e
```

c#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			H,5H)-ACRIDINEDIONE			
			6-ETHYL-2-METHYL-4,6-DIHYDRO-2H-[1	7414	334023-40-4	23
			,4]OXAZINO[3,2-C]QUINOLINE-3,5-DIO			
			NE §§ 6-ETHYL-2-METHYL-2H-1-OXA-4,			
			6-PHENANTHROLINE-3,5(4H,6H)-DIONE			
			§§ 6-ETHYL-2-METHYL-6,10B-DIHYDRO-			
			2H-[1,4]OXAZINO[3,2-C]QUINOLINE-3,			
			5-DIONE			
			4-(METHOXYMETHYL)-6-METHYL-2-PHENO	7413	332057-36-0	12
			XYNICOTINONITRILE §§ PYRIDINE-3-CA			
			RBONITRILE, 4-METHOXYMETHYL-6-METH			
			YL-2-PHENOXY-			
22	32.408	0.02	D:\DATABASE\DEMO.L			
			4-(METHOXYMETHYL)-6-METHYL-2-PHENO	7413	332057-36-0	22
			XYNICOTINONITRILE §§ PYRIDINE-3-CA			
			RBONITRILE, 4-METHOXYMETHYL-6-METH			
			YL-2-PHENOXY-			
			1-Hexadecanamine §§ Hexadecylamine	4902	000143-27-1	10
			§§ n-Cetylamine §§ n-Hexadecylami			
			ne			
			2-METHOXY-4-(METHOXYMETHYL)-6-METH	7347	063644-84-8	10
			YLNICOTINONITRILE §§ PYRIDINE-3-CA			
			RBONITRILE, 2,4-DIMETHOXY-6-METHYL			
23	32.743	0.01	D:\DATABASE\DEMO.L			
			4-(METHOXYMETHYL)-6-METHYL-2-PHENO	7413	332057-36-0	10
			XYNICOTINONITRILE §§ PYRIDINE-3-CA			
			RBONITRILE, 4-METHOXYMETHYL-6-METH			
			YL-2-PHENOXY-			
			1-Heptadecanamine §§ Heptadecylami	4935	004200-95-7	9
			ne §§ n-Heptadecylamine §§ Margary			
			lamine			
			1,12-DODECANEDIAMINE §§ DODECANE-1	4751	999004-75-2	9
			,12-DIAMINE			
24	32.975	0.01	D:\DATABASE\DEMO.L			
			9-(4-HYDROXYPHENYL)-3,3,6,6-TETRAM	7482	999007-48-3	32
			ETHYL-3,4,6,7,8A,9-HEXAHYDRO-1,8(2			
			H,5H)-ACRIDINEDIONE			
			4-(METHOXYMETHYL)-6-METHYL-2-PHENO	7413	332057-36-0	30
			XYNICOTINONITRILE §§ PYRIDINE-3-CA			
			RBONITRILE, 4-METHOXYMETHYL-6-METH			
			YL-2-PHENOXY-			
			L-Alanine, N-glycyl- §§ Alanine, N	4366	003695-73-6	22
			-glycyl-, L- §§ Glcylalanine §§ Gl			
			y-ala			
25	33.493	0.11	D:\DATABASE\DEMO.L			
			PHENANTHRENE, 7-ETHENYL-1,2,3,4,4A	481161	018319-61-4	84
			,5,6,7,8,9,10,10A-DODECAHYDRO-1,1,			
			4A,7-TETRAMETHYL-, [4AS-(4A.ALPHA.			
			,7.ALPHA.,10A.BETA.)]- §§ PINARA-8			
			(9),15-DIENE §§ PODOCARP-8-ENE, 13			
			.ALPHA.-METHYL-13-VINYL-			
			KAURA-5,16-DIEN-18-OL §§ KAURA-5,1	492904	023837-99-2	80
			6-DIEN-18(OR 19)-OL §§ KAURA-5,16-			
			DIEN-19-OL			
			Kaura-5,16-dien-18(or 19)-ol §§ Ka	492860	023837-99-2	56

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Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			ura-5,16-dien-18-ol #			
26	33.677	0.01	D:\DATABASE\DEMO.L			
			4-(METHOXYMETHYL)-6-METHYL-2-PHENO XYNICOTINONITRILE §§ PYRIDINE-3-CA RBONITRILE, 4-METHOXYMETHYL-6-METH YL-2-PHENOXY-	7413	332057-36-0	22
			1-DODECANAMINE §§ 1-AMINODODECANE §§ 1-DODECYLAMINE §§ ALAMINE 4	4661	000124-22-1	14
			1-Dodecanamine §§ Dodecylamine §§ n-Dodecylamine §§ Alamine 4	4652	000124-22-1	14
27	33.731	0.00	D:\DATABASE\DEMO.L			
			1-Hexadecanamine §§ Hexadecylamine §§ n-Cetylamine §§ n-Hexadecylami ne	4902	000143-27-1	25
			1-DODECANAMINE §§ 1-AMINODODECANE §§ 1-DODECYLAMINE §§ ALAMINE 4	4661	000124-22-1	14
			1-Dodecanamine §§ Dodecylamine §§ n-Dodecylamine §§ Alamine 4	4652	000124-22-1	14
28	33.785	0.02	D:\DATABASE\DEMO.L			
			Ethyl 2-((diethoxyphosphoryl)oxy)-3,3,3-trifluoropropanoate	3375	999003-37-6	9
			3H-[1]BENZOTHIENO[3,2-D]AZONINE-3-CARBONITRILE, 1,2,4,5,6,7-HEXAHYDR O-7-METHOXY- §§ 7-METHOXY-2,3,4,5, 6,7-HEXAHYDRO-1H-[L]BENZOTHIENO[3, 2-D]AZONINE-3-CARBONITRILE	7435	099659-20-8	6
29	33.855	0.05	D:\DATABASE\DEMO.L			
			1-Methyl-10,18-bisnorabieta-8,11,1 3-triene	466158	999466-16-6	94
			10,13-DIMETHYL-4,5,6,7,8,9,10,11,1 2,13,14,15-DODECAHYDRO-1H-CYCLOPEN TA[A]PHENANTHRENE §§ ANDROSTA-2,16 -DIENE	466180	999466-18-8	93
			s-Indacen-1(2H)-one, 3,5,6,7-tetra hydro-3,3,4,5,5,8-hexamethyl- §§ 3 ,3,4,5,5,8-Hexamethyl-3,5,6,7-tetr ahydro-s-indacen-1(2H)-one #	466171	038754-94-8	89
30	34.131	0.02	D:\DATABASE\DEMO.L			
			2,2,3,3,4,4,5,5-OCTAFLUORO-N-(3-ME THOXYPHENYL)PENTANAMIDE §§ PENTANA MIDE, 2,2,3,3,4,4,5,5-OCTAFLUORO-N -(3-METHOXYPHENYL)-	7474	339166-43-7	9
31	34.190	0.02	D:\DATABASE\DEMO.L			
			N-(1-ETHYLPROPYL)-3,4-DIMETHYL-2,6 -DINITROANILINE §§ BENZENAMINE, N- (1-ETHYLPROPYL)-3,4-DIMETHYL-2,6-D INITRO- §§ 3,4-DIMETHYL-2,6-DINITR O-N-(1-ETHYLPROPYL)ANILINE §§ 3,4- XYLIDINE, 2,6-DINITRO-N-(1-ETHYLPR OPYL)-	3317	040487-42-1	7
			Ethanediamide, N-allyl-N'-(2 ,5-dimethylphenyl)-	7392	331864-72-3	7
			.ALPHA.-METHYL-4-METHOXY-STYRENE §	1191	999001-19-1	2

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nknown Spectrum:   Apex
ntegration Events: ChemStation Integrator - autoint1.e

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              § 1-ISOPROPENYL-4-METHOXYBENZENE §
              § 4-ISOPROPENYLPHENYL METHYL ETHER

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              METHYL PIMARA-8,15-DIEN-18-OATE §§ 466513 003582-26-1 55
               1-PHENANTHRENECARBOXYLIC ACID, 7-
              ETHENYL-1,2,3,4,4A,5,6,7,8,9,10,10
              A-DODECAHYDRO-1,4A,7-TRIMETHYL-, M
              ETHYL ESTER, [1R-(1.ALPHA.,4A.BETA
              .,7.BETA.,10A.ALPHA.)]- §§ METHYL
              8,15-PIMARADIEN-18-OATE
              METHYL PIMARA-8,15-DIEN-18-OATE §§ 466512 019907-21-2 46
               1-PHENANTHRENECARBOXYLIC ACID, 7-
              ETHENYL-1,2,3,4,4A,5,6,7,8,9,10,10
              A-DODECAHYDRO-1,4A,7-TRIMETHYL-, M
              ETHYL ESTER, [1R-(1.ALPHA.,4A.BETA
              .,7.ALPHA.,10A.ALPHA.)]- §§ METHYL
               8,15-ISOPIMARADIEN-18-OATE
              1-Phenanthrenecarboxylic acid, 7-e 466506 019907-21-2 46
              thenyl-1,2,3,4,4a,5,6,7,8,9,10,10a
              -dodecahydro-1,4a,7-trimethyl-, me
              thyl ester, [1R-(1.alpha.,4a.beta.
              ,7.alpha.,10a.alpha.)]- §§ Podocar
              p-8-en-15-oic acid, 13.beta.-methy
              l-13-vinyl-, methyl ester

  34.525  0.09 D:\DATABASE\DEMO.L
              (+)1A7,4A,9,10,10A-DODECAHYDRO-1,4 481209 000000-00-0 38
              A,7-TRIMETHYL-7-VINYL-1-PHENANTHRE
              NCARBALDEHYDSHYL 4,AZC.BETA.THIOME
              THYL](12-YL2ETHYLTHIOYLENC1ETHYLDE
              THYL3-YLAPHTHC]TAOXM.BETA.ANO6, [U
              CH0ALFPAL[YL9
              PIMARA-8,15-DIENE §§ PHENANTHRENE, 481165 055255-56-6 38
               7-ETHENYL-1,2,3,4,4A,5,6,7,8,9,10
              ,10A-DODECAHYDRO-1,1,4A,7-TETRAMET
              HYL- §§ 7.ALPHA.-ETHENYL-1,1,4A,7.
              BETA.-TETRAMETHYL-1,2,3,4,4A,5,6,7
              ,8,9,10,10A-DODECAHYDROPHENANTHREN
              8-p-Tolyl-8-aza-spiro[4.5]decane-7 398754 999398-75-8 38
              ,9-dione

  34.666  0.01 D:\DATABASE\DEMO.L
              2H-3,9A-METHANO-1-BENZOXEPIN, OCTA   3110 005956-09-2 18
              HYDRO-2,2,5A,9-TETRAMETHYL-, [3R-(
              3.ALPHA.,5A.ALPHA.,9.ALPHA.,9A.ALP
              HA.)]- §§ .BETA.-AGAROFURAN, DIHYD
              RO- §§ .BETA.-DIHYDROAGAROFURAN §§
               2H-3,9A-METHANO-1-BENZOXEPIN, OCT
              AHYDRO-2,2,5A,9-TETRAMETHYL-
              1-Heptadecanamine §§ Heptadecylami   4935 004200-95-7 10
              ne §§ n-Heptadecylamine §§ Margary
              lamine
              Tridecylamine §§ n-Tridecylamine §   4735 002869-34-3 10
              § 1-Aminotridecane §§ 1-Tridecanam
              ine

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Misc :
ALS Vial : 1 Sample Multiplier: 1

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Integration Events: ChemStation Integrator - autointl.e

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			PHA.,.ALPHA.'DIOL			
36	34.903	0.03	D:\DATABASE\DEMO.L			
			2-HYDROXY-5-METHOXY-3-NITROBENZALDEHYDE §§ 2-HYDROXY-5-METHYL-3-NITROBENZALDEHYDE §§ 5-METHOXY-3-NITROSALICYLALDEHYDE	7328	066620-31-3	9
			1-(2,6-DICHLORO-BENZYL)-3,5-DIMETHYL-1H-PYRAZOL-4-YLAMINE §§ 1-(2,6-DICHLOROBENZYL)-3,5-DIMETHYL-1H-PYRAZOL-4-AMINE §§ 1-(2,6-DICHLOROBENZYL)-3,5-DIMETHYL-1H-PYRAZOL-4-YLAMINE	7421	999007-42-2	6
			1,3-BENZENEDIMETHANOL, 2-HYDROXY-5-(1-METHYLETHYL)- §§ 2,6-BIS(HYDROXYMETHYL)-4-ISOPROPYLPHENOL §§ 2,6-BIS(HYDROXYMETHYL)-4-ISOPROPYLPHENOL (IMPURE) §§ 2,6-BIS-HYDROXYMETHYL-4-ISOPROPYLPHENOL	330	054845-41-9	2
37	35.028	0.05	D:\DATABASE\DEMO.L			
			Benzene, (2,2-dimethoxyethyl)- §§ Acetaldehyde, phenyl-, dimethyl acetal §§ .alpha.-Tolylaldehyde dimethyl acetal §§ Hyacylene F	122348	000101-48-4	50
			Benzene, 1-[(dimethoxymethyl)-1-ethyl]-4-methoxycarbonyl-1-ethyl-	123523	999123-52-6	40
			4-(Dimethyl(prop-2-enyl)silyloxy)octane	123131	999123-13-4	40
38	35.136	0.03	D:\DATABASE\DEMO.L			
			1H-INDEN-2-AMINE, 2,3-DIHYDRO-4-METHOXY- §§ 1-METHOXY-6-AMINOINDANE §§ 4-METHOXYINDAN-2-AMINE	354405	076413-92-8	25
			O-CYCLOHEXYL N,N-DIETHYL PHOSPHORAMIDO CYANIDATE §§ PHOSPHORAMIDOCYANIDIC ACID, DIETHYL-, CYCLOHEXYL ESTER	355166	999355-16-9	22
			2-[4-(2-OXIRANYLMETHOXY)PHENYL]ACETAMIDE §§ 4-OXIRANYLMETHOXY-BENZENEACETANIDE	354845	029122-69-8	22
39	35.173	0.04	D:\DATABASE\DEMO.L			
			1H-INDEN-2-AMINE, 2,3-DIHYDRO-4-METHOXY- §§ 1-METHOXY-6-AMINOINDANE §§ 4-METHOXYINDAN-2-AMINE	354405	076413-92-8	25
			Benzene, 1,4-bis(1-hydroxy-2-propyl)-	354653	999354-65-6	22
			BIS(TRIMETHYLSILYL)PEROXIDE	354518	000000-00-0	14
40	35.303	0.03	D:\DATABASE\DEMO.L			
			6-METHOXY-5-NITRO-2-PHENYLQUINOXALINE	123667	000000-00-0	22
			2-Pyrrol[tert-butyl(dimethyl)silyl]oxymorphopropan-1-ol	122672	999122-67-5	22
			6-Dimethyl(dichloromethyl)silyloxy tridecane	124167	999124-17-0	14

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Integration Events: ChemStation Integrator - autoint1.e

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			p-Heptyloxyaniline $$ 4-n-Heptyloxyaniline	228109	039905-44-7	47
			Acetamide, N-(2-hydroxyphenyl)- $$ Acetanilide, 2'-hydroxy- $$ o-(Acetylamino)phenol $$ o-Acetamidophenol	227250	000614-80-2	47
			2-Methyl-2H-pyrazole-3-carboxylic acid, [1-(4-nitrophenyl)ethylidene]hydrazide	229060	999229-06-3	43
42	35.481	0.78	D:\DATABASE\DEMO.L			
			BENZ[A]ANTHRACENONE	513655	099707-96-7	83
			Xanthen-9-one, 1-hydroxy-3,5,8-trimethoxy- $$ 5,8-Dimethylbellidifolin $$ 1-Hydroxy-3,5,8-trimethoxyxanthen-9-one $$ 1-Hydroxy-3,5,8-trimethoxy-9H-xanthen-9-one #	504583	049599-09-9	48
			Silane, dimethyl(2-methyloct-5-yn-4-yloxy)hexyloxy-	466397	999466-40-5	44
43	35.654	0.08	D:\DATABASE\DEMO.L			
			(4-Ethylphenyl)-(2-methylbenzo[4,5]imidazo[1,2-a] pyrimidin-4-yl)amine	504586	999504-59-8	44
			2,7-Phenanthrenediol, 1,2,3,4,4a,9,10,10a-octahydro-1,1,4a-trimethyl-8-(1-methylethyl)-, [2S-(2.alpha.,4a.alpha.,10a.beta.)]- $$ Podocarpa-8,11,13-triene-3.beta.,13-diol, 14-isopropyl- $$ Totaradiol $$ 3.beta.-Hydroxytotarol	504581	003772-56-3	44
			ROSIN ACIDS	504611	000000-00-0	38
44	35.757	0.25	D:\DATABASE\DEMO.L			
			DEHYDROABIETIC ACID	464556	000000-00-0	97
			METHYL ABIETA-8,11,13-TRIEN-18-OATE $$ 1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,9,10,10A-OCTAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL)-, METHYL ESTER, [1R-(1.ALPHA.,4A.BETA.,10A.ALPHA.)]- $$ DEHYDROABIETIC ACID METHYL ESTER $$ METHYL DEHYDROABIETATE	464550	001235-74-1	95
			1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methylethyl)-, methyl ester, [1R-(1.alpha.,4a.beta.,10a.alpha.)]- $$ Podocarpa-8,11,13-trien-15-oic acid, 13-isopropyl-, methyl ester $$ Methyl dehydroabietat	464538	001235-74-1	95
45	35.908	0.07	D:\DATABASE\DEMO.L			
			KAUR-16-EN-18-OIC ACID $$ KAUR-16-EN-18-OIC ACID, (4.BETA.)- $$ (-)-KAURNENOIC ACID $$ (4-BETA)-KAUR-16-EN-18-OIC ACID	168418	020316-84-1	47
			1H-Pyrazole-1-acetamide, 4-iodo-N-(phenylmethyl)-	170579	999170-58-2	25
			ANTI-(Z)-BIS(PENCHYLIDENE) EPOXIDE	250745	000000-00-0	14

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Data File : WLM-10prsen-180c-2jm.D
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5	36.011	0.09	D:\DATABASE\DEMO.L 2.BETA.BENZYL-8.BETA.-HYDROXY-4,6-DIMETHYL-3,5,7-TRIOXATETRACYCLO[7.2.1.0(4,11).0(6,10)]DODECANE	503165	000000-00-0	50
			A-NORPREGN-3(5)-ENE, 3,20-DIMETHYL - §§ 3,20-DIMETHYL-A-NOR-3(5)-PREGNENE §§ DICYCLOPENTA[A,F]NAPHTHALENE, A-NORPREGN-3(5)-ENE DERIV.	503129	062008-73-5	35
			KAUR-16-EN-18-OIC ACID §§ KAUR-16-EN-18-OIC ACID, (4.BETA.)- §§ (-)-KAURNENOIC ACID §§ (4-BETA)-KAUR-16-EN-18-OIC ACID	168418	020316-84-1	30
7	36.086	0.37	D:\DATABASE\DEMO.L INDOLIZINO[1,2-B]QUINOLIN-9(11H)-ONE, 8-[(FORMYLOXY)METHYL]-7-(1-OXOPROPYL)- §§ 8-FORMYLOXYMETHYL-7-(1-OXOPROPYL)INDOLIZINO)1,2-B)QUINOLIM-9(11H)-ONE	504762	054318-62-6	95
			1-Hydroxy-6-(3-isopropenyl-cyclopent-1-enyl)-6-methyl-heptan-2-one	257257	999257-26-0	55
			KAUR-16-EN-18-OIC ACID §§ KAUR-16-EN-18-OIC ACID, (4.BETA.)- §§ (-)-KAURNENOIC ACID §§ (4-BETA)-KAUR-16-EN-18-OIC ACID	168418	020316-84-1	49
8	36.276	0.05	D:\DATABASE\DEMO.L (4-Ethylphenyl)-(2-methylbenzo[4,5]imidazo[1,2-a] pyrimidin-4-yl)amine	504586	999504-59-8	44
			PIMARA-8(14),15-DIEN-18-OIC ACID §§ 1-PHENANTHRENECARBOXYLIC ACID, 7-ETHENYL-1,2,3,4,4A,4B,5,6,7,9,10,10A-DODECAHYDRO-1,4A,7-TRIMETHYL-, [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,7.BETA.,10A.ALPHA.)]- §§ (+)-PIMARIC ACID §§ .ALPHA.-PIMARIC ACID	504608	000127-27-5	25
			Andrographolide §§ 2(3H)-Furanone, 3-[2-[decahydro-6-hydroxy-5-(hydroxymethyl)-5,8a-dimethyl-2-methylene-1-naphthalenyl]ethylidene]dihydro-4-hydroxy-	171071	005508-58-7	25
9	36.384	0.17	D:\DATABASE\DEMO.L METHYL ABIETA-7,13-DIEN-18-OATE §§ 1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL)-, METHYL ESTER, [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A.ALPHA.)]- §§ ABALYN §§ ABIETIC ACID METHYL ESTER	480551	000127-25-3	91
			METHYL ABIETA-7,13-DIEN-18-OATE §§ 1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL)-, METHYL ESTER, [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A.ALPHA.)]- §§ ABALYN §§ ABIETIC ACID METHYL ESTER	480550	000127-25-3	90

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nknown Spectrum:   Apex
ntegration Events: ChemStation Integrator - autoint1.e

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                Methyl abietate §§ 1-Phenanthrenec 480547 000127-25-3 90
                arboxylic acid, 1,2,3,4,4a,4b,5,6,
                10,10a-decahydro-1,4a-dimethyl-7-(
                1-methylethyl)-, methyl ester, [1R
                -(1.alpha.,4a.beta.,4b.alpha.,10a.
                alpha.)]- §§ Podocarpa-7,13-dien-1
                5-oic acid, 13-isopropyl-, methyl
                ester §§ Abalyn

  36.465  0.03 D:\DATABASE\DEMO.L
                KAUR-16-EN-18-OIC ACID §§ KAUR-16- 168418 020316-84-1 70
                EN-18-OIC ACID, (4.BETA.)- §§ (-)-
                KAURNENOIC ACID §§ (4-BETA)-KAUR-1
                6-EN-18-OIC ACID
                Abietic acid §§ 1-Phenanthrenecarb 513378 000514-10-3 66
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid
                Androst-5-en-17-ol, 4,4-dimethyl-  513436 999513-44-9 52

  36.594  0.53 D:\DATABASE\DEMO.L
                O-HYDROGEN PERDEUTERIO HEXADECANOI 504545 039756-30-4 90
                C ACID
                1-PHENANTHRENECARBOXYLIC ACID, 7-E 466436 005835-26-7 87
                THENYL-1,2,3,4,4A,4B,5,6,7,8,10,10
                A-DODECAHYDRO-1,4A,7-TRIMETHYL-, [
                1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,7.
                ALPHA.,10A.ALPHA.)]- §§ ISOPIMARIC
                 ACID §§ PODOCARP-7-EN-15-OIC ACID
                , 13.BETA.-METHYL-13-VINYL-
                BENZ[A]ANTHRACEMONE                513655 099707-96-7 87

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                1H-NAPHTHO[2,3-C]PYRAN-5,10-DIONE, 513557 084018-44-0 91
                 3,4-DIHYDRO-7,9-DIMETHOXY-1,3-DIM
                ETHYL-, TRANS-(.+-.)- §§ (+,-)-DEO
                XYQUINONE A DIMETHYL ETHER §§ (+,-
                )-TRANS-7,9-DIMETHOXY-1,3-DIMETHYL
                -3,4,5,10-TETRAHYDRONAPHTHO[2,3-C]
                PYRAN-5,10-DIONE
                1H-NAPHTHO[2,3-C]PYRAN-5,10-DIONE, 513558 084018-43-9 91
                 3,4-DIHYDRO-7,9-DIMETHOXY-1,3-DIM
                ETHYL-, CIS-(.+-.)- §§ (+,-)-CIS-7
                ,9-DIMETHOXY-1,3-DIMETHYL-3,4,5,10
                -TETRAHYDRONAPHTHO[2,3-C]PYRAN-5,1
                0-DIONE
                Palustric acid §§ Podocarpa-8,13-d 513439 001945-53-5 66
                ien-15-oic acid, 13-isopropyl- §§
                1-Phenanthrenecarboxylic acid, 1,2
                ,3,4,4a,5,6,9,10,10a-decahydro-1,4
                a-dimethyl-7-(1-methylethyl)-, (1R
                -(1.alpha.,4a.beta.,10a.alpha.))-
                §§ 8,13-Abietadien-18-oic acid

  36.956  0.41 D:\DATABASE\DEMO.L
                1-Phenanthrenecarboxylic acid, 1,2 503093 001740-19-8 99
```

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsen-180c-2jm.D
Acq On : 12 Oct 2019 8:00
Operator :
Sample :
Misc :
ALS Vial : 1 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autointl.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			,3,4,4a,9,10,10a-octahydro-1,4a-di methyl-7-(1-methylethyl)-, [1R-(1. alpha.,4a.beta.,10a.alpha.)]- §§ P odocarpa-8,11,13-trien-15-oic acid , 13-isopropyl- §§ Abieta-8,11,13- trien-18-oic acid §§ Abietic acid, dehydro-			
			1-PHENANTHRENECARBOXYLIC ACID, 1,2 ,3,4,4A,9,10,10A-OCTAHYDRO-1,4A-DI METHYL-7-(1-METHYLETHYL)-, [1R-(1. ALPHA.,4A.BETA.,10A.ALPHA.)]- §§ (-)-DEHYDROABIETIC ACID §§ 1,2,3,4, 4A,9,10,10A-OCTAHYDRO-1,4A-DIMETHY L-7-(1-METHYLETHYL)-1-PHENANTHRENE CARBOXYLIC ACID	503110	001740-19-8	99
			ABIETA-8,11,13-TRIEN-18-OIC ACID § § PODOCARPA-8,11,13-TRIEN-15-SAEUR E, 13-ISOPROPYL-	503106	999503-11-8	99
54	37.026	0.51	D:\DATABASE\DEMO.L			
			1-PHENANTHRENECARBOXYLIC ACID, 1,2 ,3,4,4A,9,10,10A-OCTAHYDRO-1,4A-DI METHYL-7-(1-METHYLETHYL)-, [1R-(1. ALPHA.,4A.BETA.,10A.ALPHA.)]- §§ (-)-DEHYDROABIETIC ACID §§ 1,2,3,4, 4A,9,10,10A-OCTAHYDRO-1,4A-DIMETHY L-7-(1-METHYLETHYL)-1-PHENANTHRENE CARBOXYLIC ACID	503110	001740-19-8	86
			1-Phenanthrenecarboxylic acid, 1,2 ,3,4,4a,9,10,10a-octahydro-1,4a-di methyl-7-(1-methylethyl)-, [1R-(1. alpha.,4a.beta.,10a.alpha.)]- §§ P odocarpa-8,11,13-trien-15-oic acid , 13-isopropyl- §§ Abieta-8,11,13- trien-18-oic acid §§ Abietic acid, dehydro-	503093	001740-19-8	86
			1-Phenanthrenecarboxylic acid, 1,2 ,3,4,4a,9,10,10a-octahydro-1,4a-di methyl-7-(1-methylethyl)-, [1R-(1. alpha.,4a.beta.,10a.alpha.)]- §§ P odocarpa-8,11,13-trien-15-oic acid , 13-isopropyl- §§ Abieta-8,11,13- trien-18-oic acid §§ Abietic acid, dehydro-	503081	001740-19-8	84
55	37.226	0.39	D:\DATABASE\DEMO.L			
			1-Phenanthrenecarboxylic acid, 1,2 ,3,4,4a,9,10,10a-octahydro-1,4a-di methyl-7-(1-methylethyl)-, [1S-(1. alpha.,4a.alpha.,10a.beta.)]- §§ P odocarpa-8,11,13-trien-16-oic acid , 13-isopropyl- §§ Callitrisic aci d §§ 4-Epiabietic acid, dehydro-	503094	005155-70-4	90
			ABIETA-8,11,13-TRIEN-18-OIC ACID § § 1-PHENANTHRENECARBOXYLIC ACID, 1 ,2,3,4,4A,9,10,10A-OCTAHYDRO-1,4A- DIMETHYL-7-(1-METHYLETHYL)-, [1S-(1.ALPHA.,4A.ALPHA.,10A.BETA.)]- §§ 13-ISOPROPYLPODOCARPA-8,11,13-TRI	503112	005155-70-4	90

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Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-180c-2jm.D
Acq On    : 12 Oct 2019    8:00
Operator  :
Sample    :
Misc      :
ALS Vial  : 1   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#     RT  Area%          Library/ID                    Ref#     CAS#   Qual
                EN-16-OIC ACID §§ 4-EPIABIETIC ACI
                D, DEHYDRO-
                1-Phenanthrenecarboxylic acid, 1,2 503081 001740-19-8 83
                ,3,4,4a,9,10,10a-octahydro-1,4a-di
                methyl-7-(1-methylethyl)-, [1R-(1.
                alpha.,4a.beta.,10a.alpha.)]- §§ P
                odocarpa-8,11,13-trien-15-oic acid
                , 13-isopropyl- §§ Abieta-8,11,13-
                trien-18-oic acid §§ Abietic acid,
                 dehydro-

56  37.361  0.10 D:\DATABASE\DEMO.L
                1,4-DIHYDRO-9-ISOPROPYLIDENE-5,6,7 513581 000000-00-0 90
                ,8-TETRAMETHOXY-1,4-METHANONAPHTHA
                LENE
                1-Phenanthrenecarboxylic acid, 1,2 503081 001740-19-8 55
                ,3,4,4a,9,10,10a-octahydro-1,4a-di
                methyl-7-(1-methylethyl)-, [1R-(1.
                alpha.,4a.beta.,10a.alpha.)]- §§ P
                odocarpa-8,11,13-trien-15-oic acid
                , 13-isopropyl- §§ Abieta-8,11,13-
                trien-18-oic acid §§ Abietic acid,
                 dehydro-
                ABIETA-7,13-DIEN-18-OIC ACID §§ 1- 168420 000514-10-3 51
                PHENANTHRENECARBOXYLIC ACID, 1,2,3
                ,4,4A,4B,5,6,10,10A-DECAHYDRO- §§
                1-PHENANTHRENECARBOXYLIC ACID, 1,2
                ,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,
                4A-DIMETHYL-7-(1-METHYLETHYL)-, [1
                R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A
                .ALPHA.)]-

57  37.691  2.78 D:\DATABASE\DEMO.L
                Abietic acid §§ 1-Phenanthrenecarb 513378 000514-10-3 99
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid
                Abietic acid §§ 1-Phenanthrenecarb 513347 000514-10-3 93
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid
                Abietic acid §§ 1-Phenanthrenecarb 513344 000514-10-3 93
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid

58  38.485  0.24 D:\DATABASE\DEMO.L
                Abietic acid §§ 1-Phenanthrenecarb 513378 000514-10-3 98
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
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```
Data Path : F:\DATA MS\daa\
Data File : WLM-10prsen-180c-2jm.D
Acq On    : 12 Oct 2019    8:00
Operator  :
Sample    :
Misc      :
ALS Vial  : 1   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#     RT  Area%          Library/ID                    Ref#     CAS#   Qual
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid
                Abietic acid §§ 1-Phenanthrenecarb 513347 000514-10-3 89
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid
                Palustric acid §§ Podocarpa-8,13-d 513439 001945-53-5 86
                ien-15-oic acid, 13-isopropyl- §§
                1-Phenanthrenecarboxylic acid, 1,2
                ,3,4,4a,5,6,9,10,10a-decahydro-1,4
                a-dimethyl-7-(1-methylethyl)-, (1R
                -(1.alpha.,4a.beta.,10a.alpha.))-
                §§ 8,13-Abietadien-18-oic acid

59  38.831  0.09 D:\DATABASE\DEMO.L
                Abietic acid §§ 1-Phenanthrenecarb 513378 000514-10-3 74
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid
                Abietic acid §§ 1-Phenanthrenecarb 513347 000514-10-3 64
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid
                Abietic acid §§ 1-Phenanthrenecarb 513344 000514-10-3 51
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid

60  39.004  0.20 D:\DATABASE\DEMO.L
                Abietic acid §§ 1-Phenanthrenecarb 513344 000514-10-3 44
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid
                Abietic acid §§ 1-Phenanthrenecarb 513378 000514-10-3 35
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid
                Abietic acid §§ 1-Phenanthrenecarb 513347 000514-10-3 35
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
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Data Path : F:\DATA MS\daa\
Data File : WLM-10prsen-180c-2jm.D
Acq On    : 12 Oct 2019    8:00
Operator  :
Sample    :
Misc      :
ALS Vial  : 1   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e

k#     RT  Area%          Library/ID                  Ref#     CAS#   Qual
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid

51  39.166  0.03 D:\DATABASE\DEMO.L
                Abietic acid §§ 1-Phenanthrenecarb 513347 000514-10-3 64
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid
                2-METHOXYESTRA-1,3,5(10)-TRIENE-3, 513604 000362-07-2 53
                17-DIOL §§ ESTRA-1,3,5(10)-TRIENE-
                3,17-DIOL, 2-METHOXY-, (17.BETA.)-
                 §§ (17BETA)-2-METHOXYESTRA-1,3,5(
                10)-TRIENE-3,17-DIOL §§ 2-HYDROXYE
                STRADIOL 2-METHYL ETHER
                Estra-1,3,5(10)-triene-3,17-diol,  513393 000362-07-2 53
                2-methoxy-, (17.beta.)- §§ Estra-1
                ,3,5(10)-triene-3,17.beta.-diol, 2
                -methoxy- §§ 2-Hydroxyestradiol 2-
                methyl ether §§ 2-Methoxyestradiol

52  39.306  0.06 D:\DATABASE\DEMO.L
                Abietic acid §§ 1-Phenanthrenecarb 513347 000514-10-3 60
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid
                Abietic acid §§ 1-Phenanthrenecarb 513378 000514-10-3 42
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid
                ABIETA-7,13-DIEN-18-OIC ACID §§ 1- 168419 000514-10-3 30
                PHENANTHRENECARBOXYLIC ACID, 1,2,3
                ,4,4A,4B,5,6,10,10A-DECAHYDRO- §§
                1-PHENANTHRENECARBOXYLIC ACID, 1,2
                ,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,
                4A-DIMETHYL-7-(1-METHYLETHYL)-, [1
                R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A
                .ALPHA.)]-

53  40.241  0.00 D:\DATABASE\DEMO.L
                KAUR-16-EN-18-OIC ACID §§ KAUR-16- 168418 020316-84-1 32
                EN-18-OIC ACID, (4.BETA.)- §§ (-)-
                KAURNEMOIC ACID §§ (4-BETA)-KAUR-1
                6-EN-18-OIC ACID
                2-PROPENE-1-SULFONIC ACID, 3-(3,4, 428799 104503-96-0 32
                5-TRIMETHOXYPHENYL)-, METHYL ESTER
                , (E)- §§ METHYL-3-(3',4',5'-TRIME
                THOXYPHENYL)-2-PROPENE-1-SULPHONAT
```

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-180c-2jm.D
Acq On : 12 Oct 2019 8:00
Operator :
Sample :
Misc :
ALS Vial : 1 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autointl.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			2-Pyrrolidinone, 3-hydroxy-4-methy l-3-phenyl-, (3S-cis)- §§ 3-Hydrox y-4-methyl-3-phenyl-2-pyrrolidinon e #	208512	104194-17-4	15
64	40.289	0.00	D:\DATABASE\DEMO.L			
			CIS-4-ETHOXY-B-METHYL-B-NITROSTYRE NE	428132	000000-00-0	25
			cis-4-Ethoxy-b-methyl-b-nitrosstyre ne	428021	999428-02-8	25
			ABIETA-7,13-DIEN-18-OIC ACID §§ 1- PHENANTHRENECARBOXYLIC ACID, 1,2,3 ,4,4A,4B,5,6,10,10A-DECAHYDRO- §§ 1-PHENANTHRENECARBOXYLIC ACID, 1,2 ,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1, 4A-DIMETHYL-7-(1-METHYLETHYL)-, [1 R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A .ALPHA.)]-	168419	000514-10-3	25
65	40.322	0.00	D:\DATABASE\DEMO.L			
			Abietic acid §§ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- §§ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- §§ L-abietic acid	513378	000514-10-3	84
			1,4-DIHYDRO-9-ISOPROPYLIDENE-5,6,7 ,8-TETRAMETHOXY-1,4-METHANONAPHTHA LENE	513581	000000-00-0	83
			PREGNANE, 20-METHYL- §§ 20-METHYL- 5.ALPHA.,17.ALPHA.-PREGNANE §§ 20- METHYL-5.ALPHA.-PREGNANE §§ 23,24- DINORCHOLANE	513674	006005-93-2	59

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsen-180c-3jmu.D
Acq On : 9 Oct 2019 17:10
Operator :
Sample :
Misc :
ALS Vial : 2 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	1.973	0.07	D:\DATABASE\DEMO.L			
			ACETIC ACID, HYDROXY-, ETHYL ESTER $$ ETHYL GLYCOLATE $$ ETHYL GLYCOLLATE $$ ETHYL HYDROXYACETATE	5374	000623-50-7	4
			ETHANOL $$ HYDROXYETHANE $$ 1-HYDROXYETHANE $$ ABSOLUTE ALCOHOL	5103	000064-17-5	4
			Acetic acid, hydroxy-, ethyl ester $$ Glycolic acid, ethyl ester $$ Ethyl glycolate $$ Ethyl hydroxyacetate	5363	000623-50-7	4
2	1.989	0.08	D:\DATABASE\DEMO.L			
			ETHANOL $$ HYDROXYETHANE $$ 1-HYDROXYETHANE $$ ABSOLUTE ALCOHOL	5099	000064-17-5	80
			Ethanol $$ Ethyl alcohol $$ Alcohol $$ Alcohol anhydrous	5086	000064-17-5	78
			ETHANOL $$ HYDROXYETHANE $$ 1-HYDROXYETHANE $$ ABSOLUTE ALCOHOL	5094	000064-17-5	78
3	2.135	0.08	D:\DATABASE\DEMO.L			
			Pentane, 2,4-dimethyl- $$ 2,4-Dimethylpentane	18750	000108-08-7	91
			PENTANE, 2,4-DIMETHYL- $$ 2,4-DIMETHYLPENTANE $$ PENTANE, 2,4-DIMETHYL	65648	000108-08-7	90
			PENTANE, 2,4-DIMETHYL- $$ 2,4-DIMETHYLPENTANE $$ PENTANE, 2,4-DIMETHYL	19002	000108-08-7	80
4	2.205	9.99	D:\DATABASE\DEMO.L			
			Hexane, 3-methyl- $$ 2-Ethylpentane $$ 3-Methylhexane	18743	000589-34-4	68
			HEXANE, 3-METHYL- $$ 3-METHYLHEXANE $$ 2-ETHYLPENTANE $$ HEXANE, 3-METHYL	18992	000589-34-4	68
			Hexane, 3-methyl- $$ 2-Ethylpentane $$ 3-Methylhexane	18754	000589-34-4	68
5	2.243	4.01	D:\DATABASE\DEMO.L			
			Cyclopentane, 1,3-dimethyl-, cis- $$ cis-1,3-Dimethylcyclopentane $$ 1,3-Dimethylcyclopentane cis $$ 1,3-Dimethylcyclopentane #	62231	002532-58-3	91
			1,3-DIMETHYLCYCLOPENTANE $$ CYCLOPENTANE, 1,3-DIMETHYL-, CIS- $$ 1,3-DIMETHYLCYCLOPENTANE (CIS) $$ 1,3-DIMETHYLCYCLOPENTANE CIS	62286	002532-58-3	91
			Cyclopentane, 1,3-dimethyl- $$ 1,3-Dimethylcyclopentane	101343	002453-00-1	91
6	2.335	6.85	D:\DATABASE\DEMO.L			
			CYCLOHEXANE, METHYL- $$ METHYLCYCLOHEXANE $$ 1-METHYLCYCLOHEXANE $$ CYCLOHEXANE, METHYL	141469	000108-87-2	96
			CYCLOHEXANE, METHYL- $$ METHYLCYCLOHEXANE $$ 1-METHYLCYCLOHEXANE $$ CYCLOHEXANE, METHYL	141470	000108-87-2	95
			CYCLOHEXANE, METHYL- $$ METHYLCYCLOHEXANE $$ 1-METHYLCYCLOHEXANE $$	141467	000108-87-2	94

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Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-180c-3jmu.D
Acq On    :  9 Oct 2019  17:10
Operator  :
Sample    :
Misc      :
ALS Vial  : 2   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autointl.e

k#     RT  Area%          Library/ID                  Ref#     CAS#   Qual
               CYCLOHEXANE, METHYL

 7   2.421 71.09 D:\DATABASE\DEMO.L
               BENZENE, METHYL- $$ METHYLBENZENE  158622 000108-88-3 91
               $$ TOLUENE $$ ANTISAL 1A
               Toluene $$ Benzene, methyl $$ Meth 158580 000108-88-3 91
               acide $$ Methylbenzene
               BENZENE, METHYL- $$ METHYLBENZENE  158625 000108-88-3 90
               $$ TOLUENE $$ ANTISAL 1A

 8   2.751  1.05 D:\DATABASE\DEMO.L
               CYCLOHEXANE, ETHYL- $$ ETHYLCYCLOH 141561 001678-91-7 93
               EXANE $$ ETHYL CYCLOHEXANE $$ ETHY
               LCYCLOHEXAN
               Cyclohexane, ethyl- $$ Ethylcycloh 141508 001678-91-7 93
               exane
               Cyclohexane, ethyl- $$ Ethylcycloh 141506 001678-91-7 93
               exane

 9  33.499  0.17 D:\DATABASE\DEMO.L
               PHENANTHRENE, 7-ETHENYL-1,2,3,4,4A 481161 018319-61-4 60
               ,5,6,7,8,9,10,10A-DODECAHYDRO-1,1,
               4A,7-TETRAMETHYL-, [4AS-(4A.ALPHA.
               ,7.ALPHA.,10A.BETA.)]- $$ PIMARA-8
               (9),15-DIENE $$ PODOCARP-8-ENE, 13
               .ALPHA.-METHYL-13-VINYL-
               1,2-BIS(4-ETHOXYPHENYL)DIAZENE 1-O 223740 004792-83-0 46
               XIDE $$ 4, 4'-BIS(ETHOXY)AZOXYBENZ
               ENE $$ 4,4'-AZOXYDIPHENETOLE $$ 4,
               4'-AZOXYPHENETOLE
               14-ISOPROPYL-3,7,11-TRIMETHYL-1,3, 181371 001898-13-1 45
               6,10-CYCLOTETRADECATETRAENE $$ 1,3
               ,6,10-CYCLOTETRADECATETRAENE, 3,7,
               11-TRIMETHYL-14-(1-METHYLETHYL)-,
               [S-(E,Z,E,E)]- $$ (+)-CEMBRENE $$
               (+)-THUNBERGEN

10  33.871  0.08 D:\DATABASE\DEMO.L
               Androst-2,16-diene                 466169 999466-17-7 96
               1-Methyl-10,18-bisnorabieta-8,11,1 466158 999466-16-6 94
               3-triene
               10,13-DIMETHYL-4,5,6,7,8,9,10,11,1 466180 999466-18-8 92
               2,13,14,15-DODECAHYDRO-1H-CYCLOPEN
               TA[A]PHENANTHRENE $$ ANDROSTA-2,16
               -DIENE

11  35.503  1.27 D:\DATABASE\DEMO.L
               Phenol, 2,4-bis(1-phenylethyl)- $$ 504578 002769-94-0 55
                2,4-Bis(1-phenylethyl)phenol #
               Xanthen-9-one, 1-hydroxy-3,5,8-tri 504583 049599-09-9 55
               methoxy- $$ 5,8-Dimethylbellidifol
               in $$ 1-Hydroxy-3,5,8-trimethoxyxa
               nthen-9-one $$ 1-Hydroxy-3,5,8-tri
               methoxy-9H-xanthen-9-one #
               (4-Ethylphenyl)-(2-methylbenzo[4,5 504586 999504-59-8 55
               ]imidazo[1,2-a] pyrimidin-4-yl)ami
               ne

12  35.649  0.12 D:\DATABASE\DEMO.L
```

```
Data Path : P:\DATA MS\GAS\
Data File : WLM-10pesen-180c-3jmu.D
Acq On    :  9 Oct 2019  17:10
Operator  :
Sample    :
Misc      :
ALS Vial  : 2   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autointl.e

#     RT  Area%          Library/ID                  Ref#     CAS#   Qual

              1-PHENANTHRENECARBOXYLIC ACID, 7-E 466436 005835-26-7 64
              THENYL-1,2,3,4,4A,4B,5,6,7,8,10,10
              A-DODECAHYDRO-1,4A,7-TRIMETHYL-, [
              1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,7.
              ALPHA.,10A.ALPHA.)]- §§ ISOPIMARIC
               ACID §§ PODOCARP-7-EN-15-OIC ACID
              , 13.BETA.-METHYL-13-VINYL-
              Phenol, 2,4-bis(1-phenylethyl)- §§ 504578 002769-94-0 49
               2,4-Bis(1-phenylethyl)phenol #
              Phenarsazine, 5,10-dihydro-10-hydr 466306 004733-19-1 46
              oxy-, 10-oxide §§ Phenarsazinic ac
              id §§ Phenarsazinic acid §§ Phenar
              sazine, 5,10-dihydro-5-hydroxy-, 5
              -oxide

3  35.757  0.26 D:\DATABASE\DEMO.L
              DEHYDROABIETIC ACID               464556 000000-00-0 97
              1-Phenanthrenecarboxylic acid, 1,2 464538 001235-74-1 93
              ,3,4,4a,9,10,10a-octahydro-1,4a-di
              methyl-7-(1-methylethyl)-, methyl
              ester, [1R-(1.alpha.,4a.beta.,10a.
              alpha.)]- §§ Podocarpa-8,11,13-tri
              en-15-oic acid, 13-isopropyl-, met
              hyl ester §§ Methyl dehydroabietat
              METHYL ABIETA-8,11,13-TRIEN-18-OAT 464550 001235-74-1 93
              E §§ 1-PHENANTHRENECARBOXYLIC ACID
              , 1,2,3,4,4A,9,10,10A-OCTAHYDRO-1,
              4A-DIMETHYL-7-(1-METHYLETHYL)-, ME
              THYL ESTER, [1R-(1.ALPHA.,4A.BETA.
              ,10A.ALPHA.)]- §§ DEHYDROABIETIC A
              CID METHYL ESTER §§ METHYL DEHYDRO
              ABIETATE

4  36.102  0.07 D:\DATABASE\DEMO.L
              Phenol, 2,4-bis(1-phenylethyl)- §§ 504578 002769-94-0 59
               2,4-Bis(1-phenylethyl)phenol #
              Palustric acid §§ Podocarpa-8,13-d 513439 001945-53-5 47
              ien-15-oic acid, 13-isopropyl- §§
              1-Phenanthrenecarboxylic acid, 1,2
              ,3,4,4a,5,6,9,10,10a-decahydro-1,4
              a-dimethyl-7-(1-methylethyl)-, (1R
              -(1.alpha.,4a.beta.,10a.alpha.))-
              §§ 8,13-Abietadien-18-oic acid
              CYCLOPROPANECARBONITRILE, 1,1'-[IM 504526 090594-32-4 43
              INOBIS(METHYLENE)]BIS[2,2,3,3-TETR
              AMETHYL- §§ 2,2,2',2',3,3,3',3'-OC
              TAMETHYL-1,1'-IMINEBIS(METHYLENE)D
              ICYCLOPROPANE-1,1'-DICARBONITRILE

5  36.383  0.06 D:\DATABASE\DEMO.L
              METHYL ABIETA-7,13-DIEN-18-OATE §§ 480551 000127-25-3 91
               1-PHENANTHRENECARBOXYLIC ACID, 1,
              2,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1
              ,4A-DIMETHYL-7-(1-METHYLETHYL)-, M
              ETHYL ESTER, [1R-(1.ALPHA.,4A.BETA
              .,4B.ALPHA.,10A.ALPHA.)]- §§ ABALY
              N §§ ABIETIC ACID METHYL ESTER
              Methyl abietate §§ 1-Phenanthrenec 258889 000127-25-3 90
              arboxylic acid, 1,2,3,4,4a,4b,5,6,
```

```
Data Path : F:\DATA MS\DAA\
Data File : WLM-10pssn-180c-3jmu.D
Acq On    :  9 Oct 2019  17:10
Operator  :
Sample    :
Misc      :
ALS Vial  : 2   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e

#     RT  Area%          Library/ID                    Ref#     CAS#   Qual
                10,10a-decahydro-1,4a-dimethyl-7-(
                1-methylethyl)-, methyl ester, [1R
                -(1.alpha.,4a.beta.,4b.alpha.,10a.
                alpha.)]- $$ Podocarpa-7,13-dien-1
                5-oic acid, 13-isopropyl-, methyl
                ester $$ Abalyn
                METHYL ABIETA-7,13-DIEN-18-OATE $$ 258918 000127-25-3 90
                 1-PHENANTHRENECARBOXYLIC ACID, 1,
                2,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1
                ,4A-DIMETHYL-7-(1-METHYLETHYL)-, M
                ETHYL ESTER, [1R-(1.ALPHA.,4A.BETA
                .,4B.ALPHA.,10A.ALPHA.)]- $$ ABALY
                N $$ ABIETIC ACID METHYL ESTER

6   36.610  0.19 D:\DATABASE\DEMO.L
                KAUR-16-EN-18-OIC ACID $$ KAUR-16- 168418 020316-84-1 86
                EN-18-OIC ACID, (4.BETA.)- $$ (-)-
                KAURNENOIC ACID $$ (4-BETA)-KAUR-1
                6-EN-18-OIC ACID
                Phenol, 2,4-bis(1-phenylethyl)- $$ 504578 002769-94-0 86
                 2,4-Bis(1-phenylethyl)phenol #
                Abietic acid $$ 1-Phenanthrenecarb 513344 000514-10-3 64
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- $$ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- $$ L-abietic acid

7   36.761  0.23 D:\DATABASE\DEMO.L
                BENZ[A]ANTHRACENONE                   513655 099707-96-7 90
                Palustric acid $$ Podocarpa-8,13-d 513439 001945-53-5 64
                ien-15-oic acid, 13-isopropyl- $$
                1-Phenanthrenecarboxylic acid, 1,2
                ,3,4,4a,5,6,9,10,10a-decahydro-1,4
                a-dimethyl-7-(1-methylethyl)-, (1R
                -(1.alpha.,4a.beta.,10a.alpha.))-
                $$ 8,13-Abietadien-18-oic acid
                Methanone, [1,4-dimethyl-7-(1-meth 513367 039665-56-0 42
                ylethyl)-2-azulenyl]phenyl- $$ 2-B
                enzoylguaiazulene $$ (7-Isopropyl-
                1,4-dimethyl-2-azulenyl)(phenyl)me
                thanone #

8   37.048  1.12 D:\DATABASE\DEMO.L
                1-Phenanthrenecarboxylic acid, 1,2 503081 001740-19-8 83
                ,3,4,4a,9,10,10a-octahydro-1,4a-di
                methyl-7-(1-methylethyl)-, [1R-(1.
                alpha.,4a.beta.,10a.alpha.)]- $$ P
                odocarpa-8,11,13-trien-15-oic acid
                , 13-isopropyl- $$ Abieta-8,11,13-
                trien-18-oic acid $$ Abietic acid,
                 dehydro-
                1-Phenanthrenecarboxylic acid, 1,2 503082 001740-19-8 51
                ,3,4,4a,9,10,10a-octahydro-1,4a-di
                methyl-7-(1-methylethyl)-, [1R-(1.
                alpha.,4a.beta.,10a.alpha.)]- $$ P
                odocarpa-8,11,13-trien-15-oic acid
                , 13-isopropyl- $$ Abieta-8,11,13-
```

```
ata Path : F:\DATA MS\daa\
ata File : WLM-10prsen-180c-3jmu.D
cq On    :  9 Oct 2019  17:10
perator  :
ample    :
isc      :
LS Vial  : 2   Sample Multiplier: 1

earch Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

nknown Spectrum:   Apex
ntegration Events: ChemStation Integrator - autoint1.e

     RT  Area%          Library/ID                    Ref#     CAS#   Qual

              trien-18-oic acid $$ Abietic acid,
               dehydro-
              1H-NAPHTHO[2,3-C]PYRAN-5,10-DIONE, 513557 084018-44-0 43
               3,4-DIHYDRO-7,9-DIMETHOXY-1,3-DIM
              ETHYL-, TRANS-(.+-.)- $$ (+,-)-DEO
              XYQUINONE A DIMETHYL ETHER $$ (+,-
              )-TRANS-7,9-DIMETHOXY-1,3-DIMETHYL
              -3,4,5,10-TETRAHYDRONAPHTHO[2,3-C]
              PYRAN-5,10-DIONE

  37.242  0.54 D:\DATABASE\DEMO.L
              Abietic acid $$ 1-Phenanthrenecarb 513378 000514-10-3 78
              oxylic acid, 1,2,3,4,4a,4b,5,6,10,
              10a-decahydro-1,4a-dimethyl-7-(1-m
              ethylethyl)-, [1R-(1.alpha.,4a.bet
              a.,4b.alpha.,10a.alpha.)]- $$ Podo
              carpa-7,13-dien-15-oic acid, 13-is
              opropyl- $$ L-abietic acid
              Abietic acid $$ 1-Phenanthrenecarb 513344 000514-10-3 70
              oxylic acid, 1,2,3,4,4a,4b,5,6,10,
              10a-decahydro-1,4a-dimethyl-7-(1-m
              ethylethyl)-, [1R-(1.alpha.,4a.bet
              a.,4b.alpha.,10a.alpha.)]- $$ Podo
              carpa-7,13-dien-15-oic acid, 13-is
              opropyl- $$ L-abietic acid
              ABIETA-7,13-DIEN-18-OIC ACID $$ 1- 168419 000514-10-3 52
              PHENANTHRENECARBOXYLIC ACID, 1,2,3
              ,4,4A,4B,5,6,10,10A-DECAHYDRO- $$
              1-PHENANTHRENECARBOXYLIC ACID, 1,2
              ,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,
              4A-DIMETHYL-7-(1-METHYLETHYL)-, [1
              R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A
              .ALPHA.)]-

  37.437  0.07 D:\DATABASE\DEMO.L
              Abietic acid $$ 1-Phenanthrenecarb 513344 000514-10-3 83
              oxylic acid, 1,2,3,4,4a,4b,5,6,10,
              10a-decahydro-1,4a-dimethyl-7-(1-m
              ethylethyl)-, [1R-(1.alpha.,4a.bet
              a.,4b.alpha.,10a.alpha.)]- $$ Podo
              carpa-7,13-dien-15-oic acid, 13-is
              opropyl- $$ L-abietic acid
              1H-2,10A-ETHANOPHENANTHRENE, KAUR- 513651 006730-83-2 60
              16-EN-18-OIC ACID DERIV. $$ KAUR-1
              6-EN-18-OIC ACID $$ KAUR-16-EN-18-
              OIC ACID, (4.ALPHA.)- $$ (-)-ENT-K
              AUR-16-EN-19-OIC ACID
              Abietic acid $$ 1-Phenanthrenecarb 513378 000514-10-3 60
              oxylic acid, 1,2,3,4,4a,4b,5,6,10,
              10a-decahydro-1,4a-dimethyl-7-(1-m
              ethylethyl)-, [1R-(1.alpha.,4a.bet
              a.,4b.alpha.,10a.alpha.)]- $$ Podo
              carpa-7,13-dien-15-oic acid, 13-is
              opropyl- $$ L-abietic acid

  37.707  2.60 D:\DATABASE\DEMO.L
              Abietic acid $$ 1-Phenanthrenecarb 513378 000514-10-3 99
              oxylic acid, 1,2,3,4,4a,4b,5,6,10,
              10a-decahydro-1,4a-dimethyl-7-(1-m
```

```
Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-180c-3jmu.D
Acq On    :  9 Oct 2019  17:10
Operator  :
Sample    :
Misc      :
ALS Vial  : 2   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e

#     RT  Area%          Library/ID                  Ref#     CAS#   Qual
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid
                Abietic acid §§ 1-Phenanthrenecarb 513344 000514-10-3 96
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid
                Abietic acid §§ 1-Phenanthrenecarb 513347 000514-10-3 94
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid
```

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsen-180c-4jm.D
Acq On : 12 Oct 2019 12:30
Operator :
Sample :
Misc :
ALS Vial : 2 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	1.962	5.54	D:\DATABASE\DEMO.L			
			Methyl Alcohol $$ Methanol $$ Carb inol $$ Methyl hydroxide	5073	000067-56-1	2
			METHANOL $$ HYDROXYMETHANE $$ ALCO HOL, METHYL $$ ALCOOL METHYLIQUE	5075	000067-56-1	2
			Methyl Alcohol $$ Methanol $$ Carb inol $$ Methyl hydroxide	5072	000067-56-1	2
2	2.070	0.01	D:\DATABASE\DEMO.L			
			DECANE-1,2-D2	22505	019165-56-1	33
			Formic acid, propyl ester $$ n-Pro pyl formate $$ Propyl formate $$ P ropyl methanoate	5233	000110-74-7	25
			3-Cyclopropyl-4-hydroxy-4,5,5-trim ethyl-oxazolidin-2-one	26504	999026-50-6	17
3	2.135	0.15	D:\DATABASE\DEMO.L			
			Pentane, 2,4-dimethyl- $$ 2,4-Dime thylpentane	18750	000108-08-7	91
			Pentane, 2,4-dimethyl- $$ 2,4-Dime thylpentane	18753	000108-08-7	90
			Pentane, 2,4-dimethyl- $$ 2,4-Dime thylpentane	18799	000108-08-7	83
4	2.200	11.62	D:\DATABASE\DEMO.L			
			HEXANE, 3-METHYL- $$ 3-METHYLHEXAN E $$ 2-ETHYLPENTANE $$ HEXANE, 3-M ETHYL	18994	000589-34-4	64
			1-PENTANOL, 2-METHYL- $$ 2-METHYLP ENTAN-1-OL $$ (+-)-2-METHYL-1-PENT ANOL $$ (+-)-2-METHYLPENTANOL	19228	000105-30-6	59
			Hexane, 3-methyl- $$ 2-Ethylpentan e $$ 3-Methylhexane	18754	000589-34-4	58
5	2.243	4.54	D:\DATABASE\DEMO.L			
			Cyclopentane, 1,3-dimethyl-, cis- $$ cis-1,3-Dimethylcyclopentane $$ 1,3-Dimethylcyclopentane cis $$ 1 ,3-Dimethylcyclopentane #	62231	002532-58-3	91
			1,3-DIMETHYLCYCLOPENTANE $$ CYCLOP ENTANE, 1,3-DIMETHYL-, CIS- $$ 1,3 -DIMETHYLCYCLOPENTANE (CIS) $$ 1,3 -DIMETHYLCYCLOPENTANE CIS	62286	002532-58-3	91
			Cyclopentane, 1,3-dimethyl- $$ 1,3 -Dimethylcyclopentane	101343	002453-00-1	91
6	2.335	6.78	D:\DATABASE\DEMO.L			
			CYCLOHEXANE, METHYL- $$ METHYLCYCL OHEXANE $$ 1-METHYLCYCLOHEXANE $$ CYCLOHEXANE, METHYL	141469	000108-87-2	96
			CYCLOHEXANE, METHYL- $$ METHYLCYCL OHEXANE $$ 1-METHYLCYCLOHEXANE $$ CYCLOHEXANE, METHYL	141470	000108-87-2	95
			CYCLOHEXANE, METHYL- $$ METHYLCYCL OHEXANE $$ 1-METHYLCYCLOHEXANE $$ CYCLOHEXANE, METHYL	141467	000108-87-2	95
7	2.421	61.33	D:\DATABASE\DEMO.L			
			Toluene $$ Benzene, methyl $$ Meth	158579	000108-88-3	91

```
Data Path : F:\DATA MS\daa\
Data File : WLM-10pesen-180c-4jm.D
Acq On    : 12 Oct 2019  12:30
Operator  :
Sample    :
Misc      :
ALS Vial  : 2   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autointl.e

k#     RT  Area%          Library/ID                   Ref#     CAS#   Qual
                acide §§ Methylbenzene
                BENZENE, METHYL- §§ METHYLBENZENE  158625 000108-88-3 91
                §§ TOLUENE §§ ANTISAL 1A
                Toluene §§ Benzene, methyl §§ Meth 158580 000108-88-3 91
                acide §§ Methylbenzene

 8   2.745  1.12 D:\DATABASE\DEMO.L
                Cyclohexane, ethyl- §§ Ethylcycloh 141506 001678-91-7 93
                exane
                Cyclohexane, ethyl- §§ Ethylcycloh 141508 001678-91-7 93
                exane
                CYCLOHEXANE, ETHYL- §§ ETHYLCYCLOH 141561 001678-91-7 93
                EXANE §§ ETHYL CYCLOHEXANE §§ ETHY
                LCYCLOHEXAN

 9   2.875  0.48 D:\DATABASE\DEMO.L
                BENZENE, METHYL- §§ METHYLBENZENE  158623 000108-88-3 90
                §§ TOLUENE §§ ANTISAL 1A
                1,3,5-CYCLOHEPTATRIENE §§ CYCLOHEP 158636 000544-25-2 90
                TA-1,3,5-TRIENE §§ CYCLOHEPTATRIEN
                E §§ CYCLOHEPTATRIENE [UN2603] [FL
                AMMABLE LIQUID]
                1,3,5-CYCLOHEPTATRIENE §§ CYCLOHEP 158637 000544-25-2 87
                TA-1,3,5-TRIENE §§ CYCLOHEPTATRIEN
                E §§ CYCLOHEPTATRIENE [UN2603] [FL
                AMMABLE LIQUID]

10  17.315  0.03 D:\DATABASE\DEMO.L
                2H-2,4A-METHANONAPHTHALENE, 1,3,4, 350801 001135-66-6 95
                5,6,7-HEXAHYDRO-1,1,5,5-TETRAMETHY
                L-, (2S)- §§ (-)-ISOLONGIFOLENE §§
                  (-)-ISOLONGIFOLINE §§ (2S)-1,3,4,
                5,6,7-HEXAHYDRO-1,1,5,5-TETRAMETHY
                L-2H-2,4A-METHANONAPHTHALENE
                2H-2,4a-Methanonaphthalene, 1,3,4, 350641 001135-66-6 95
                5,6,7-hexahydro-1,1,5,5-tetramethy
                l-, (2S)- §§ 2H-2,4a-Methanonaphth
                alene, 1,3,4,5,6,7-hexahydro-1,1,5
                ,5-tetramethyl-, (2S,4aR)-(-)- §§
                Isolongifolene §§ (-)-Isolongifoli
                ne
                2H-2,4A-METHANONAPHTHALENE, 1,3,4, 350804 001135-66-6 95
                5,6,7-HEXAHYDRO-1,1,5,5-TETRAMETHY
                L-, (2S)- §§ (-)-ISOLONGIFOLENE §§
                  (-)-ISOLONGIFOLINE §§ (2S)-1,3,4,
                5,6,7-HEXAHYDRO-1,1,5,5-TETRAMETHY
                L-2H-2,4A-METHANONAPHTHALENE

11  17.698  0.00 D:\DATABASE\DEMO.L
                (2,6,6-TRIMETHYLBICYCLO[3.1.1]HEPT   4518 999004-51-9 10
                -3-YL)METHANAMINE §§ (2,6,6-TRIMET
                HYLBICYCLO[3.1.1]HEPT-3-YL)METHYLA
                MINE
                Ethanol, 2-bromo- §§ Ethylene brom   5441 000540-51-2  9
                ohydrin §§ Glycol bromohydrin §§ 1
                -Bromo-2-ethanol
                3-(3-OXO-3H-BENZO[F]CHROMEN-2-YL)-   7476 999007-47-7  9
                2,4(1H,3H)-QUINOLINEDIONE §§ 4-HYD
                ROXY-3-(2-OXO-2H-1-OXA-3-PHENANTHR
```

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsen-180c-4jm.D
Acq On : 12 Oct 2019 12:30
Operator :
Sample :
Misc :
ALS Vial : 2 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			YL)-2(1H)-QUINOLINONE			
12	17.725	0.01	D:\DATABASE\DEMO.L			
			2,2,3,3,4,4,5,5-OCTAFLUORO-N-(3-METHOXYPHENYL)PENTANAMIDE §§ PENTANAMIDE, 2,2,3,3,4,4,5,5-OCTAFLUORO-N-(3-METHOXYPHENYL)-	7474	339166-43-7	9
			Propanedioic acid, (hydroxyimino)-, diethyl ester §§ Bis-(ethoxycarbonyl)hydroxyiminomethane §§ Diethyl 2-(hydroxyimino)malonate #	2893	006829-41-0	4
			3-(3-OXO-3H-BENZO[F]CHROMEN-2-YL)-2,4(1H,3H)-QUINOLINEDIONE §§ 4-HYDROXY-3-(2-OXO-2H-1-OXA-3-PHENANTHRYL)-2(1H)-QUINOLINONE	7476	999007-47-7	4
13	28.610	0.01	D:\DATABASE\DEMO.L			
			4-(METHOXYMETHYL)-6-METHYL-2-PHENOXYNICOTINONITRILE §§ PYRIDINE-3-CARBONITRILE, 4-METHOXYMETHYL-6-METHYL-2-PHENOXY-	7413	332057-36-0	25
			4-BROMO-N-[(6-METHYL-2-PYRIDYL)AMINOMETHYL]PHTHALIMIDE §§ 5-BROMO-2-{[(6-METHYL-2-PYRIDINYL)AMINO]METHYL}-1H-ISOINDOLE-1,3(2H)-DIONE	7473	999007-47-4	9
			1-Dodecanamine §§ Dodecylamine §§ n-Dodecylamine §§ Alamine 4	4652	000124-22-1	4
14	30.215	0.00	D:\DATABASE\DEMO.L			
			4-(METHOXYMETHYL)-6-METHYL-2-PHENOXYNICOTINONITRILE §§ PYRIDINE-3-CARBONITRILE, 4-METHOXYMETHYL-6-METHYL-2-PHENOXY-	7413	332057-36-0	22
			METHYL (2E,4E)-5-(1-HYDROXY-2,6,6-TRIMETHYL-4-OXO-2-CYCLOHEXEN-1-YL)-3-METHYL-2,4-PENTADIENOATE §§ 2,4-PENTADIENOIC ACID, 5-(1-HYDROXY-2,6,6-TRIMETHYL-4-OXO-2-CYCLOHEXEN-1-YL)-3-METHYL-, METHYL ESTER, (R)-(Z,E)- §§ METHYL ABSCISATE	3305	007200-31-9	10
			4-BROMO-N-[(6-METHYL-2-PYRIDYL)AMINOMETHYL]PHTHALIMIDE §§ 5-BROMO-2-{[(6-METHYL-2-PYRIDINYL)AMINO]METHYL}-1H-ISOINDOLE-1,3(2H)-DIONE	7473	999007-47-4	9
15	30.306	0.03	D:\DATABASE\DEMO.L			
			Phenanthrene, 7-ethenyl-1,2,3,4,4a,5,6,7,8,9,10,10a-dodecahydro-1,1,4a,7-tetramethyl- §§ Pimara-8,15-diene #	481092	055255-56-6	87
			Naphthalene, decahydro-1,1,4a-trimethyl-6-methylene-5-(3-methyl-2,4-pentadienyl)-, [4aS-(4a.alpha.,5.alpha.,8a.beta.)]- §§ Labda-8(20),12,14-triene §§ Biformen §§ Biformene	481091	005957-33-5	83
			1,1,4A-TRIMETHYL-6-METHYLENE-5-[(2E)-3-METHYL-2,4-PENTADIENYL]DECAHYDRONAPHTHALENE §§ NAPHTHALENE, DEC	481156	005957-33-5	83

```
Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-180c-4jm.D
Acq On    : 12 Oct 2019  12:30
Operator  :
Sample    :
Misc      :
ALS Vial  : 2   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e

k#     RT  Area%          Library/ID                    Ref#     CAS#   Qual
                AHYDRO-1,1,4A-TRIMETHYL-6-METHYLEN
                E-5-(3-METHYL-2,4-PENTADIENYL)-, [
                4AS-(4A.ALPHA.,5.ALPHA.,8A.BETA.)]
                - $$ BIFORMEN $$ BIFORMENE

16  30.549  0.01 D:\DATABASE\DEMO.L
                4-(METHOXYMETHYL)-6-METHYL-2-PHENO   7413 332057-36-0 25
                XYNICOTINONITRILE $$ PYRIDINE-3-CA
                RBONITRILE, 4-METHOXYMETHYL-6-METH
                YL-2-PHENOXY-
                1-Dodecanamine $$ Dodecylamine $$    4652 000124-22-1  9
                n-Dodecylamine $$ Alamine 4
                1-DODECANAMINE $$ 1-AMINODODECANE    4661 000124-22-1  9
                $$ 1-DODECYLAMINE $$ ALAMINE 4

17  30.712  0.01 D:\DATABASE\DEMO.L
                4-(METHOXYMETHYL)-6-METHYL-2-PHENO   7413 332057-36-0 27
                XYNICOTINONITRILE $$ PYRIDINE-3-CA
                RBONITRILE, 4-METHOXYMETHYL-6-METH
                YL-2-PHENOXY-
                1-Dodecanamine $$ Dodecylamine $$    4652 000124-22-1  9
                n-Dodecylamine $$ Alamine 4
                1-DODECANAMINE $$ 1-AMINODODECANE    4661 000124-22-1  9
                $$ 1-DODECYLAMINE $$ ALAMINE 4

18  30.879  0.01 D:\DATABASE\DEMO.L
                4H-1-BENZOPYRAN-4-ONE, 3-HYDROXY-2 468099 104197-23-1 43
                -(PHENYL-D5)- $$ 3-HYDROXY-2',3',4
                ',5',6'-PENTADEUTEROFLAVONE
                13-.ALPHA.-METHYLANDROSTA          468266 000000-00-0 32
                4-(METHOXYMETHYL)-6-METHYL-2-PHENO   7413 332057-36-0 22
                XYNICOTINONITRILE $$ PYRIDINE-3-CA
                RBONITRILE, 4-METHOXYMETHYL-6-METH
                YL-2-PHENOXY-

19  31.187  0.01 D:\DATABASE\DEMO.L
                4H-1-BENZOPYRAN-4-ONE, 3-HYDROXY-2 468099 104197-23-1 47
                -(PHENYL-D5)- $$ 3-HYDROXY-2',3',4
                ',5',6'-PENTADEUTEROFLAVONE
                Pyran-4-one, 3-acetyl-2-(2-aminoph 468125 999468-13-3 38
                enylamino)-6-methyl-
                13-.ALPHA.-METHYLANDROST-9,11-E    468253 000000-00-0 37

20  31.695  0.03 D:\DATABASE\DEMO.L
                6-ETHYL-2-METHYL-4,6-DIHYDRO-2H-[1   7414 334023-40-4 10
                ,4]OXAZINO[3,2-C]QUINOLINE-3,5-DIO
                NE $$ 6-ETHYL-2-METHYL-2H-1-OXA-4,
                6-PHENANTHROLINE-3,5(4H,6H)-DIONE
                $$ 6-ETHYL-2-METHYL-6,10B-DIHYDRO-
                2H-[1,4]OXAZINO[3,2-C]QUINOLINE-3,
                5-DIONE
                (+-)METHYL HERITOL                    484 000000-00-0 10
                3H-[1]BENZOTHIENO[3,2-D]AZONINE-3-   7435 099659-20-8  7
                CARBONITRILE, 1,2,4,5,6,7-HEXAHYDR
                O-7-METHOXY- $$ 7-METHOXY-2,3,4,5,
                6,7-HEXAHYDRO-1H-[1]BENZOTHIENO[3,
                2-D]AZONINE-3-CARBONITRILE

21  31.824  0.00 D:\DATABASE\DEMO.L
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```
Data Path : F:\DATA MS\daa\
Data File : WLM-10green-180c-4jm.D
Acq On    : 12 Oct 2019  12:30
Operator  :
Sample    :
Misc      :
ALS Vial  : 2   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autointl.e

Pk#     RT  Area%          Library/ID                  Ref#     CAS#   Qual
                N-Carbethoxymethylimine, formylmal   3288 999003-28-9  1
                onic acid diethyl ester
                DIETHYL 2-({[2-ETHOXY-2-OXOETHYL]I   3294 999003-29-5  1
                MINO}METHYL)MALONATE $$ N-CARBETOX
                YMETHYLIMINE, FORMYLMALONIC ACID D
                IETHYL ESTER
                ETHYL ESTER OF TRICHLOROACRYLIC AC   2997 000000-00-0  1
                ID

22  31.997  0.04 D:\DATABASE\DEMO.L
                Naphthalene, 1,2,3,4-tetrahydro-1-  373089 081603-43-2 47
                methyl-8-(1-methylethyl)- $$ 8-Iso
                propyl-1-methyl-1,2,3,4-tetrahydro
                naphthalene #
                5-Quinolinamine, 8-ethoxy-          373098 999373-10-2 38
                2-BUTYL-5-HEXYLINDANE $$ INDAN, 2-  398767 025446-32-6 35
                BUTYL-5-HEXYL- $$ 2-N-BUTYL-1-N-HE
                XYL-2,3-DIHYDROINDENE $$ 2-N-BUTYL
                -5-N-HEXYL-(2,3-DIHYDROINDENE)

23  32.100  0.02 D:\DATABASE\DEMO.L
                2(1H)-Phenanthrenone, 3,4,4a,9,10,  481103 055255-51-1 46
                10a-hexahydro-7-methoxy-1,1,4a-tri
                methyl- $$ 13-Methoxypodocarpa-8,1
                1,13-trien-3-one #
                3,5-Bis(trifluoromethyl)-4-hydroxy  481094 999481-10-6 43
                acetophenone
                4'-METHYL-1',4'-DIHYDRO-[2,3']BIQU  481121 999481-13-3 43
                INOLINYL

24  32.392  0.01 D:\DATABASE\DEMO.L
                1H-BENZIMIDAZOLE, 2-(4-THIAZOLYL)-  419260 000148-79-8 49
                 $$ 1H-BENZIMIDAZOLE, 2- (4-THIAZO
                LYL)- $$ 2-(1,3-THIAZOL-4-YL)-1H-B
                ENZIMIDAZOLE $$ 2-(1,3-THIAZOL-4-Y
                L)BENZIMIDAZOLE
                1,4-Pentanediamine, N(4)-(6-methox  419707 000090-34-6 47
                y-8-quinolinyl)- $$ Neo-Quipenyl $
                $ Primachin $$ Primaquine
                1,3,5-TRIAZINE-2,4-DIAMINE, 6-(3-M  419264 029366-76-5 47
                ETHYLPHENYL)- $$ 1,3,5-TRIAZINE-2,
                 4-DIAMINE, 6- (3-METHYLPHENYL)- $
                $ 2-(M-METHYLPHENYL)-4,6-DIAMINO-S
                -TRIAZINE $$ S-TRIAZINE, 2,4-DIAMI
                NO-6-M-TOLYL-

25  32.419  0.01 D:\DATABASE\DEMO.L
                3,5-DIETHYL-2-(2-FURYL)PYRIDINE $$  419329 078563-73-2 30
                 3,5-DIETHYL-4-(2-FURYL)PYRIDINE
                4-NITRO-2-NAPHTHALDEHYDE            419272 000000-00-0 27
                5-Trifluoromethyl-3-methylthiazoli  419133 186791-22-0 27
                dine-2-thione $$ 3-Methyl-5-(trifl
                uoromethyl)-1,3-thiazolidine-2-thi
                one #

26  32.764  0.01 D:\DATABASE\DEMO.L
                1-Hexadecanamine $$ Hexadecylamine   4902 000143-27-1 16
                 $$ n-Cetylamine $$ n-Hexadecylami
                ne
```

```
Data Path : P:\DATA MS\GCMS\
Data File : WLM-10pmsen-180c-4jm.D
Acq On    : 12 Oct 2019  12:30
Operator  :
Sample    :
Misc      :
ALS Vial  : 2   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autointl.e

#     RT  Area%          Library/ID                    Ref#     CAS#   Qual

              4-(METHOXYMETHYL)-6-METHYL-2-PHENO   7413 332057-36-0 16
              XYNICOTINONITRILE $$ PYRIDINE-3-CA
              RBONITRILE, 4-METHOXYMETHYL-6-METH
              YL-2-PHENOXY-
              1-Heptadecanamine $$ Heptadecylami   4935 004200-95-7  9
              ne $$ n-Heptadecylamine $$ Margary
              lamine

7  32.980  0.01 D:\DATABASE\DEMO.L
              4-(METHOXYMETHYL)-6-METHYL-2-PHENO   7413 332057-36-0 16
              XYNICOTINONITRILE $$ PYRIDINE-3-CA
              RBONITRILE, 4-METHOXYMETHYL-6-METH
              YL-2-PHENOXY-
              1-PENTADECANAMINE $$ 1-PENTADECYLA   4879 002570-26-5  9
              MINE $$ N-PENTADECYLAMINE $$ PENTA
              DECANE, 1-AMINO-
              1-Tetradecanamine $$ Tetradecylami   4817 002016-42-4  9
              ne $$ Armeen 14 $$ Myristylamine

8  33.380  0.00 D:\DATABASE\DEMO.L
              1-Hexadecanamine $$ Hexadecylamine   4902 000143-27-1 27
               $$ n-Cetylamine $$ n-Hexadecylami
              ne
              2-METHOXY-4-(METHOXYMETHYL)-6-METH   7347 063644-84-8 12
              YLNICOTINONITRILE $$ PYRIDINE-3-CA
              RBONITRILE, 2,4-DIMETHOXY-6-METHYL
              1-Tetradecanamine $$ Tetradecylami   4817 002016-42-4 10
              ne $$ Armeen 14 $$ Myristylamine

9  33.499  0.11 D:\DATABASE\DEMO.L
              ANDROST-5-ENE, 4,4-DIMETHYL-, (13. 492912 073495-94-0 90
              ALPHA.)- $$ 4,4-DIMETHYL-13.ALPHA.
              -ANDROST-5-ENE
              (+)1A7,4A,9,10,10A-DODECAHYDRO-1,4 481209 000000-00-0 53
              A,7-TRIMETHYL-7-VINYL-1-PHENANTHRE
              NCARBALDEHYDSHYL 4,A2C.BETA.THIOME
              THYL](12-YL2ETHYLTHIOYLENC1ETHYLDE
              THYL3-YLAPHTHC]TAOXM.BETA.AMO6, [U
              CH0ALFPAL[YL9
              KAURA-5,16-DIEN-18-OL $$ KAURA-5,1 492904 023837-99-2 50
              6-DIEN-18(OR 19)-OL $$ KAURA-5,16-
              DIEN-19-OL

0  33.618  0.00 D:\DATABASE\DEMO.L
              4-BROMO-N-[(6-METHYL-2-PYRIDYL)AMI   7473 999007-47-4 22
              NOMETHYL]PHTHALIMIDE $$ 5-BROMO-2-
              {[(6-METHYL-2-PYRIDINYL)AMINO]METH
              YL}-1H-ISOINDOLE-1,3(2H)-DIONE
              2-METHOXY-4-(METHOXYMETHYL)-6-METH   7347 063644-84-8 22
              YLNICOTINONITRILE $$ PYRIDINE-3-CA
              RBONITRILE, 2,4-DIMETHOXY-6-METHYL
              1-Hexadecanamine $$ Hexadecylamine   4902 000143-27-1 12
               $$ n-Cetylamine $$ n-Hexadecylami
              ne

1  33.661  0.00 D:\DATABASE\DEMO.L
              4-(METHOXYMETHYL)-6-METHYL-2-PHENO   7413 332057-36-0 25
              XYNICOTINONITRILE $$ PYRIDINE-3-CA
              RBONITRILE, 4-METHOXYMETHYL-6-METH
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Data Path : F:\DATA MS\daa\
Data File : WLM-10green-180c-4jm.D
Acq On    : 12 Oct 2019  12:30
Operator  :
Sample    :
Misc      :
ALS Vial  : 2   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#     RT  Area%          Library/ID                    Ref#     CAS#   Qual
                YL-2-PHENOXY-
                1-Hexadecanamine §§ Hexadecylamine    4902 000143-27-1 12
                 §§ n-Cetylamine §§ n-Hexadecylami
                ne
                3-(3-OXO-3H-BENZO[F]CHROMEN-2-YL)-    7476 999007-47-7 10
                2,4(1H,3H)-QUINOLINEDIONE §§ 4-HYD
                ROXY-3-(2-OXO-2H-1-OXA-3-PHENANTHR
                YL)-2(1H)-QUINOLINONE

32  33.791  0.03 D:\DATABASE\DEMO.L
                7-BENZYLOXY-2-HYDROXY-2H-[1,4]BENZ 166364 000000-00-0 11
                OXAZIN-3(4H)-ONE
                7-BENZYLOXY-2,4-DIHYDROXY-2H-[1,4] 167385 000000-00-0 10
                BENZOXAZIN-3(4H)-ONE
                9-Benzyladenine N(1)-oxide §§ 9-Be 164412 004261-16-9 10
                nzyl-1-oxido-9H-purin-6-ylamine #

33  33.861  0.07 D:\DATABASE\DEMO.L
                10,13-DIMETHYL-4,5,6,7,8,9,10,11,1 466180 999466-18-8 95
                2,13,14,15-DODECAHYDRO-1H-CYCLOPEN
                TA[A]PHENANTHRENE §§ ANDROSTA-2,16
                -DIENE
                1-Methyl-10,18-bisnorabieta-8,11,1 466158 999466-16-6 94
                3-triene
                4-(N-METHYLAMINO)-6,7-(1,2,3,4-TET 466219 000000-00-0 90
                RAHYDRO-1,1,4,4-TETRAMETHYLBENZO)I
                NDOLE

34  34.131  0.01 D:\DATABASE\DEMO.L
                1-Tetradecanamine §§ Tetradecylami    4817 002016-42-4 10
                ne §§ Armeen 14 §§ Myristylamine
                Ethanamine, 2-methoxy- §§ Ethylami    3693 000109-85-3  9
                ne, 2-methoxy- §§ .beta.-Methoxyet
                hylamine §§ Methoxyethylamine
                1-Undecanamine §§ Undecylamine §§     4554 007307-55-3  9
                n-Undecylamine §§ Hendecylamine

35  34.196  0.01 D:\DATABASE\DEMO.L
                2-METHOXY-4-(METHOXYMETHYL)-6-METH    7347 063644-84-8 12
                YLNICOTINONITRILE §§ PYRIDINE-3-CA
                RBONITRILE, 2,4-DIMETHOXY-6-METHYL
                1-Hexadecanamine §§ Hexadecylamine    4902 000143-27-1 10
                 §§ n-Cetylamine §§ n-Hexadecylami
                ne
                1,12-Dodecanediamine §§ 1,12-Diami    4748 002783-17-7  9
                nododecane §§ Dodecamethylenediami
                ne §§ Dodecylenediamine

36  34.309  0.04 D:\DATABASE\DEMO.L
                1-Phenanthrenecarboxylic acid, 7-e 466507 003582-26-1 86
                thenyl-1,2,3,4,4a,5,6,7,8,9,10,10a
                -dodecahydro-1,4a,7-trimethyl-, me
                thyl ester, [1R-(1.alpha.,4a.beta.
                ,7.beta.,10a.alpha.)]- §§ Podocarp
                -8-en-15-oic acid, 13.alpha.-methy
                l-13-vinyl-, methyl ester
                METHYL PIMARA-8(14),15-DIEN-18-OAT 466514 001686-54-0 62
                E §§ 1-PHENANTHRENECARBOXYLIC ACID
                , 7-ETHENYL-1,2,3,4,4A,4B,5,6,7,9,
```

Data Path : F:\DATA MS\daa\
Data File : WLM-10pmen-180c-4jm.D
Acq On : 12 Oct 2019 12:30
Operator :
Sample :
Misc :
ALS Vial : 2 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autointl.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			10,10A-DODECAHYDRO-1,4A,7-TRIMETHY L-, METHYL ESTER, [1R-(1.ALPHA.,4A .BETA.,4B.ALPHA.,7.ALPHA.,10A.ALPH A.)]- $$ ISODEXTROPIMARIC ACID MET HYL ESTER			
			METHYL PIMARA-8,15-DIEN-18-OATE $$ 1-PHENANTHRENECARBOXYLIC ACID, 7- ETHENYL-1,2,3,4,4A,5,6,7,8,9,10,10 A-DODECAHYDRO-1,4A,7-TRIMETHYL-, M ETHYL ESTER, [1R-(1.ALPHA.,4A.BETA .,7.BETA.,10A.ALPHA.)]- $$ METHYL 8,15-PIMARADIEN-18-OATE	466513	003582-26-1	60
37	34.541	0.04	D:\DATABASE\DEMO.L			
			ABIETA-7,13-DIEN-18-OIC ACID $$ 1- PHENANTHRENECARBOXYLIC ACID, 1,2,3 ,4,4A,4B,5,6,10,10A-DECAHYDRO- $$ 1-PHENANTHRENECARBOXYLIC ACID, 1,2 ,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1, 4A-DIMETHYL-7-(1-METHYLETHYL)-, [1 R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A .ALPHA.)]-	168420	000514-10-3	46
			KAUR-16-EN-18-OIC ACID $$ KAUR-16- EN-18-OIC ACID, (4.BETA.)- $$ (-)- KAURNENOIC ACID $$ (4-BETA)-KAUR-1 6-EN-18-OIC ACID	168418	020316-84-1	15
			4H-[1,2,4]Triazole-3-thiol, 4-benz yl-5-furan-2-yl-	165414	999165-41-7	10
38	34.606	0.00	D:\DATABASE\DEMO.L			
			1-Hexadecanamine $$ Hexadecylamine $$ n-Cetylamine $$ n-Hexadecylami ne	4902	000143-27-1	11
			2-METHOXY-4-(METHOXYMETHYL)-6-METH YLNICOTINONITRILE $$ PYRIDINE-3-CA RBONITRILE, 2,4-DIMETHOXY-6-METHYL	7347	063644-84-8	10
			1-Tetradecanamine $$ Tetradecylami ne $$ Armeen 14 $$ Myristylamine	4815	002016-42-4	10
39	34.650	0.00	D:\DATABASE\DEMO.L			
			2-METHOXY-4-(METHOXYMETHYL)-6-METH YLNICOTINONITRILE $$ PYRIDINE-3-CA RBONITRILE, 2,4-DIMETHOXY-6-METHYL	7347	063644-84-8	22
			1-Hexadecanamine $$ Hexadecylamine $$ n-Cetylamine $$ n-Hexadecylami ne	4902	000143-27-1	10
			4-BROMO-N-[(6-METHYL-2-PYRIDYL)AMI NOMETHYL]PHTHALIMIDE $$ 5-BROMO-2- {[(6-METHYL-2-PYRIDINYL)AMINO]METH YL}-1H-ISOINDOLE-1,3(2H)-DIONE	7473	999007-47-4	10
40	34.677	0.00	D:\DATABASE\DEMO.L			
			2-((E)-[((E)-2-([(E)-(2-HYDROXYPHE NYL)METHYLIDENE]AMINO)PROPYL)IMINO]METHYL)PHENOL $$ .ALPHA.,.ALPHA.' -(1-METHYLETHYLENEDIIMINO)DI-ORTHO -CRESOL $$ .ALPHA.,.ALPHA.'-DIPROP YLENEDINITRILODI-O-CRESOL $$ ALPHA ,ALPHA'-(1-METHYLETHYLENEDIIMINO)D	45719	000094-91-7	25

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsen-180c-4jm.D
Acq On : 12 Oct 2019 12:30
Operator :
Sample :
Misc :
ALS Vial : 2 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			I-ORTHO-CRESOL			
			Morphinan-14-ol, 3-methoxy-17-meth yl- §§ (-)-14-Hydroxy-3-methoxy-17 -methylmorphinan §§ 3-Methoxy-17-m ethylmorphinan-14-ol #	45783	001639-74-3	25
			3-METHOXY-17-METHYLMORPHINAN-14-OL §§ MORPHINAN-14-OL, 3-METHOXY-17- METHYL- §§ (-)-14-HYDROXY-3-METHOX Y-17-METHYLMORPHINAN	45788	001639-74-3	25
41	34.725	0.00	D:\DATABASE\DEMO.L			
			2H-3,9A-METHANO-1-BENZOXEPIN, OCTA HYDRO-2,2,5A,9-TETRAMETHYL-, [3R-(3.ALPHA.,5A.ALPHA.,9.ALPHA.,9A.ALP HA.)]- §§ .BETA.-AGAROFURAN, DIHYD RO- §§ .BETA.-DIHYDROAGAROFURAN §§ 2H-3,9A-METHANO-1-BENZOXEPIN, OCT AHYDRO-2,2,5A,9-TETRAMETHYL-	3110	005956-09-2	9
42	34.785	0.01	D:\DATABASE\DEMO.L			
			2H-3,9A-METHANO-1-BENZOXEPIN, OCTA HYDRO-2,2,5A,9-TETRAMETHYL-, [3R-(3.ALPHA.,5A.ALPHA.,9.ALPHA.,9A.ALP HA.)]- §§ .BETA.-AGAROFURAN, DIHYD RO- §§ .BETA.-DIHYDROAGAROFURAN §§ 2H-3,9A-METHANO-1-BENZOXEPIN, OCT AHYDRO-2,2,5A,9-TETRAMETHYL-	3110	005956-09-2	9
			Acetic acid, 4-(3-acetylamino-2-ox opropyl)phenyl ester §§ 4-[3-(Acet ylamino)-2-oxopropyl]phenyl acetat e #	4924	061172-74-5	7
			Diethyl 3-chloro-2-hydroxypropylma lonate	3235	999003-23-6	4
43	34.909	0.01	D:\DATABASE\DEMO.L			
			Diethyl 3-chloro-2-hydroxypropylma lonate	3235	999003-23-6	9
			DIETHYL 2-(3-CHLORO-2-HYDROXYPROPY L)MALONATE §§ DIETHYL 3-CHLORO-2-H YDROXYPROPYLMALONATE	3236	999003-23-7	9
			2H-3,9A-METHANO-1-BENZOXEPIN, OCTA HYDRO-2,2,5A,9-TETRAMETHYL-, [3R-(3.ALPHA.,5A.ALPHA.,9.ALPHA.,9A.ALP HA.)]- §§ .BETA.-AGAROFURAN, DIHYD RO- §§ .BETA.-DIHYDROAGAROFURAN §§ 2H-3,9A-METHANO-1-BENZOXEPIN, OCT AHYDRO-2,2,5A,9-TETRAMETHYL-	3110	005956-09-2	6
44	34.936	0.01	D:\DATABASE\DEMO.L			
			2-Propenamide, N-octyl-3-phenyl- § § (2E)-n-Octyl-3-phenyl-2-propenam ide #	283082	055030-48-3	25
			2-((E)-[((E)-2-([(E)-(2-HYDROXYPHE NYL)METHYLIDENE]AMINO)PROPYL)IMINO]METHYL)PHENOL §§ .ALPHA.,.ALPHA.' -(1-METHYLETHYLENEDIIMINO)DI-ORTHO -CRESOL §§ .ALPHA.,.ALPHA.'-DIPROP YLENEDINITRILODI-O-CRESOL §§ ALPHA ,ALPHA'-(1-METHYLETHYLENEDIIMINO)D	45719	000094-91-7	25

Data File : WLW-10pTWB-1800-4jm.D
Acq On : 12 Oct 2019 12:30
Operator :
Sample :
Misc :
ALS Vial : 2 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			I-ORTHO-CRESOL			
			(2E)-N-OCTYL-3-PHENYL-2-PROPENAMID E $$ 2-PROPENAMIDE, N-OCTYL-3-PHEN YL- $$ N-N-OCTYL-3-PHENYLPROPENAMI DE	283089	055030-48-3	25
45	35.028	0.03	D:\DATABASE\DEMO.L			
			Benzene, (2,2-dimethoxyethyl)- $$ Acetaldehyde, phenyl-, dimethyl ac etal $$ .alpha.-Tolylaldehyde dime thyl acetal $$ Hyacylene P	122348	000101-48-4	53
			5,5-DIMETHYL-2-(TRIMETHYLSILYL)-1, 2,3,4,4A,5,6,7-OCTAHYDRO-2-NAPHTHA LENOL $$ 5,5-DIMETHYL-2-TRIMETHYLS ILANYL-1,2,3,4,4A,5,6,7-OCTAHYDRO-NAPHTHALEN-2-OL	123410	999123-41-3	42
			t-Butyldimethyl(2-methylcyclohex-1 -enylmethoxy)silane	123280	999123-28-3	42
46	35.120	0.01	D:\DATABASE\DEMO.L			
			2-((E)-[((E)-2-([(E)-(2-HYDROXYPHE NYL)METHYLIDENE]AMINO)PROPYL)IMINO]METHYL)PHENOL $$ .ALPHA.,.ALPHA.' -(1-METHYLETHYLENEDIIMINO)DI-ORTHO -CRESOL $$ .ALPHA.,.ALPHA.'-DIPROP YLENEDINITRILODI-O-CRESOL $$ ALPHA ,ALPHA'-(1-METHYLETHYLENEDIIMINO)D I-ORTHO-CRESOL	45719	000094-91-7	38
			Benzenepropanoic acid, tert-butyld imethylsilyl ester $$ tert-Butyl(d imethyl)silyl 3-phenylpropanoate #	123517	078324-01-3	10
			3-(3'-CHLOROPHENYL)-4-METHYL-.DELT A.(4)-THIAZOLINE-2-THIONE	427153	116350-75-5	9
47	35.141	0.01	D:\DATABASE\DEMO.L			
			2-((E)-[((E)-2-([(E)-(2-HYDROXYPHE NYL)METHYLIDENE]AMINO)PROPYL)IMINO]METHYL)PHENOL $$ .ALPHA.,.ALPHA.' -(1-METHYLETHYLENEDIIMINO)DI-ORTHO -CRESOL $$ .ALPHA.,.ALPHA.'-DIPROP YLENEDINITRILODI-O-CRESOL $$ ALPHA ,ALPHA'-(1-METHYLETHYLENEDIIMINO)D I-ORTHO-CRESOL	45719	000094-91-7	41
			Andrographolide $$ 2(3H)-Furanone, 3-[2-[decahydro-6-hydroxy-5-(hydr oxymethyl)-5,8a-dimethyl-2-methyla ne-1-naphthalenyl]ethylidene]dihyd ro-4-hydroxy-	171071	005508-58-7	16
			1-benzylindole	162408	999162-41-1	10
48	35.179	0.01	D:\DATABASE\DEMO.L			
			KAUR-16-EN-18-OIC ACID $$ KAUR-16-EN-18-OIC ACID, (4.BETA.)- $$ (-)-KAURNENOIC ACID $$ (4-BETA)-KAUR-16-EN-18-OIC ACID	168418	020316-84-1	53
			CIS-4-ETHOXY-B-METHYL-B-NITROSTYRE NE	428132	000000-00-0	46
			cis-4-Ethoxy-b-methyl-b-nitrostyrene	428021	999428-02-8	46

Data Path : F:\DATA MS\daa\
Data File : WLM-10prsen-180c-4jm.D
Acq On : 12 Oct 2019 12:30
Operator :
Sample :
Misc :
ALS Vial : 2 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
49	35.201	0.01	D:\DATABASE\DEMO.L			
			KAUR-16-EN-18-OIC ACID §§ KAUR-16-EN-18-OIC ACID, (4.BETA.)- §§ (-)-KAURNENOIC ACID §§ (4-BETA)-KAUR-16-EN-18-OIC ACID	168418	020316-84-1	50
			[1,2,4]Triazolo[1,5-a]pyrimidine-6-carboxylic acid, 5-ethyl-7-(4-fluorophenyl)-4,7-dihydro-, methyl ester	428797	999428-80-4	46
			PYRIMIDINE, 2-(5-NITRO-3-THIENYL)- §§ 2-(5'-NITRO-3'-THIENYL)PYRIMIDINE	428099	057059-17-3	27
50	35.303	0.02	D:\DATABASE\DEMO.L			
			KAUR-16-EN-18-OIC ACID §§ KAUR-16-EN-18-OIC ACID, (4.BETA.)- §§ (-)-KAURNENOIC ACID §§ (4-BETA)-KAUR-16-EN-18-OIC ACID	168418	020316-84-1	41
			BUTYL 2-(METHYLAMINO)BENZOATE §§ ANTHRANILIC ACID, N-METHYL-, BUTYL ESTER §§ N-BUTYL O-METHYLAMINOBENZOATE	209256	015236-34-7	35
			[1,2,4]Triazolo[1,5-a]pyrimidine-6-carboxylic acid, 5-ethyl-7-(4-fluorophenyl)-4,7-dihydro-, methyl ester	428797	999428-80-4	35
51	35.395	0.03	D:\DATABASE\DEMO.L			
			2-(ACETYLAMINO)PHENYL ACETATE §§ ACETIC ACID 2-ACETYLAMINO-PHENYL ESTER	227934	999227-93-7	47
			p-Heptyloxyaniline §§ 4-n-Heptyloxyaniline	228109	039905-44-7	47
			1,3,4-Thiadiazol-2-amine, 5-[[(4-fluorophenyl)methyl]thio]-	228627	999228-63-0	46
52	35.492	1.11	D:\DATABASE\DEMO.L			
			(+-)-CIS-3,4,6,9-TETRAHYDRO-10-HYDROXY-7-METHOXY-1,3,8-TRIMETHYL-1H-NAPHTHO[2,3-C]PYRAN-6,9-DIONE[(+-)-VENTILAGONE 7-METHYL ETHYL]	504601	124821-09-6	90
			ROSIN ACIDS	504611	000000-00-0	70
			Xanthen-9-one, 1-hydroxy-3,5,8-trimethoxy- §§ 5,8-Dimethylbellidifolin §§ 1-Hydroxy-3,5,8-trimethoxyxanthen-9-one §§ 1-Hydroxy-3,5,8-trimethoxy-9H-xanthen-9-one #	504583	049599-09-9	52
53	35.660	0.12	D:\DATABASE\DEMO.L			
			1-PHENANTHRENECARBOXYLIC ACID, 7-ETHENYL-1,2,3,4,4A,4B,5,6,7,8,10,10A-DODECAHYDRO-1,4A,7-TRIMETHYL-, [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,7.ALPHA.,10A.ALPHA.)]- §§ ISOPIMARIC ACID §§ PODOCARP-7-EN-15-OIC ACID, 13.BETA.-METHYL-13-VINYL-	466436	005835-26-7	52
			3-((1-Amino-2-naphthyl)methylene)-2-benzofuran-1(3H)-one peak 1	504402	999504-41-4	44

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Data Path : F:\DATA MS\daa\
Data File : WLM-10pr4en-180c-4jm.D
Acq On    : 12 Oct 2019  12:30
Operator  :
Sample    :
Misc      :
ALS Vial  : 2   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e

#     RT  Area%          Library/ID                  Ref#     CAS#   Qual
                Androst-5-en-17-ol, 4,4-dimethyl-  513436 999513-44-9 41

4  35.757  0.26 D:\DATABASE\DEMO.L
                DEHYDROABIETIC ACID                464556 000000-00-0 97
                METHYL ABIETA-8,11,13-TRIEN-18-OAT 464549 001235-74-1 90
                E §§ 1-PHENANTHRENECARBOXYLIC ACID
                , 1,2,3,4,4A,9,10,10A-OCTAHYDRO-1,
                4A-DIMETHYL-7-(1-METHYLETHYL)-, ME
                THYL ESTER, [1R-(1.ALPHA.,4A.BETA.
                ,10A.ALPHA.)]- §§ DEHYDROABIETIC A
                CID METHYL ESTER §§ METHYL DEHYDRO
                ABIETATE
                METHYL ABIETA-8,11,13-TRIEN-18-OAT 464548 001235-74-1 81
                E §§ 1-PHENANTHRENECARBOXYLIC ACID
                , 1,2,3,4,4A,9,10,10A-OCTAHYDRO-1,
                4A-DIMETHYL-7-(1-METHYLETHYL)-, ME
                THYL ESTER, [1R-(1.ALPHA.,4A.BETA.
                ,10A.ALPHA.)]- §§ DEHYDROABIETIC A
                CID METHYL ESTER §§ METHYL DEHYDRO
                ABIETATE

5  35.903  0.12 D:\DATABASE\DEMO.L
                BENZ[A]ANTHRACENONE                513655 099707-96-7 72
                PIMARA-8(14),15-DIEN-18-OIC ACID § 504609 000127-27-5 51
                § 1-PHENANTHRENECARBOXYLIC ACID, 7
                -ETHENYL-1,2,3,4,4A,4B,5,6,7,9,10,
                10A-DODECAHYDRO-1,4A,7-TRIMETHYL-,
                 [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,
                7.BETA.,10A.ALPHA.)]- §§ (+)-PINAR
                IC ACID §§ .ALPHA.-PIMARIC ACID
                Pimaric acid §§ 1-Phenanthrenecarb 466434 000127-27-5 49
                oxylic acid, 7-ethenyl-1,2,3,4,4a,
                4b,5,6,7,9,10,10a-dodecahydro-1,4a
                ,7-trimethyl-, [1R-(1.alpha.,4a.be
                ta.,4b.alpha.,7.beta.,10a.alpha.)]
                - §§ Podocarp-8(14)-en-15-oic acid
                , 13.alpha.-methyl-13-vinyl- §§ D-
                pimaric acid

6  35.995  0.05 D:\DATABASE\DEMO.L
                Pimaric acid §§ 1-Phenanthrenecarb 466434 000127-27-5 70
                oxylic acid, 7-ethenyl-1,2,3,4,4a,
                4b,5,6,7,9,10,10a-dodecahydro-1,4a
                ,7-trimethyl-, [1R-(1.alpha.,4a.be
                ta.,4b.alpha.,7.beta.,10a.alpha.)]
                - §§ Podocarp-8(14)-en-15-oic acid
                , 13.alpha.-methyl-13-vinyl- §§ D-
                pimaric acid
                Androst-5-en-17-ol, 4,4-dimethyl-  513436 999513-44-9 50
                ABIETA-7,13-DIEN-18-OIC ACID §§ 1- 168419 000514-10-3 44
                PHENANTHRENECARBOXYLIC ACID, 1,2,3
                ,4,4A,4B,5,6,10,10A-DECAHYDRO- §§
                1-PHENANTHRENECARBOXYLIC ACID, 1,2
                ,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,
                4A-DIMETHYL-7-(1-METHYLETHYL)-, [1
                R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A
                .ALPHA.)]-

7  36.022  0.04 D:\DATABASE\DEMO.L
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Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-180c-4jm.D
Acq On    : 12 Oct 2019  12:30
Operator  :
Sample    :
Misc      :
ALS Vial  : 2   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autointl.e

#     RT  Area%          Library/ID                  Ref#     CAS#   Qual
                Palustric acid §§ Podocarpa-8,13-d 513439 001945-53-5 64
                ien-15-oic acid, 13-isopropyl- §§
                1-Phenanthrenecarboxylic acid, 1,2
                ,3,4,4a,5,6,9,10,10a-decahydro-1,4
                a-dimethyl-7-(1-methylethyl)-, (1R
                -(1.alpha.,4a.beta.,10a.alpha.))-
                §§ 8,13-Abietadien-18-oic acid
                Androst-5-en-17-ol, 4,4-dimethyl-  513436 999513-44-9 49
                1-PHENANTHRENECARBOXYLIC ACID, 7-E 466436 005835-26-7 48
                THENYL-1,2,3,4,4A,4B,5,6,7,8,10,10
                A-DODECAHYDRO-1,4A,7-TRIMETHYL-, [
                1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,7.
                ALPHA.,10A.ALPHA.)]- §§ ISOPIMARIC
                 ACID §§ PODOCARP-7-EN-15-OIC ACID
                , 13.BETA.-METHYL-13-VINYL-

8  36.092  0.13 D:\DATABASE\DEMO.L
                Palustric acid §§ Podocarpa-8,13-d 513439 001945-53-5 47
                ien-15-oic acid, 13-isopropyl- §§
                1-Phenanthrenecarboxylic acid, 1,2
                ,3,4,4a,5,6,9,10,10a-decahydro-1,4
                a-dimethyl-7-(1-methylethyl)-, (1R
                -(1.alpha.,4a.beta.,10a.alpha.))-
                §§ 8,13-Abietadien-18-oic acid
                Pimaric acid §§ 1-Phenanthrenecarb 466434 000127-27-5 45
                oxylic acid, 7-ethenyl-1,2,3,4,4a,
                4b,5,6,7,9,10,10a-dodecahydro-1,4a
                ,7-trimethyl-, [1R-(1.alpha.,4a.be
                ta.,4b.alpha.,7.beta.,10a.alpha.)]
                - §§ Podocarp-8(14)-en-15-oic acid
                , 13.alpha.-methyl-13-vinyl- §§ D-
                pimaric acid
                3-DIETHYLBORYL-2-TRIMETHYLGERMANYL 250295 000000-00-0 38
                -2-PENTENE

9  36.157  0.03 D:\DATABASE\DEMO.L
                1H-NAPHTHO[2,3-C]PYRAN-5,10-DIONE, 513558 084018-43-9 72
                 3,4-DIHYDRO-7,9-DIMETHOXY-1,3-DIM
                ETHYL-, CIS-(.+-.)- §§ (+,-)-CIS-7
                ,9-DIMETHOXY-1,3-DIMETHYL-3,4,5,10
                -TETRAHYDRONAPHTHO[2,3-C]PYRAN-5,1
                0-DIONE
                1-PHENANTHRENECARBOXYLIC ACID, 7-E 466436 005835-26-7 48
                THENYL-1,2,3,4,4A,4B,5,6,7,8,10,10
                A-DODECAHYDRO-1,4A,7-TRIMETHYL-, [
                1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,7.
                ALPHA.,10A.ALPHA.)]- §§ ISOPIMARIC
                 ACID §§ PODOCARP-7-EN-15-OIC ACID
                , 13.BETA.-METHYL-13-VINYL-
                Palustric acid §§ Podocarpa-8,13-d 513439 001945-53-5 47
                ien-15-oic acid, 13-isopropyl- §§
                1-Phenanthrenecarboxylic acid, 1,2
                ,3,4,4a,5,6,9,10,10a-decahydro-1,4
                a-dimethyl-7-(1-methylethyl)-, (1R
                -(1.alpha.,4a.beta.,10a.alpha.))-
                §§ 8,13-Abietadien-18-oic acid

0  36.184  0.04 D:\DATABASE\DEMO.L
                Palustric acid §§ Podocarpa-8,13-d 513439 001945-53-5 53
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Data File : WLM-10prsen-180c-4jm.D
Acq On    : 12 Oct 2019  12:30
Operator  :
Sample    :
Misc      :
ALS Vial  : 2   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e

#     RT  Area%          Library/ID                    Ref#     CAS#   Qual
                ien-15-oic acid, 13-isopropyl- §§
                1-Phenanthrenecarboxylic acid, 1,2
                ,3,4,4a,5,6,9,10,10a-decahydro-1,4
                a-dimethyl-7-(1-methylethyl)-, (1R
                -(1.alpha.,4a.beta.,10a.alpha.))-
                §§ 8,13-Abietadien-18-oic acid
                Androst-5-en-17-ol, 4,4-dimethyl-  513436 999513-44-9 38
                1-PHENANTHRENECARBOXYLIC ACID, 7-E 466436 005835-26-7 38
                THENYL-1,2,3,4,4A,4B,5,6,7,8,10,10
                A-DODECAHYDRO-1,4A,7-TRIMETHYL-, [
                1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,7.
                ALPHA.,10A.ALPHA.)]- §§ ISOPIMARIC
                 ACID §§ PODOCARP-7-EN-15-OIC ACID
                , 13.BETA.-METHYL-13-VINYL-

1  36.384  0.19 D:\DATABASE\DEMO.L
                METHYL ABIETA-7,13-DIEN-18-OATE §§ 258918 000127-25-3 95
                 1-PHENANTHRENECARBOXYLIC ACID, 1,
                2,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1
                ,4A-DIMETHYL-7-(1-METHYLETHYL)-, M
                ETHYL ESTER, [1R-(1.ALPHA.,4A.BETA
                .,4B.ALPHA.,10A.ALPHA.)]- §§ ABALY
                N §§ ABIETIC ACID METHYL ESTER
                Methyl abietate §§ 1-Phenanthrenec 258889 000127-25-3 95
                arboxylic acid, 1,2,3,4,4a,4b,5,6,
                10,10a-decahydro-1,4a-dimethyl-7-(
                1-methylethyl)-, methyl ester, [1R
                -(1.alpha.,4a.beta.,4b.alpha.,10a.
                alpha.)]- §§ Podocarpa-7,13-dien-1
                5-oic acid, 13-isopropyl-, methyl
                ester §§ Abalyn
                METHYL ABIETA-7,13-DIEN-18-OATE §§ 480551 000127-25-3 94
                 1-PHENANTHRENECARBOXYLIC ACID, 1,
                2,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1
                ,4A-DIMETHYL-7-(1-METHYLETHYL)-, M
                ETHYL ESTER, [1R-(1.ALPHA.,4A.BETA
                .,4B.ALPHA.,10A.ALPHA.)]- §§ ABALY
                N §§ ABIETIC ACID METHYL ESTER

2  36.605  0.37 D:\DATABASE\DEMO.L
                KAUR-16-EN-18-OIC ACID §§ KAUR-16- 168418 020316-84-1 87
                EN-18-OIC ACID, (4.BETA.)- §§ (-)-
                KAURNENOIC ACID §§ (4-BETA)-KAUR-1
                6-EN-18-OIC ACID
                Palustric acid §§ Podocarpa-8,13-d 513439 001945-53-5 70
                ien-15-oic acid, 13-isopropyl- §§
                1-Phenanthrenecarboxylic acid, 1,2
                ,3,4,4a,5,6,9,10,10a-decahydro-1,4
                a-dimethyl-7-(1-methylethyl)-, (1R
                -(1.alpha.,4a.beta.,10a.alpha.))-
                §§ 8,13-Abietadien-18-oic acid
                PIMARA-8(14),15-DIEN-18-OIC ACID § 504608 000127-27-5 46
                § 1-PHENANTHRENECARBOXYLIC ACID, 7
                -ETHENYL-1,2,3,4,4A,4B,5,6,7,9,10,
                10A-DODECAHYDRO-1,4A,7-TRIMETHYL-,
                 [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,
                7.BETA.,10A.ALPHA.)]- §§ (+)-PIMAR
                IC ACID §§ .ALPHA.-PIMARIC ACID
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Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-180c-4jm.D
Acq On    : 12 Oct 2019  12:30
Operator  :
Sample    :
Misc      :
ALS Vial  : 2   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autointl.e

#     RT  Area%          Library/ID                  Ref#     CAS#   Qual
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3  36.746  0.33 D:\DATABASE\DEMO.L
                1H-NAPHTHO[2,3-C]PYRAN-5,10-DIONE, 513557 084018-44-0 91
                 3,4-DIHYDRO-7,9-DIMETHOXY-1,3-DIM
                ETHYL-, TRANS-(.+-.)- §§ (+,-)-DEO
                XYQUINONE A DIMETHYL ETHER §§ (+,-
                )-TRANS-7,9-DIMETHOXY-1,3-DIMETHYL
                -3,4,5,10-TETRAHYDRONAPHTHO[2,3-C]
                PYRAN-5,10-DIONE
                Palustric acid §§ Podocarpa-8,13-d 513439 001945-53-5 53
                ien-15-oic acid, 13-isopropyl- §§
                1-Phenanthrenecarboxylic acid, 1,2
                ,3,4,4a,5,6,9,10,10a-decahydro-1,4
                a-dimethyl-7-(1-methylethyl)-, (1R
                -(1.alpha.,4a.beta.,10a.alpha.))-
                §§ 8,13-Abietadien-18-oic acid
                Pimaric acid §§ 1-Phenanthrenecarb 466434 000127-27-5 53
                oxylic acid, 7-ethenyl-1,2,3,4,4a,
                4b,5,6,7,9,10,10a-dodecahydro-1,4a
                ,7-trimethyl-, [1R-(1.alpha.,4a.be
                ta.,4b.alpha.,7.beta.,10a.alpha.)]
                - §§ Podocarp-8(14)-en-15-oic acid
                , 13.alpha.-methyl-13-vinyl- §§ D-
                pimaric acid

4  36.837  0.07 D:\DATABASE\DEMO.L
                1H-NAPHTHO[2,3-C]PYRAN-5,10-DIONE, 513558 084018-43-9 91
                 3,4-DIHYDRO-7,9-DIMETHOXY-1,3-DIM
                ETHYL-, CIS-(.+-.)- §§ (+,-)-CIS-7
                ,9-DIMETHOXY-1,3-DIMETHYL-3,4,5,10
                -TETRAHYDRONAPHTHO[2,3-C]PYRAN-5,1
                0-DIONE
                1H-NAPHTHO[2,3-C]PYRAN-5,10-DIONE, 513557 084018-44-0 91
                 3,4-DIHYDRO-7,9-DIMETHOXY-1,3-DIM
                ETHYL-, TRANS-(.+-.)- §§ (+,-)-DEO
                XYQUINONE A DIMETHYL ETHER §§ (+,-
                )-TRANS-7,9-DIMETHOXY-1,3-DIMETHYL
                -3,4,5,10-TETRAHYDRONAPHTHO[2,3-C]
                PYRAN-5,10-DIONE
                Abietic acid §§ 1-Phenanthrenecarb 513378 000514-10-3 83
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid

5  37.037  1.15 D:\DATABASE\DEMO.L
                ABIETA-7,13-DIEN-18-OIC ACID §§ 1- 168419 000514-10-3 60
                PHENANTHRENECARBOXYLIC ACID, 1,2,3
                ,4,4A,4B,5,6,10,10A-DECAHYDRO- §§
                1-PHENANTHRENECARBOXYLIC ACID, 1,2
                ,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,
                4A-DIMETHYL-7-(1-METHYLETHYL)-, [1
                R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A
                .ALPHA.)]-
                ABIETA-8,11,13-TRIEN-18-OIC ACID § 503106 999503-11-8 56
                § PODOCARPA-8,11,13-TRIEN-15-SAEUR
                E, 13-ISOPROPYL-
                Abietic acid §§ 1-Phenanthrenecarb 513344 000514-10-3 55
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```
Data Path : F:\DATA MS\2019\
Data File : WLM-10pegen-180c-4jm.D
Acq On    : 12 Oct 2019  12:30
Operator  :
Sample    :
Misc      :
ALS Vial  : 2   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#     RT  Area%          Library/ID                    Ref#     CAS#   Qual
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid

 66  37.242  0.63 D:\DATABASE\DEMO.L
                ABIETA-7,13-DIEN-18-OIC ACID §§ 1- 168419 000514-10-3 78
                PHENANTHRENECARBOXYLIC ACID, 1,2,3
                ,4,4A,4B,5,6,10,10A-DECAHYDRO- §§
                1-PHENANTHRENECARBOXYLIC ACID, 1,2
                ,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,
                4A-DIMETHYL-7-(1-METHYLETHYL)-, [1
                R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A
                .ALPHA.)]-
                1H-2,10A-ETHANOPHENANTHRENE, KAUR- 513651 006730-83-2 60
                16-EN-18-OIC ACID DERIV. §§ KAUR-1
                6-EN-18-OIC ACID §§ KAUR-16-EN-18-
                OIC ACID, (4.ALPHA.)- §§ (-)-ENT-K
                AUR-16-EN-19-OIC ACID
                Abietic acid §§ 1-Phenanthrenecarb 513344 000514-10-3 55
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid

 67  37.405  0.21 D:\DATABASE\DEMO.L
                ABIETA-7,13-DIEN-18-OIC ACID §§ 1- 168420 000514-10-3 92
                PHENANTHRENECARBOXYLIC ACID, 1,2,3
                ,4,4A,4B,5,6,10,10A-DECAHYDRO- §§
                1-PHENANTHRENECARBOXYLIC ACID, 1,2
                ,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,
                4A-DIMETHYL-7-(1-METHYLETHYL)-, [1
                R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A
                .ALPHA.)]-
                Abietic acid §§ 1-Phenanthrenecarb 513378 000514-10-3 91
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid
                ABIETA-7,13-DIEN-18-OIC ACID §§ 1- 168419 000514-10-3 83
                PHENANTHRENECARBOXYLIC ACID, 1,2,3
                ,4,4A,4B,5,6,10,10A-DECAHYDRO- §§
                1-PHENANTHRENECARBOXYLIC ACID, 1,2
                ,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,
                4A-DIMETHYL-7-(1-METHYLETHYL)-, [1
                R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A
                .ALPHA.)]-

 68  37.486  0.18 D:\DATABASE\DEMO.L
                1,4-DIHYDRO-9-ISOPROPYLIDENE-5,6,7 513581 000000-00-0 90
                ,8-TETRAMETHOXY-1,4-METHANONAPHTHA
                LENE
                1H-2,10A-ETHANOPHENANTHRENE, KAUR- 513651 006730-83-2 64
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Data Path : F:\DATA MS\daa\
Data File : WLM-10prsan-180c-4jm.D
Acq On    : 12 Oct 2019  12:30
Operator  :
Sample    :
Misc      :
ALS Vial  : 2   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e

c#     RT  Area%          Library/ID                   Ref#     CAS#   Qual
                16-EN-18-OIC ACID DERIV. §§ KAUR-1
                6-EN-18-OIC ACID §§ KAUR-16-EN-18-
                OIC ACID, (4.ALPHA.)- §§ (-)-ENT-K
                AUR-16-EN-19-OIC ACID
                Abietic acid §§ 1-Phenanthrenecarb 513344 000514-10-3 60
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid

59  37.685  2.43 D:\DATABASE\DEMO.L
                Abietic acid §§ 1-Phenanthrenecarb 513378 000514-10-3 99
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid
                Abietic acid §§ 1-Phenanthrenecarb 513347 000514-10-3 93
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid
                Abietic acid §§ 1-Phenanthrenecarb 513344 000514-10-3 90
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid

70  38.490  0.15 D:\DATABASE\DEMO.L
                Abietic acid §§ 1-Phenanthrenecarb 513378 000514-10-3 91
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid
                Abietic acid §§ 1-Phenanthrenecarb 513347 000514-10-3 86
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid
                .beta.-Pimaric acid §§ .delta.6,8( 513374 000079-54-9 83
                14)-Abietadienoic acid §§ l-Pimari
                c acid §§ l-Sapietic acid

71  38.836  0.04 D:\DATABASE\DEMO.L
                Abietic acid §§ 1-Phenanthrenecarb 513378 000514-10-3 90
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
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```
  Data Path : F:\DATA MS\daa\
  Data File : WLM-10prsen-180c-4jm.D
  Acq On    : 12 Oct 2019  12:30
  Operator  :
  Sample    :
  Misc      :
  ALS Vial  : 2   Sample Multiplier: 1

  Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

  Unknown Spectrum:   Apex
  Integration Events: ChemStation Integrator - autoint1.e

Pk#     RT  Area%          Library/ID                    Ref#     CAS#   Qual
                  a.,4b.alpha.,10a.alpha.)]- §§ Podo
                  carpa-7,13-dien-15-oic acid, 13-is
                  opropyl- §§ L-abietic acid
                  Abietic acid §§ 1-Phenanthrenecarb 513344 000514-10-3 84
                  oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                  10a-decahydro-1,4a-dimethyl-7-(1-m
                  ethylethyl)-, [1R-(1.alpha.,4a.bet
                  a.,4b.alpha.,10a.alpha.)]- §§ Podo
                  carpa-7,13-dien-15-oic acid, 13-is
                  opropyl- §§ L-abietic acid
                  Abietic acid §§ 1-Phenanthrenecarb 513347 000514-10-3 55
                  oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                  10a-decahydro-1,4a-dimethyl-7-(1-m
                  ethylethyl)-, [1R-(1.alpha.,4a.bet
                  a.,4b.alpha.,10a.alpha.)]- §§ Podo
                  carpa-7,13-dien-15-oic acid, 13-is
                  opropyl- §§ L-abietic acid

 72  39.004  0.09 D:\DATABASE\DEMO.L
                  ABIETA-7,13-DIEN-18-OIC ACID §§ 1- 168420 000514-10-3 55
                  PHENANTHRENECARBOXYLIC ACID, 1,2,3
                  ,4,4A,4B,5,6,10,10A-DECAHYDRO- §§
                  1-PHENANTHRENECARBOXYLIC ACID, 1,2
                  ,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,
                  4A-DIMETHYL-7-(1-METHYLETHYL)-, [1
                  R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A
                  .ALPHA.)]-
                  ABIETA-7,13-DIEN-18-OIC ACID §§ 1- 168419 000514-10-3 55
                  PHENANTHRENECARBOXYLIC ACID, 1,2,3
                  ,4,4A,4B,5,6,10,10A-DECAHYDRO- §§
                  1-PHENANTHRENECARBOXYLIC ACID, 1,2
                  ,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,
                  4A-DIMETHYL-7-(1-METHYLETHYL)-, [1
                  R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A
                  .ALPHA.)]-
                  6-Hydroxy-7-isopropyl-1,4a-dimethy 513428 022595-48-8 53
                  l-1,2,3,4,4a,9,10,10a-octahydro-1-
                  phenanthrenemethanol, (1.alpha., 4
                  a.beta., 10a.alpha)- §§ Abieta-8,1
                  1,13-triene-12,18-diol #
```

Library Search Report

Data Path : F:\DATA MS\daa\
Data File : WLM-200c-10prsan-1jmu.D
Acq On : 9 Oct 2019 16:21
Operator :
Sample :
Misc :
ALS Vial : 1 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	1.967	0.40	D:\DATABASE\DEMO.L			
			Acetic acid, hydroxy- $$ Glycolic acid $$ .alpha.-Hydroxyacetic acid $$ Glycollic acid	5206	000079-14-1	4
			GLYCOLIC-ACID $$ HYDROXY-ACETIC ACID $$ HYDROXYACETIC ACID	5208	999005-20-9	4
			ACETIC ACID, HYDROXY- $$ 2-HYDROXY ACETIC ACID $$ .ALPHA.-HYDROXYACETIC ACID $$ ACETIC ACID, HYDROXY	5209	000079-14-1	4
2	2.135	0.09	D:\DATABASE\DEMO.L			
			Pentane, 2,4-dimethyl- $$ 2,4-Dimethylpentane	18750	000108-08-7	87
			PENTANE, 2,4-DIMETHYL- $$ 2,4-DIMETHYLPENTANE $$ PENTANE, 2,4-DIMETHYL	18833	000108-08-7	80
			PENTANE, 2,4-DIMETHYL- $$ 2,4-DIMETHYLPENTANE $$ PENTANE, 2,4-DIMETHYL	19002	000108-08-7	80
3	2.205	10.43	D:\DATABASE\DEMO.L			
			Hexane, 3-methyl- $$ 2-Ethylpentane $$ 3-Methylhexane	18811	000589-34-4	72
			Hexane, 3-methyl- $$ 2-Ethylpentane $$ 3-Methylhexane	18754	000589-34-4	68
			Hexane, 3-methyl- $$ 2-Ethylpentane $$ 3-Methylhexane	18743	000589-34-4	68
4	2.243	4.23	D:\DATABASE\DEMO.L			
			Cyclopentane, 1,3-dimethyl- $$ 1,3-Dimethylcyclopentane	101343	002453-00-1	91
			Cyclopentane, 1,3-dimethyl-, cis- $$ cis-1,3-Dimethylcyclopentane $$ 1,3-Dimethylcyclopentane cis $$ 1,3-Dimethylcyclopentane #	62231	002532-58-3	91
			1,3-DIMETHYLCYCLOPENTANE $$ CYCLOPENTANE, 1,3-DIMETHYL-, CIS- $$ 1,3-DIMETHYLCYCLOPENTANE (CIS) $$ 1,3-DIMETHYLCYCLOPENTANE CIS	62286	002532-58-3	91
5	2.335	7.19	D:\DATABASE\DEMO.L			
			CYCLOHEXANE, METHYL- $$ METHYLCYCLOHEXANE $$ 1-METHYLCYCLOHEXANE $$ CYCLOHEXANE, METHYL	141469	000108-87-2	96
			CYCLOHEXANE, METHYL- $$ METHYLCYCLOHEXANE $$ 1-METHYLCYCLOHEXANE $$ CYCLOHEXANE, METHYL	141467	000108-87-2	95
			CYCLOHEXANE, METHYL- $$ METHYLCYCLOHEXANE $$ 1-METHYLCYCLOHEXANE $$ CYCLOHEXANE, METHYL	141470	000108-87-2	95
6	2.421	70.31	D:\DATABASE\DEMO.L			
			BENZENE, METHYL- $$ METHYLBENZENE $$ TOLUENE $$ ANTISAL 1A	158622	000108-88-3	91
			Toluene $$ Benzene, methyl $$ Methylbenzene	158580	000108-88-3	91
			BENZENE, METHYL- $$ METHYLBENZENE $$ TOLUENE $$ ANTISAL 1A	158625	000108-88-3	90

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Data Path : F:\DATA MS\daa\
Data File : WLM-200c-10prsan-1jmu.D
Acq On    :  9 Oct 2019  16:21
Operator  :
Sample    :
Misc      :
ALS Vial  : 1   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e
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Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
7	2.751	1.09	D:\DATABASE\DEMO.L			
			Cyclohexane, ethyl- $$ Ethylcycloh	141508	001678-91-7	93
			exane			
			Cyclohexane, ethyl- $$ Ethylcycloh	141506	001678-91-7	93
			exane			
			CYCLOHEXANE, ETHYL- $$ ETHYLCYCLOH	141561	001678-91-7	93
			EXANE $$ ETHYL CYCLOHEXANE $$ ETHY			
			LCYCLOHEXAN			
8	33.499	0.16	D:\DATABASE\DEMO.L			
			5-HYDROXY-1,3,4-TRIMETHOXY-7-METHY	492890	000000-00-0	90
			L-6-PROPARGYNAPHTHALENE			
			ANDROST-5-ENE, 4,4-DIMETHYL-, (13.	492912	073495-94-0	90
			ALPHA.)- $$ 4,4-DIMETHYL-13.ALPHA.			
			-ANDROST-5-ENE			
			KAURA-5,16-DIEN-18-OL $$ KAURA-5,1	492904	023837-99-2	51
			6-DIEN-18(OR 19)-OL $$ KAURA-5,16-			
			DIEN-19-OL			
9	33.871	0.09	D:\DATABASE\DEMO.L			
			Androst-2,16-diene	466169	999466-17-7	95
			1-Methyl-10,18-bisnorabieta-8,11,1	466158	999466-16-6	94
			3-triene			
			10,13-DIMETHYL-4,5,6,7,8,9,10,11,1	466180	999466-18-8	91
			2,13,14,15-DODECAHYDRO-1H-CYCLOPEN			
			TA[A]PHENANTHRENE $$ ANDROSTA-2,16			
			-DIENE			
10	35.503	1.06	D:\DATABASE\DEMO.L			
			(+-)-CIS-3,4,6,9-TETRAHYDRO-10-HYD	504601	124821-09-6	90
			ROXY-7-METHOXY-1,3,8-TRIMETHYL-1H-			
			NAPHTHO[2,3-C]PYRAN-6,9-DIONE[(+-)			
			-VENTILAGONE 7-METHYL ETHYL]			
			BENZ[A]ANTHRACENONE	513655	099707-96-7	87
			Xanthen-9-one, 1-hydroxy-3,5,8-tri	504583	049599-09-9	55
			methoxy- $$ 5,8-Dimethylbellidifol			
			in $$ 1-Hydroxy-3,5,8-trimethoxyxa			
			nthen-9-one $$ 1-Hydroxy-3,5,8-tri			
			methoxy-9H-xanthen-9-one #			
11	35.665	0.08	D:\DATABASE\DEMO.L			
			O-HYDROGEN PERDEUTERIO HEXADECANOI	504545	039756-30-4	53
			C ACID			
			Phenol, 2,4-bis(1-phenylethyl)- $$	504578	002769-94-0	51
			2,4-Bis(1-phenylethyl)phenol #			
			4-METHYL-2-PHENYL[1]BENZOPYRANO-[3	504527	000000-00-0	44
			,4-C]PYRIDIN-5-ONE			
12	35.757	0.18	D:\DATABASE\DEMO.L			
			DEHYDROABIETIC ACID	464556	000000-00-0	97
			1-Phenanthrenecarboxylic acid, 1,2	464538	001235-74-1	95
			,3,4,4a,9,10,10a-octahydro-1,4a-di			
			methyl-7-(1-methylethyl)-, methyl			
			ester, [1R-(1.alpha.,4a.beta.,10a.			
			alpha.)]- $$ Podocarpa-8,11,13-tri			
			en-15-oic acid, 13-isopropyl-, met			
			hyl ester $$ Methyl dehydroabietat			
			METHYL ABIETA-8,11,13-TRIEN-18-OAT	464550	001235-74-1	95
			E $$ 1-PHENANTHRENECARBOXYLIC ACID			
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Data Path : F:\DATA MS\daa\
Data File : WLM-200c-10pssn-1jmu.D
Acq On : 9 Oct 2019 16:21
Operator :
Sample :
Misc :
ALS Vial : 1 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			, 1,2,3,4,4A,9,10,10A-OCTAHYDRO-1, 4A-DIMETHYL-7-(1-METHYLETHYL)-, ME THYL ESTER, [1R-(1.ALPHA.,4A.BETA. ,10A.ALPHA.)]- §§ DEHYDROABIETIC A CID METHYL ESTER §§ METHYL DEHYDRO ABIETATE			
13	36.389	0.06	D:\DATABASE\DEMO.L			
			METHYL ABIETA-7,13-DIEN-18-OATE §§ 1-PHENANTHRENECARBOXYLIC ACID, 1, 2,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1 ,4A-DIMETHYL-7-(1-METHYLETHYL)-, M ETHYL ESTER, [1R-(1.ALPHA.,4A.BETA .,4B.ALPHA.,10A.ALPHA.)]- §§ ABALY N §§ ABIETIC ACID METHYL ESTER	480551	000127-25-3	93
			METHYL ABIETA-7,13-DIEN-18-OATE §§ 1-PHENANTHRENECARBOXYLIC ACID, 1, 2,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1 ,4A-DIMETHYL-7-(1-METHYLETHYL)-, M ETHYL ESTER, [1R-(1.ALPHA.,4A.BETA .,4B.ALPHA.,10A.ALPHA.)]- §§ ABALY N §§ ABIETIC ACID METHYL ESTER	258918	000127-25-3	92
			Methyl abietate §§ 1-Phenanthrenec arboxylic acid, 1,2,3,4,4a,4b,5,6, 10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, methyl ester, [1R -(1.alpha.,4a.beta.,4b.alpha.,10a. alpha.)]- §§ Podocarpa-7,13-dien-1 5-oic acid, 13-isopropyl-, methyl ester §§ Abalyn	258889	000127-25-3	92
14	36.610	0.15	D:\DATABASE\DEMO.L			
			ROSIN ACIDS	504611	000000-00-0	83
			PHENOL, 5-[2-(3-HYDROXY-4-METHOXYP HENYL)ETHENYL]-2,3-DIMETHOXY-, (Z) - §§ 2,3-DIMETHOXY-5-[2-(3-HYDROXY -4-METHOXYPHENYL)ETHENYL]PHENOL (Z) §§ COMBRETASTATIN A3	513563	111394-45-7	78
			PINE ROSIN MIXTURE	504612	000000-00-0	78
15	36.756	0.25	D:\DATABASE\DEMO.L			
			Pimaric acid §§ 1-Phenanthrenecarb oxylic acid, 7-ethenyl-1,2,3,4,4a, 4b,5,6,7,9,10,10a-dodecahydro-1,4a ,7-trimethyl-, [1R-(1.alpha.,4a.be ta.,4b.alpha.,7.beta.,10a.alpha.)] - §§ Podocarp-8(14)-en-15-oic acid , 13.alpha.-methyl-13-vinyl- §§ D-pimaric acid	466434	000127-27-5	64
			1-PHENANTHRENECARBOXYLIC ACID, 7-E THENYL-1,2,3,4,4A,4B,5,6,7,8,10,10 A-DODECAHYDRO-1,4A,7-TRIMETHYL-, [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,7. ALPHA.,10A.ALPHA.)]- §§ ISOPIMARIC ACID §§ PODOCARP-7-EN-15-OIC ACID , 13.BETA.-METHYL-13-VINYL-	466436	005835-26-7	59
			KAUR-16-EN-18-OIC ACID §§ KAUR-16- EN-18-OIC ACID, (4.BETA.)- §§ (-)- KAURNENOIC ACID §§ (4-BETA)-KAUR-1	168418	020316-84-1	58

```
Data Path : F:\DATA MS\daa\
Data File : WLM-200c-10prsan-1jmu.D
Acq On    :  9 Oct 2019  16:21
Operator  :
Sample    :
Misc      :
ALS Vial  : 1   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autointl.e

k#     RT  Area%          Library/ID                  Ref#     CAS#   Qual
               6-EN-18-OIC ACID

16  37.048  1.10 D:\DATABASE\DEMO.L
                ABIETA-8,11,13-TRIEN-18-OIC ACID § 503106 999503-11-8 72
                § PODOCARPA-8,11,13-TRIEN-15-SAEUR
                E, 13-ISOPROPYL-
                1-PHENANTHRENECARBOXYLIC ACID, 1,2 503110 001740-19-8 70
                ,3,4,4A,9,10,10A-OCTAHYDRO-1,4A-DI
                METHYL-7-(1-METHYLETHYL)-, [1R-(1.
                ALPHA.,4A.BETA.,10A.ALPHA.)]- §§ (
                -)-DEHYDROABIETIC ACID §§ 1,2,3,4,
                4A,9,10,10A-OCTAHYDRO-1,4A-DIMETHY
                L-7-(1-METHYLETHYL)-1-PHENANTHRENE
                CARBOXYLIC ACID
                1-Phenanthrenecarboxylic acid, 1,2 503093 001740-19-8 70
                ,3,4,4a,9,10,10a-octahydro-1,4a-di
                methyl-7-(1-methylethyl)-, [1R-(1.
                alpha.,4a.beta.,10a.alpha.)]- §§ P
                odocarpa-8,11,13-trien-15-oic acid
                , 13-isopropyl- §§ Abieta-8,11,13-
                trien-18-oic acid §§ Abietic acid,
                 dehydro-

17  37.242  0.69 D:\DATABASE\DEMO.L
                Abietic acid §§ 1-Phenanthrenecarb 513344 000514-10-3 46
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid
                ABIETA-7,13-DIEN-18-OIC ACID §§ 1- 168419 000514-10-3 45
                PHENANTHRENECARBOXYLIC ACID, 1,2,3
                ,4,4A,4B,5,6,10,10A-DECAHYDRO- §§
                1-PHENANTHRENECARBOXYLIC ACID, 1,2
                ,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,
                4A-DIMETHYL-7-(1-METHYLETHYL)-, [1
                R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A
                .ALPHA.)]-
                KAURA-9(11),16-DIEN-18-OIC ACID, ( 503118 022338-67-6 42
                4.ALPHA.)- §§ (-)-KAUR-9(11),16-DI
                EN-19-OIC ACID §§ GRANDIFLORENIC A
                CID §§ KAURA-5,16-DIEN-18(OR 19)-O
                IC ACID

18  37.707  2.41 D:\DATABASE\DEMO.L
                Abietic acid §§ 1-Phenanthrenecarb 513378 000514-10-3 99
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid
                Abietic acid §§ 1-Phenanthrenecarb 513347 000514-10-3 94
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
```

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Data Path : F:\DATA MS\daa\
Data File : WLM-200c-10prsen-1jmu.D
Acq On    :  9 Oct 2019  16:21
Operator  :
Sample    :
Misc      :
ALS Vial  : 1   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e

#     RT  Area%          Library/ID                Ref#     CAS#   Qual

               opropyl- $$ L-abietic acid
               Abietic acid $$ 1-Phenanthrenecarb 513344 000514-10-3 93
               oxylic acid, 1,2,3,4,4a,4b,5,6,10,
               10a-decahydro-1,4a-dimethyl-7-(1-m
               ethylethyl)-, [1R-(1.alpha.,4a.bet
               a.,4b.alpha.,10a.alpha.)]- $$ Podo
               carpa-7,13-dien-15-oic acid, 13-is
               opropyl- $$ L-abietic acid
```

```
Data Path : F:\DATA MS\daa\
Data File : WLM-200c-10prsan-2jm.D
Acq On    : 12 Oct 2019  10:27
Operator  :
Sample    :
Misc      :
ALS Vial  : 4   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e

k#     RT  Area%          Library/ID                    Ref#     CAS#   Qual
-------------------------------------------------------------------------------
1   1.962  4.04 D:\DATABASE\DEMO.L
                Methyl Alcohol $$ Methanol $$ Carb   5073 000067-56-1  2
                inol $$ Methyl hydroxide
                METHANOL $$ HYDROXYMETHANE $$ ALCO   5075 000067-56-1  2
                HOL, METHYL $$ ALCOOL METHYLIQUE
                Methyl Alcohol $$ Methanol $$ Carb   5072 000067-56-1  2
                inol $$ Methyl hydroxide

2   2.135  0.12 D:\DATABASE\DEMO.L
                Pentane, 2,4-dimethyl- $$ 2,4-Dime  18753 000108-08-7 91
                thylpentane
                Pentane, 2,4-dimethyl- $$ 2,4-Dime  18799 000108-08-7 90
                thylpentane
                PENTANE, 2,4-DIMETHYL- $$ 2,4-DIME  19001 000108-08-7 90
                THYLPENTANE $$ PENTANE, 2,4-DIMETH
                YL

3   2.200 10.42 D:\DATABASE\DEMO.L
                HEXANE, 3-METHYL- $$ 3-METHYLHEXAN  18994 000589-34-4 64
                E $$ 2-ETHYLPENTANE $$ HEXANE, 3-M
                ETHYL
                HEPTANE $$ ALIPHATIC HYDROCARBON $   18986 000142-82-5 62
                $ DIPROPYL METHANE $$ DIPROPYLMETH
                ANE
                HEXANE, 3-METHYL- $$ 3-METHYLHEXAN  18992 000589-34-4 58
                E $$ 2-ETHYLPENTANE $$ HEXANE, 3-M
                ETHYL

4   2.243  4.11 D:\DATABASE\DEMO.L
                1,3-DIMETHYLCYCLOPENTANE $$ CYCLOP  62286 002532-58-3 91
                ENTANE, 1,3-DIMETHYL-, CIS- $$ 1,3
                -DIMETHYLCYCLOPENTANE (CIS) $$ 1,3
                -DIMETHYLCYCLOPENTANE CIS
                Cyclopentane, 1,3-dimethyl- $$ 1,3 101343 002453-00-1 91
                -Dimethylcyclopentane
                Cyclopentane, 1,3-dimethyl-, cis-   62231 002532-58-3 91
                $$ cis-1,3-Dimethylcyclopentane $$
                 1,3-Dimethylcyclopentane cis $$ 1
                ,3-Dimethylcyclopentane #

5   2.335  6.52 D:\DATABASE\DEMO.L
                CYCLOHEXANE, METHYL- $$ METHYLCYCL 141469 000108-87-2 96
                OHEXANE $$ 1-METHYLCYCLOHEXANE $$
                CYCLOHEXANE, METHYL
                CYCLOHEXANE, METHYL- $$ METHYLCYCL 141470 000108-87-2 95
                OHEXANE $$ 1-METHYLCYCLOHEXANE $$
                CYCLOHEXANE, METHYL
                CYCLOHEXANE, METHYL- $$ METHYLCYCL 141467 000108-87-2 95
                OHEXANE $$ 1-METHYLCYCLOHEXANE $$
                CYCLOHEXANE, METHYL

6   2.421 62.65 D:\DATABASE\DEMO.L
                Toluene $$ Benzene, methyl $$ Meth 158580 000108-88-3 91
                acide $$ Methylbenzene
                Toluene $$ Benzene, methyl $$ Meth 158579 000108-88-3 91
                acide $$ Methylbenzene
                BENZENE, METHYL- $$ METHYLBENZENE  158625 000108-88-3 91
                $$ TOLUENE $$ ANTISAL 1A
```

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Data File : WLM-200c-10pxaa-2jm.D
Acq On    : 12 Oct 2019  10:27
Operator  :
Sample    :
Misc      :
ALS Vial  : 4   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autointl.e

#     RT  Area%          Library/ID                    Ref#     CAS#   Qual

7   2.745  1.20 D:\DATABASE\DEMO.L
               CYCLOHEXANE, ETHYL- §§ ETHYLCYCLOH 141562 001678-91-7 81
               EXANE §§ ETHYL CYCLOHEXANE §§ ETHY
               LCYCLOHEXAN
               CYCLOHEXANE, ETHYL- §§ ETHYLCYCLOH 141528 001678-91-7 81
               EXANE §§ ETHYL CYCLOHEXANE §§ ETHY
               LCYCLOHEXAN
               CYCLOHEXANE, ETHYL- §§ ETHYLCYCLOH 141564 001678-91-7 81
               EXANE §§ ETHYL CYCLOHEXANE §§ ETHY
               LCYCLOHEXAN

8   2.870  0.56 D:\DATABASE\DEMO.L
               BENZENE, METHYL- §§ METHYLBENZENE  158623 000108-88-3 90
               §§ TOLUENE §§ ANTISAL 1A
               1,3,5-CYCLOHEPTATRIENE §§ CYCLOHEP 158637 000544-25-2 90
               TA-1,3,5-TRIENE §§ CYCLOHEPTATRIEN
               E §§ CYCLOHEPTATRIENE [UN2603] [FL
               AMMABLE LIQUID]
               1,3,5-CYCLOHEPTATRIENE §§ CYCLOHEP 158604 000544-25-2 87
               TA-1,3,5-TRIENE §§ CYCLOHEPTATRIEN
               E §§ CYCLOHEPTATRIENE [UN2603] [FL
               AMMABLE LIQUID]

9  17.309  0.03 D:\DATABASE\DEMO.L
               2H-2,4a-Methanonaphthalene, 1,3,4, 350641 001135-66-6 95
               5,6,7-hexahydro-1,1,5,5-tetramethy
               l-, (2S)- §§ 2H-2,4a-Methanonaphth
               alene, 1,3,4,5,6,7-hexahydro-1,1,5
               ,5-tetramethyl-, (2S,4aR)-(-)- §§
               Isolongifolene §§ (-)-Isolongifoli
               ne
               2H-2,4A-METHANONAPHTHALENE, 1,3,4, 350804 001135-66-6 95
               5,6,7-HEXAHYDRO-1,1,5,5-TETRAMETHY
               L-, (2S)- §§ (-)-ISOLONGIFOLENE §§
                (-)-ISOLONGIFOLINE §§ (2S)-1,3,4,
               5,6,7-HEXAHYDRO-1,1,5,5-TETRAMETHY
               L-2H-2,4A-METHANONAPHTHALENE
               2H-2,4A-METHANONAPHTHALENE, 1,3,4, 350805 001135-66-6 95
               5,6,7-HEXAHYDRO-1,1,5,5-TETRAMETHY
               L-, (2S)- §§ (-)-ISOLONGIFOLENE §§
                (-)-ISOLONGIFOLINE §§ (2S)-1,3,4,
               5,6,7-HEXAHYDRO-1,1,5,5-TETRAMETHY
               L-2H-2,4A-METHANONAPHTHALENE

0  17.703  0.01 D:\DATABASE\DEMO.L
               3,6,8-Nonatrienoic acid, 5-methyl-   2929 999002-93-0 10
               , ethyl ester
               3,6,8-NONATRIENOIC ACID, 5-METHYL-   2933 000000-00-0 10
               , ETHYLESTER
               2-(1-Cyano-3-methyl-but-2-enylamin    733 999000-73-3  9
               o)-succinonitrile

1  28.605  0.01 D:\DATABASE\DEMO.L
               4-(METHOXYMETHYL)-6-METHYL-2-PHENO   7413 332057-36-0 10
               XYNICOTINONITRILE §§ PYRIDINE-3-CA
               RBONITRILE, 4-METHOXYMETHYL-6-METH
               YL-2-PHENOXY-
               4-BROMO-N-[(6-METHYL-2-PYRIDYL)AMI   7473 999007-47-4  9
               NOMETHYL]PHTHALIMIDE §§ 5-BROMO-2-
```

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  Data Path : F:\DATA MS\daa\
  Data File : WLM-200c-10prsan-2jm.D
  Acq On    : 12 Oct 2019  10:27
  Operator  :
  Sample    :
  Misc      :
  ALS Vial  : 4   Sample Multiplier: 1

  Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

  Unknown Spectrum:   Apex
  Integration Events: ChemStation Integrator - autoint1.e
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Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			{[(6-METHYL-2-PYRIDINYL)AMINO]METH YL}-1H-ISOINDOLE-1,3(2H)-DIONE			
			3-(3-OXO-3H-BENZO[F]CHROMEN-2-YL)- 2,4(1H,3H)-QUINOLINEDIONE §§ 4-HYD ROXY-3-(2-OXO-2H-1-OXA-3-PHENANTHR YL)-2(1H)-QUINOLINONE	7476	999007-47-7	9
12	30.220	0.02	D:\DATABASE\DEMO.L			
			2-AMINO-4-(4'-METHYLPHENYL)THIAZOL	402705	000000-00-0	30
			1,5-METHANO-8H-PYRIDO[1,2-A][1,5]D IAZOCIN-8-ONE, 1,2,3,4,5,6-HEXAHYD RO-, (1R)- §§ (-)-CYTISINE §§ 1, 5 -METHANO-8H-PYRIDO[1,2-A][1,5]DIAZ OCIN-8-ONE, 1,2,3,4,5, 6-HEXAHYDRO -, (1R)- §§ 1,2,3,4,5,6-HEXAHYDRO-1,5-METHANO-8H-PYRIDO(1,2-A)(1,5)D IAZOCIN-8-ONE	402738	000485-35-8	30
			2-Cyano-6-methoxybenzothiazole §§ 6-Methoxy-1,3-benzothiazole-2-carb onitrile #	402420	000943-03-3	27
13	30.301	0.03	D:\DATABASE\DEMO.L			
			PIMARA-8,15-DIENE §§ PHENANTHRENE, 7-ETHENYL-1,2,3,4,4A,5,6,7,8,9,10 ,10A-DODECAHYDRO-1,1,4A,7-TETRAMET HYL- §§ 7.ALPHA.-ETHENYL-1,1,4A,7. BETA.-TETRAMETHYL-1,2,3,4,4A,5,6,7 ,8,9,10,10A-DODECAHYDROPHENANTHREN	481165	055255-56-6	99
			Phenanthrene, 7-ethenyl-1,2,3,4,4a ,5,6,7,8,9,10,10a-dodecahydro-1,1, 4a,7-tetramethyl- §§ Pimara-8,15-d iene #	481092	055255-56-6	99
			PHENANTHRENE, 7-ETHENYL-1,2,3,4,4A ,5,6,7,8,9,10,10A-DODECAHYDRO-1,1, 4A,7-TETRAMETHYL-, [4AS-(4A.ALPHA. ,7.ALPHA.,10A.BETA.)]- §§ PIMARA-8 (9),15-DIENE §§ PODOCARP-8-ENE, 13 .ALPHA.-METHYL-13-VINYL-	481161	018319-61-4	91
14	30.544	0.04	D:\DATABASE\DEMO.L			
			Naphtho[2,3-b]furan-8(4H)-one, 4a, 5,6,7,8a,9-hexahydro-	402491	999402-49-5	30
			2H-1-BENZOPYRAN-2-ONE, 8-HYDROXY-4 ,7-DIMETHYL- §§ 8-HYDROXY-4,7-DIME THYLCOUMARIN	402726	077869-46-6	30
			7H-Chromen-7-one, 8-hydroxy-2,4-di methyl-	402491	999402-43-5	30
15	30.711	0.01	D:\DATABASE\DEMO.L			
			9-(4-HYDROXYPHENYL)-3,3,6,6-TETRAM ETHYL-3,4,6,7,8A,9-HEXAHYDRO-1,8(2 H,5H)-ACRIDINEDIONE	7482	999007-48-3	25
			4-(METHOXYMETHYL)-6-METHYL-2-PHENO XYNICOTINONITRILE §§ PYRIDINE-3-CA RBONITRILE, 4-METHOXYMETHYL-6-METH YL-2-PHENOXY-	7413	332057-36-0	16
			4-BROMO-N-[(6-METHYL-2-PYRIDYL)AMI NOMETHYL]PHTHALIMIDE §§ 5-BROMO-2- {[(6-METHYL-2-PYRIDINYL)AMINO]METH	7473	999007-47-4	12

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Data Path : F:\DATA MS\daa\
Data File : WLM-200c-10pesan-2jm.D
Acq On    : 12 Oct 2019  10:27
Operator  :
Sample    :
Misc      :
ALS Vial  : 4   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autointl.e

k#     RT  Area%          Library/ID                  Ref#     CAS#   Qual
_____________________________________________________________________________
               YL}-1H-ISOINDOLE-1,3(2H)-DIONE

16  30.873  0.02 D:\DATABASE\DEMO.L
               3-Phenyl-4-azafluorene §§ 2-Phenyl 467987 033777-97-8 72
               -5H-indeno[1,2-b]pyridine #
               5-METHYLBENZO[C]ACRIDINE §§ BENZ[C 468083 003519-87-7 72
               ]ACRIDINE, 5-METHYL- §§ 5-METHYLBE
               NZ(C)ACRIDINE §§ 5-METHYLBENZO(C)A
               CRIDINE
               3-PHENYL-4-AZAFLUORENE             468090 033777-97-8 64

17  31.192  0.03 D:\DATABASE\DEMO.L
               8H-Pyrano[2,3-a]benzothiophen-8-on 467956 999467-96-4 72
               e, 4-formamido-6-methyl-
               9H-Carbazole, 9-phenyl- §§ Carbazo 467916 001150-62-5 72
               le, 9-phenyl- §§ N-Phenylcarbazole
                §§ 9-Phenylcarbazole
               5-METHYLBENZO[C]ACRIDINE §§ BENZ[C 468083 003519-87-7 72
               ]ACRIDINE, 5-METHYL- §§ 5-METHYLBE
               NZ(C)ACRIDINE §§ 5-METHYLBENZO(C)A
               CRIDINE

18  31.262  0.00 D:\DATABASE\DEMO.L
               4-(METHOXYMETHYL)-6-METHYL-2-PHENO   7413 332057-36-0 25
               XYNICOTINONITRILE §§ PYRIDINE-3-CA
               RBONITRILE, 4-METHOXYMETHYL-6-METH
               YL-2-PHENOXY-
               6-ETHYL-2-METHYL-4,6-DIHYDRO-2H-[1   7414 334023-40-4  9
               ,4]OXAZINO[3,2-C]QUINOLINE-3,5-DIO
               NE §§ 6-ETHYL-2-METHYL-2H-1-OXA-4,
               6-PHENANTHROLINE-3,5(4H,6H)-DICNE
               §§ 6-ETHYL-2-METHYL-6,10B-DIHYDRO-
               2H-[1,4]OXAZINO[3,2-C]QUINOLINE-3,
               5-DICNE
               2,2'-(1,4-Piperazinediyl)bis[N-(4-   7524 293766-05-9  9
               methoxyphenyl)succinimide]

19  31.689  0.06 D:\DATABASE\DEMO.L
               3,4-DIHYDRO-7,12-DIMETHYLBENZ[A]AN 482069 000000-00-0 90
               THRACENE
               (+-)-(3S*,4AS*,9AS*)-7-HYDROXY-3,6 482050 000000-00-0 83
               ,8,9,9-PENTAMETHYL-1,2,3,4,4A,9A-H
               EXAHYDROFLURENE
               3(2H)-PYRIDAZINONE, 2-[4-METHOXY-3 481976 120129-92-2 83
               -(1-METHYLETHYL)PHENYL]-6-METHYL-
               §§ 2-(3-ISOPROPYL-4-METHOXYPHENYL)
               -6-METHYLPYRIDAZIN-3(2H)-ONE

20  31.830  0.01 D:\DATABASE\DEMO.L
               4-(METHOXYMETHYL)-6-METHYL-2-PHENO   7413 332057-36-0 22
               XYNICOTINONITRILE §§ PYRIDINE-3-CA
               RBONITRILE, 4-METHOXYMETHYL-6-METH
               YL-2-PHENOXY-
               3-(3-OXO-3H-BENZO[F]CHROMEN-2-YL)-   7476 999007-47-7  9
               2,4(1H,3H)-QUINOLINEDICNE §§ 4-HYD
               ROXY-3-(2-OXO-2H-1-OXA-3-PHENANTHR
               YL)-2(1H)-QUINOLINONE
               2-METHOXY-4-(METHOXYMETHYL)-6-METH   7347 063644-84-8  9
               YLNICOTINONITRILE §§ PYRIDINE-3-CA
```

```
Data Path : F:\DATA MS\daa\
Data File : WLM-200c-10prsan-2jm.D
Acq On    : 12 Oct 2019  10:27
Operator  :
Sample    :
Misc      :
ALS Vial  : 4   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autointl.e

k#     RT  Area%          Library/ID                   Ref#     CAS#   Qual
                RBONITRILE, 2,4-DIMETHOXY-6-METHYL

21  31.981  0.07 D:\DATABASE\DEMO.L
                (+-)-(3S*,4aS*,9aS*)-7-HYDROXY-3,6 482050 000000-00-0 90
                ,8,9,9-PENTAMETHYL-1,2,3,4,4a,9a-H
                EXAHYDROFLURENE
                3(2H)-PYRIDAZINONE, 2-[4-METHOXY-3 481976 120129-92-2 90
                -(1-METHYLETHYL)PHENYL]-6-METHYL-
                §§ 2-(3-ISOPROPYL-4-METHOXYPHENYL)
                -6-METHYLPYRIDAZIN-3(2H)-ONE
                3,4-DIHYDRO-7,12-DIMETHYLBENZ[A]AN 482069 000000-00-0 90
                THRACENE

22  32.100  0.03 D:\DATABASE\DEMO.L
                2-METHYL-1,2-DIHYDRO-2,2'-BIQUINOL 481149 000000-00-0 43
                YL
                3-METHYL-3-PHENYL-3H-NAPHTHO[2,3-B 481155 000000-00-0 43
                ]PYRAN
                Pyrido[3,4-d]pyridazine-4,5(3H,6H) 480936 160033-05-6 35
                -dione, 1-(2-furfuryl)-7-methyl- §
                § 1-(2-Furylmethyl)-7-methylpyrido
                [3,4-d]pyridazine-4,5(3H,6H)-dione
                 #

23  32.337  0.01 D:\DATABASE\DEMO.L
                4-(METHOXYMETHYL)-6-METHYL-2-PHENO   7413 332057-36-0 35
                XYNICOTINONITRILE §§ PYRIDINE-3-CA
                RBONITRILE, 4-METHOXYMETHYL-6-METH
                YL-2-PHENOXY-
                1,3-OXATHIOL-1-IUM, 4-HYDROXY-2-[(   7423 096088-83-4 14
                1-METHYLETHYL)THIO]-5-(TRIFLUOROAC
                ETYL)-, HYDROXIDE, INNER SALT §§ 2
                -ISOPROPYLTHIO-5-TRIFLUORACETYL-1,
                3-OXATHIOLYIUM-4-OLAT
                1-Dodecanamine §§ Dodecylamine §§    4652 000124-22-1  9
                n-Dodecylamine §§ Alamine 4

24  32.386  0.02 D:\DATABASE\DEMO.L
                2,5-Dimethyl-1-(p-anisyl)pyrrole § 419191 005044-27-9 60
                § 1-(4-Methoxyphenyl)-2,5-dimethyl
                -1H-pyrrole #
                1-(4-METHOXYPHENYL)-2,5-DIMETHYL-1 419322 005044-27-9 53
                H-PYRROLE §§ 2,5-DIMETHYL-1-(P-ANI
                SYL)PYRROLE
                (2E)-(1,3,3-TRIMETHYL-1,3-DIHYDRO- 419319 000084-83-3 53
                2H-INDOL-2-YLIDENE)ETHANAL §§ ACET
                ALDEHYDE, (1,3-DIHYDRO-1,3,3-TRIME
                THYL-2H-INDOL-2-YLIDENE)- §§ (1, 3
                ,3-TRIMETHYLINDOLIN-2-YLIDENE)ACET
                ALDEHYDE §§ (1,3,3-TRIMETHYLINDOLI
                N-2-YLIDENE)ACETALDEHYDE

25  32.456  0.01 D:\DATABASE\DEMO.L
                4-(METHOXYMETHYL)-6-METHYL-2-PHENO   7413 332057-36-0 16
                XYNICOTINONITRILE §§ PYRIDINE-3-CA
                RBONITRILE, 4-METHOXYMETHYL-6-METH
                YL-2-PHENOXY-
                2-(3-BUTOXY-2-HYDROXYPROPYL)MALONO   7415 331648-87-4 12
                HYDRAZIDE §§ MALONODIHYDRAZIDE, 2-
```

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Data Path : F:\DATA MS\daa\
Data File : WLM-200c-10prsan-2jm.D
Acq On    : 12 Oct 2019  10:27
Operator  :
Sample    :
Misc      :
ALS Vial  : 4   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autointl.e

c#     RT  Area%          Library/ID                    Ref#     CAS#   Qual
                (3-BUTOXY-2-HYDROXYPROPYL)-
                2-METHOXY-4-(METHOXYMETHYL)-6-METH   7347 063644-84-8 12
                YLNICOTINONITRILE $$ PYRIDINE-3-CA
                RBONITRILE, 2,4-DIMETHOXY-6-METHYL

26  32.591  0.01 D:\DATABASE\DEMO.L
                1-Octadecanamine $$ Octadecylamine   4961 000124-30-1 14
                 $$ n-Octadecylamine $$ n-Stearyla
                mine
                4-(METHOXYMETHYL)-6-METHYL-2-PHENO   7413 332057-36-0 12
                XYNICOTINONITRILE $$ PYRIDINE-3-CA
                RBONITRILE, 4-METHOXYMETHYL-6-METH
                YL-2-PHENOXY-
                1-Hexadecanamine $$ Hexadecylamine   4902 000143-27-1 12
                 $$ n-Cetylamine $$ n-Hexadecylami
                ne

27  32.759  0.01 D:\DATABASE\DEMO.L
                L-Alanine, N-glycyl- $$ Alanine, N   4366 003695-73-6  9
                -glycyl-, L- $$ Glcylalanine $$ Gl
                y-ala
                1,12-DODECANEDIAMINE $$ DODECANE-1   4755 002783-17-7  9
                ,12-DIAMINE $$ 1, 12-DIAMINODODECA
                NE $$ 1, 12-DODECANEDIAMINE
                1-Dodecanamine $$ Dodecylamine $$    4653 000124-22-1  9
                n-Dodecylamine $$ Alamine 4

28  32.980  0.01 D:\DATABASE\DEMO.L
                2-METHOXY-4-(METHOXYMETHYL)-6-METH   7347 063644-84-8 12
                YLNICOTINONITRILE $$ PYRIDINE-3-CA
                RBONITRILE, 2,4-DIMETHOXY-6-METHYL
                1,3-OXATHIOL-1-IUM, 4-HYDROXY-2-[(   7423 096088-83-4 11
                1-METHYLETHYL)THIO]-5-(TRIFLUOROAC
                ETYL)-, HYDROXIDE, INNER SALT $$ 2
                -ISOPROPYLTHIO-5-TRIFLUORACETYL-1,
                3-OXATHIOLYIUM-4-OLAT
                Taurolidine $$ 2H-1,2,4-Thiadiazin   4983 019388-87-5 10
                e, 4,4'-methylenebis[tetrahydro-,
                1,1,1',1'-tetraoxide $$ 4,4'-Methy
                lenebis(tetrahydro-1,2,4-thiadiazi
                ne 1,1-dioxide) $$ Taurolin

29  33.029  0.00 D:\DATABASE\DEMO.L
                4-(METHOXYMETHYL)-6-METHYL-2-PHENO   7413 332057-36-0 22
                XYNICOTINONITRILE $$ PYRIDINE-3-CA
                RBONITRILE, 4-METHOXYMETHYL-6-METH
                YL-2-PHENOXY-
                1-Hexadecanamine $$ Hexadecylamine   4902 000143-27-1 16
                 $$ n-Cetylamine $$ n-Hexadecylami
                ne
                1-OCTADECANAMINE $$ OCTADECAN-1-AM   4965 000124-30-1 14
                INE $$ 1-AMINOOCTADECANE $$ 1-OCTA
                DECANAMIN

30  33.142  0.01 D:\DATABASE\DEMO.L
                3-METHOXY-17-METHYLMORPHINAN-14-OL  45788 001639-74-3 45
                 $$ MORPHINAN-14-OL, 3-METHOXY-17-
                METHYL- $$ (-)-14-HYDROXY-3-METHOX
                Y-17-METHYLMORPHINAN
```

Data Path : F:\DATA MS\daa\
Data File : WLM-200c-10prsan-2jm.D
Acq On : 12 Oct 2019 10:27
Operator :
Sample :
Misc :
ALS Vial : 4 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			Morphinan-14-ol, 3-methoxy-17-meth yl- §§ (-)-14-Hydroxy-3-methoxy-17 -methylmorphinan §§ 3-Methoxy-17-m ethylmorphinan-14-ol #	45783	001639-74-3	45
			(1'S,3R)-N-(1-CYCLOHEXYLETHYL)-3-H YDROXY-3-PHENYLPROPIONAMID	45648	100929-25-7	17
31	33.326	0.01	D:\DATABASE\DEMO.L			
			Tridecylamine §§ n-Tridecylamine § § 1-Aminotridecane §§ 1-Tridecanam ine	4737	002869-34-3	14
			1-Tetradecanamine §§ Tetradecylami ne §§ Armeen 14 §§ Myristylamine	4817	002016-42-4	14
			1-Hexadecanamine §§ Hexadecylamine §§ n-Cetylamine §§ n-Hexadecylami ne	4902	000143-27-1	10
32	33.369	0.01	D:\DATABASE\DEMO.L			
			2-METHOXY-4-(METHOXYMETHYL)-6-METH YLNICOTINONITRILE §§ PYRIDINE-3-CA RBONITRILE, 2,4-DIMETHOXY-6-METHYL	7347	063644-84-8	27
			1-Tetradecanamine §§ Tetradecylami ne §§ Armeen 14 §§ Myristylamine	4817	002016-42-4	11
			1-Hexadecanamine §§ Hexadecylamine §§ n-Cetylamine §§ n-Hexadecylami ne	4902	000143-27-1	10
33	33.493	0.13	D:\DATABASE\DEMO.L			
			KAURA-5,16-DIEN-18-OL §§ KAURA-5,1 6-DIEN-18(OR 19)-OL §§ KAURA-5,16- DIEN-19-OL	492904	023837-99-2	83
			Kaura-5,16-dien-18(or 19)-ol §§ Ka ura-5,16-dien-18-ol #	492860	023837-99-2	80
			4-METHYL-4'-ACETYL-P-TERPHENYL	503749	999503-76-1	50
34	33.682	0.02	D:\DATABASE\DEMO.L			
			2-METHOXY-4-(METHOXYMETHYL)-6-METH YLNICOTINONITRILE §§ PYRIDINE-3-CA RBONITRILE, 2,4-DIMETHOXY-6-METHYL	7347	063644-84-8	14
			2-(3-Methyl-1,5-dinitro-3-aza-bicy clo[3.3.1]non-6-en-6-yloxy)-ethano	45784	999045-78-6	12
			Morphinan-14-ol, 3-methoxy-17-meth yl- §§ (-)-14-Hydroxy-3-methoxy-17 -methylmorphinan §§ 3-Methoxy-17-m ethylmorphinan-14-ol #	45783	001639-74-3	11
35	33.785	0.03	D:\DATABASE\DEMO.L			
			7-BENZYLOXY-2,4-DIHYDROXY-2H-[1,4] BENZOXAZIN-3(4H)-ONE	167385	000000-00-0	43
			Naphthalene, 6-ethyl-1,2,3,4-tetra hydro-1,1,4,4-tetramethyl-7-(1-met hylethenyl)- §§ 6-Ethyl-7-isopropa nyl-1,1,4,4-tetramethyl-1,2,3,4-te trahydronaphthalene #	466156	301643-35-6	35
			4-ISOPROPYL-1,1,6,6-TETRAMETHYL-1, 2,3,6,7,8-HEXAHYDRO-AS-INDACENE §§ AS-INDACENE, 1,2,3,6,7,8-HEXAHYDR O-1,1,6,6-TETRAMETHYL-4-(1-METHYLE THYL)- §§ 1,1,6,6-TETRAMETHYL-4-IS	466223	017465-47-3	35

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Data Path : F:\DATA MS\daa\
Data File : WLM-200c-10prsan-2jm.D
Acq On    : 12 Oct 2019  10:27
Operator  :
Sample    :
Misc      :
ALS Vial  : 4   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autointl.e

Pk#     RT  Area%          Library/ID                   Ref#     CAS#   Qual
                OPROPYL-1,2,3,6,7,8-HEXAHYDRO-A8-I
                NDACENE

36  33.855  0.10 D:\DATABASE\DEMO.L
                1-Methyl-10,18-bisnorabieta-8,11,1 466158 999466-16-6 94
                3-triene
                10,13-DIMETHYL-4,5,6,7,8,9,10,11,1 466180 999466-18-8 93
                2,13,14,15-DODECAHYDRO-1H-CYCLOPEN
                TA[A]PHENANTHRENE $$ ANDROSTA-2,16
                -DIENE
                3,3,4,5,5,8-HEXAMETHYL-3,5,6,7-TET 466221 038754-94-8 72
                RAHYDRO-8-INDACEN-1(2H)-ONE $$ 8-I
                NDACEN-1(2H)-ONE, 3,5,6,7-TETRAHYD
                RO-3,3,4,5,5,8-HEXAMETHYL- $$ 3,3,
                4,5,5,8-HEXAMETHYL-1-8-HYDRINDACEN
                ONE

37  34.125  0.01 D:\DATABASE\DEMO.L
                No matches found

38  34.185  0.00 D:\DATABASE\DEMO.L
                1-Hexadecanamine $$ Hexadecylamine   4902 000143-27-1 10
                 $$ n-Cetylamine $$ n-Hexadecylami
                ne
                4-(METHOXYMETHYL)-6-METHYL-2-PHENO   7413 332057-36-0 10
                XYNICOTINONITRILE $$ PYRIDINE-3-CA
                RBONITRILE, 4-METHOXYMETHYL-6-METH
                YL-2-PHENOXY-
                1-Tetradecanamine $$ Tetradecylami   4817 002016-42-4 10
                ne $$ Armeen 14 $$ Myristylamine

39  34.212  0.00 D:\DATABASE\DEMO.L
                2-((E)-[((E)-2-([(E)-(2-HYDROXYPHE  45719 000094-91-7 22
                NYL)METHYLIDENE]AMINO)PROPYL)IMINO
                ]METHYL)PHENOL $$ .ALPHA.,.ALPHA.'
                -(1-METHYLETHYLENEDIIMINO)DI-ORTHO
                -CRESOL $$ .ALPHA.,.ALPHA.'-DIPROP
                YLENEDINITRILODI-O-CRESOL $$ ALPHA
                ,ALPHA'-(1-METHYLETHYLENEDIIMINO)D
                I-ORTHO-CRESOL
                Sarcosine, N-(3-cyclopentylpropion  45577 999045-57-9  1
                yl)-, isobutyl ester

40  34.304  0.05 D:\DATABASE\DEMO.L
                METHYL PIMARA-8,15-DIEN-18-OATE $$ 466513 003582-26-1 53
                 1-PHENANTHRENECARBOXYLIC ACID, 7-
                ETHENYL-1,2,3,4,4A,5,6,7,8,9,10,10
                A-DODECAHYDRO-1,4A,7-TRIMETHYL-, M
                ETHYL ESTER, [1R-(1.ALPHA.,4A.BETA
                .,7.BETA.,10A.ALPHA.)]- $$ METHYL
                8,15-PIMARADIEN-18-OATE
                METHYL PIMARA-7,15-DIEN-18-OATE $$ 466517 001686-62-0 49
                 1-PHENANTHRENECARBOXYLIC ACID, 7-
                ETHENYL-1,2,3,4,4A,4B,5,6,7,8,10,1
                0A-DODECAHYDRO-1,4A,7-TRIMETHYL-,
                METHYL ESTER, [1R-(1.ALPHA.,4A.BET
                A.,4B.ALPHA.,7.ALPHA.,10A.ALPHA.)]
                - $$ ISOPIMARATE $$ ISOPIMARIC ACI
                D, METHYL ESTER
```

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Data Path : F:\DATA MS\daa\
Data File : WLM-200c-10prsan-2jm.D
Acq On    : 12 Oct 2019  10:27
Operator  :
Sample    :
Misc      :
ALS Vial  : 4   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e

k#     RT  Area%          Library/ID                   Ref#     CAS#    Qual
                1-Phenanthrenecarboxylic acid, 7-e 466506 019907-21-2 25
                thenyl-1,2,3,4,4a,5,6,7,8,9,10,10a
                -dodecahydro-1,4a,7-trimethyl-, me
                thyl ester, [1R-(1.alpha.,4a.beta.
                ,7.alpha.,10a.alpha.)]- §§ Podocar
                p-8-en-15-oic acid, 13.beta.-methy
                l-13-vinyl-, methyl ester

41  34.406  0.00 D:\DATABASE\DEMO.L
                1-Hexadecanamine §§ Hexadecylamine   4902 000143-27-1 11
                 §§ n-Cetylamine §§ n-Hexadecylami
                ne
                GLYCINE, N-[[(4-METHOXYPHENYL)METH   7411 108536-10-3 10
                OXY]CARBONYL]-N-METHYL- §§ PNZ-SAR
                2,2'-(1,4-Piperazinediyl)bis[N-(4-   7524 293766-05-9 10
                methoxyphenyl)succinimide]

42  34.541  0.05 D:\DATABASE\DEMO.L
                1,2,4-TRIAZOLO(3,4-C)(1,2,4)-BENZO 282352 000000-00-0 53
                TRIAZIN-1(5H)-ONE
                1-Phenanthrenecarboxaldehyde, 7-et 481182 000472-39-9 53
                henyl-1,2,3,4,4a,4b,5,6,7,9,10,10a
                -dodecahydro-1,4a,7-trimethyl-, [1
                R-(1.alpha.,4a.beta.,4b.alpha.,7.b
                eta.,10a.alpha.)]- §§ Podocarp-8(1
                4)-en-15-al, 13.alpha.-methyl-13-v
                inyl- §§ Cryptopinon §§ Cryptopino
                ne
                PIMARA-8(14),15-DIEN-18-AL §§ 1-PH 481208 000472-39-9 53
                ENANTHRENECARBOXALDEHYDE, 7-ETHENY
                L-1,2,3,4,4A,4B,5,6,7,9,10,10A-DOD
                ECAHYDRO-1,4A,7-TRIMETHYL-, [1R-(1
                .ALPHA.,4A.BETA.,4B.ALPHA.,7.BETA.
                ,10A.ALPHA.)]- §§ CRYPTOPINON §§ C
                RYPTOPINONE

43  34.671  0.00 D:\DATABASE\DEMO.L
                No matches found

44  34.730  0.02 D:\DATABASE\DEMO.L
                N-ISOPROPYL-2,2-DIMETHOXY-3,3-DIME   7369 000000-00-0 10
                THYL-1-BUTYLAMINE
                3-TRIDEUTEROMETHOXY-4-METHYL-2(5H)   2514 000000-00-0  9
                -FURANONE
                3,5,7,8-TETRACHLOROUNDECAFLUORO-OC   3535 000000-00-0  4
                TANOIC ACID

45  34.822  0.00 D:\DATABASE\DEMO.L
                2-((E)-[((E)-2-([(E)-(2-HYDROXYPHE  45719 000094-91-7 64
                NYL)METHYLIDENE]AMINO)PROPYL)IMINO
                ]METHYL)PHENOL §§ .ALPHA.,.ALPHA.'
                -(1-METHYLETHYLENEDIIMINO)DI-ORTHO
                -CRESOL §§ .ALPHA.,.ALPHA.'-DIPROP
                YLENEDINITRILODI-O-CRESOL §§ ALPHA
                ,ALPHA'-(1-METHYLETHYLENEDIIMINO)D
                I-ORTHO-CRESOL
                2-PYRIDINEPROPANOIC ACID, .ALPHA.-   5863 999005-86-4  9
                METHYL-.BETA.-OXO-, ETHYL ESTER §§
                 ETHYL 2-METHYL-3-OXO-3-(2-PYRIDIN
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```
Data Path : F:\DATA MS\daa\
Data File : WLM-200c-10prsan-2jm.D
Acq On    : 12 Oct 2019  10:27
Operator  :
Sample    :
Misc      :
ALS Vial  : 4   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autointl.e

Pk#     RT  Area%          Library/ID                    Ref#     CAS#   Qual
                YL)PROPANOATE
                2H-3,9A-METHANO-1-BENZOXEPIN, OCTA   3110 005956-09-2  8
                HYDRO-2,2,5A,9-TETRAMETHYL-, [3R-(
                3.ALPHA.,5A.ALPHA.,9.ALPHA.,9A.ALP
                HA.)]- §§ .BETA.-AGAROFURAN, DIHYD
                RO- §§ .BETA.-DIHYDROAGAROFURAN §§
                 2H-3,9A-METHANO-1-BENZOXEPIN, OCT
                AHYDRO-2,2,5A,9-TETRAMETHYL-

46  34.936  0.03 D:\DATABASE\DEMO.L
                (2E)-N-OCTYL-3-PHENYL-2-PROPENAMID 283089 055030-48-3 40
                E §§ 2-PROPENAMIDE, N-OCTYL-3-PHEN
                YL- §§ N-N-OCTYL-3-PHENYLPROPENAMI
                DE
                2-Propenamide, N-octyl-3-phenyl- § 283082 055030-48-3 40
                § (2E)-n-Octyl-3-phenyl-2-propenam
                ide #
                1,2,4-TRIAZOLO(3,4-C)(1,2,4)-BENZO 282352 000000-00-0 35
                TRIAZIN-1(5H)-ONE

47  35.022  0.03 D:\DATABASE\DEMO.L
                4,5-Bis-dimethoxymethyl-octanedioi 124248 999124-25-1 50
                c acid, dimethyl ester
                1-Dimethyl(prop-2-enyl)silyloxy-10 123536 999123-53-9 47
                -undecene
                METHYL (2E)-3,7-DIMETHYL-2,6-OCTAD 122646 002349-14-6 47
                IENOATE §§ 2,6-OCTADIENOIC ACID, 3
                ,7-DIMETHYL-, METHYL ESTER §§ METH
                YL 3,7-DIMETHYL-2,6-OCTADIENOATE §
                § METHYL ESTER OF 3,7-DIMETHYL-2,6
                -OCTADIENEOIC ACID

48  35.119  0.02 D:\DATABASE\DEMO.L
                KAUR-16-EN-18-OIC ACID §§ KAUR-16- 168418 020316-84-1 35
                EN-18-OIC ACID, (4.BETA.)- §§ (-)-
                KAURNENOIC ACID §§ (4-BETA)-KAUR-1
                6-EN-18-OIC ACID
                Benzoic acid, 2-(methylamino)-, 2- 209232 065505-24-0 25
                methylpropyl ester §§ iso-Butyl N-
                methyl anthranilate §§ Isobutyl 2-
                (methylamino)benzoate #
                2-METHYLPROPYL N-METHYLANTHRANILAT 209257 000000-00-0 25

49  35.141  0.01 D:\DATABASE\DEMO.L
                KAUR-16-EN-18-OIC ACID §§ KAUR-16- 168418 020316-84-1 49
                EN-18-OIC ACID, (4.BETA.)- §§ (-)-
                KAURNENOIC ACID §§ (4-BETA)-KAUR-1
                6-EN-18-OIC ACID
                2-((E)-[((E)-2-([(E)-(2-HYDROXYPHE  45719 000094-91-7 43
                NYL)METHYLIDENE]AMINO)PROPYL)IMINO
                ]METHYL)PHENOL §§ .ALPHA.,.ALPHA.'
                -(1-METHYLETHYLENEDIIMINO)DI-ORTHO
                -CRESOL §§ .ALPHA.,.ALPHA.'-DIPROP
                YLENEDINITRILODI-O-CRESOL §§ ALPHA
                ,ALPHA'-(1-METHYLETHYLENEDIIMINO)D
                I-ORTHO-CRESOL
                Benzonitrile, m-phenethyl- §§ 3-(2 162409 034176-91-5 10
                -Phenylethyl)benzonitrile #
```

Data Path : F:\DATA MS\daa\
Data File : WLM-200c-10prsan-2jm.D
Acq On : 12 Oct 2019 10:27
Operator :
Sample :
Misc :
ALS Vial : 4 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

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50	35.173	0.03	D:\DATABASE\DEMO.L			
			KAUR-16-EN-18-OIC ACID §§ KAUR-16-EN-18-OIC ACID, (4.BETA.)- §§ (-)-KAURNENOIC ACID §§ (4-BETA)-KAUR-16-EN-18-OIC ACID	168418	020316-84-1	38
			Acetamide, N-(2,6-dimethylphenyl)-2-[5-(4-methoxyphenyl)tetrazol-2-yl]-	287822	999287-82-5	10
			Benzonitrile, m-phenethyl- §§ 3-(2-Phenylethyl)benzonitrile #	162409	034176-91-5	10
51	35.308	0.03	D:\DATABASE\DEMO.L			
			KAUR-16-EN-18-OIC ACID §§ KAUR-16-EN-18-OIC ACID, (4.BETA.)- §§ (-)-KAURNENOIC ACID §§ (4-BETA)-KAUR-16-EN-18-OIC ACID	168418	020316-84-1	62
			2,4B-DIMETHYL-8-METHYLENE-2-VINYL-1,2,3,4,4A,4B,5,6,7,8,8A,9-DODECAHYDROPHENANTHRENE §§ PHENANTHRENE, 7-ETHENYL-1,2,3,4,4A,4B,5,6,7,8,10,10A-DODECAHYDRO-4A,7-DIMETHYL-1-METHYLENE-, [4AS-(4A.ALPHA.,4B.BETA.,7.BETA.,10A.BETA.)]-	165412	026549-04-2	25
			2-METHYLPROPYL N-METHYLANTHRANILAT	209257	000000-00-0	25
52	35.389	0.04	D:\DATABASE\DEMO.L			
			2-(ACETYLAMINO)PHENYL ACETATE §§ ACETIC ACID 2-ACETYLAMINO-PHENYL ESTER	227934	999227-93-7	43
			6,6-Dimethylhepta-2,4-diene	226916	999226-91-9	41
			PHOSPHORIC ACID, 4-HYDROXY-3-(TRIMETHYLSILYL)PHENYL DIMETHYL ESTER §§ DIMETHYL-4-HYDROXY-3-TRIMETHYLSILYLPHENYL PHOSPHATE	229092	094420-62-9	38
53	35.492	1.32	D:\DATABASE\DEMO.L			
			Phenol, 2,4-bis(1-phenylethyl)- §§ 2,4-Bis(1-phenylethyl)phenol #	504578	002769-94-0	60
			1-[1-(4-METHYLTHIO)HEXYLIDENE]-4-PHENYLCYCLOHEXANE	504561	113035-73-7	58
			Xanthen-9-one, 1-hydroxy-3,5,8-trimethoxy- §§ 5,8-Dimethylbellidifolin §§ 1-Hydroxy-3,5,8-trimethoxyxanthen-9-one §§ 1-Hydroxy-3,5,8-trimethoxy-9H-xanthen-9-one #	504583	049599-09-9	48
54	35.665	0.14	D:\DATABASE\DEMO.L			
			Xanthen-9-one, 1-hydroxy-3,5,8-trimethoxy- §§ 5,8-Dimethylbellidifolin §§ 1-Hydroxy-3,5,8-trimethoxyxanthen-9-one §§ 1-Hydroxy-3,5,8-trimethoxy-9H-xanthen-9-one #	504583	049599-09-9	47
			Phenol, 2,4-bis(1-phenylethyl)- §§ 2,4-Bis(1-phenylethyl)phenol #	504578	002769-94-0	47
			4,5-Dihydrobenzo[d]isoxazole, 3-methyl-4,6-diphenyl-	504377	999504-38-9	45
55	35.757	0.30	D:\DATABASE\DEMO.L			
			DEHYDROABIETIC ACID	464556	000000-00-0	97

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  Data File : WLM-200c-10prsan-2jm.D
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  Operator  :
  Sample    :
  Misc      :
  ALS Vial  : 4   Sample Multiplier: 1

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  Unknown Spectrum:   Apex
  Integration Events: ChemStation Integrator - autoint1.e

Pk#     RT  Area%          Library/ID                    Ref#     CAS#    Qual
                1-Phenanthrenecarboxylic acid, 1,2 464536 001235-74-1 93
                ,3,4,4a,9,10,10a-octahydro-1,4a-di
                methyl-7-(1-methylethyl)-, methyl
                ester, [1R-(1.alpha.,4a.beta.,10a.
                alpha.)]- §§ Podocarpa-8,11,13-tri
                en-15-oic acid, 13-isopropyl-, met
                hyl ester §§ Methyl dehydroabietat
                METHYL ABIETA-8,11,13-TRIEN-18-OAT 464549 001235-74-1 89
                E §§ 1-PHENANTHRENECARBOXYLIC ACID
                , 1,2,3,4,4A,9,10,10A-OCTAHYDRO-1,
                4A-DIMETHYL-7-(1-METHYLETHYL)-, ME
                THYL ESTER, [1R-(1.ALPHA.,4A.BETA.
                ,10A.ALPHA.)]- §§ DEHYDROABIETIC A
                CID METHYL ESTER §§ METHYL DEHYDRO
                ABIETATE

 56  35.897  0.18 D:\DATABASE\DEMO.L
                Androst-5-en-17-ol, 4,4-dimethyl-  513436 999513-44-9 46
                2-ACETYL-4,9-DIMETHOXY-7-METHYL-5H 513538 092611-83-1 45
                -FURO[3,2-G][1]-BENZOPYRAN-5-ONE
                1-PHENANTHRENECARBOXYLIC ACID, 7-E 466436 005835-26-7 44
                THENYL-1,2,3,4,4A,4B,5,6,7,8,10,10
                A-DODECAHYDRO-1,4A,7-TRIMETHYL-, [
                1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,7.
                ALPHA.,10A.ALPHA.)]- §§ ISOPIMARIC
                 ACID §§ PODOCARP-7-EN-15-OIC ACID
                , 13.BETA.-METHYL-13-VINYL-

 57  35.994  0.04 D:\DATABASE\DEMO.L
                1,4-DIHYDRO-9-ISOPROPYLIDENE-5,6,7 513581 000000-00-0 90
                ,8-TETRAMETHOXY-1,4-METHANONAPHTHA
                LENE
                PHENOL, 5-[2-(3-HYDROXY-4-METHOXYP 513563 111394-45-7 72
                HENYL)ETHENYL]-2,3-DIMETHOXY-, (Z)
                - §§ 2,3-DIMETHOXY-5-[2-(3-HYDROXY
                -4-METHOXYPHENYL)ETHENYL]PHENOL (Z
                ) §§ COMBRETASTATIN A3
                Abietic acid §§ 1-Phenanthrenecarb 513378 000514-10-3 50
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid

 58  36.011  0.03 D:\DATABASE\DEMO.L
                1-Hydroxy-3,7,8-trimethoxyxanthen- 504580 020882-69-3 42
                9-one §§ 8-Hydroxy-1,2,6-trimethox
                y-9H-xanthen-9-one #
                3"N-BUTYL[3]STAFFANE-3-CARBOXYLIC  168299 000000-00-0 38
                ACID
                KAUR-16-EN-18-OIC ACID §§ KAUR-16- 168418 020316-84-1 38
                EN-18-OIC ACID, (4.BETA.)- §§ (-)-
                KAURNENOIC ACID §§ (4-BETA)-KAUR-1
                6-EN-18-OIC ACID

 59  36.092  0.20 D:\DATABASE\DEMO.L
                Androst-5-en-17-ol, 4,4-dimethyl-  513436 999513-44-9 55
                1-PHENANTHRENECARBOXYLIC ACID, 7-E 466436 005835-26-7 51
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Data Path : F:\DATA MS\daa\
Data File : WLM-200c-10prsan-2jm.D
Acq On : 12 Oct 2019 10:27
Operator :
Sample :
Misc :
ALS Vial : 4 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autointl.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			THENYL-1,2,3,4,4A,4B,5,6,7,8,10,10A-DODECAHYDRO-1,4A,7-TRIMETHYL-, [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,7.ALPHA.,10A.ALPHA.)]- §§ ISOPIMARIC ACID §§ PODOCARP-7-EN-15-OIC ACID, 13.BETA.-METHYL-13-VINYL-			
			Palustric acid §§ Podocarpa-8,13-dien-15-oic acid, 13-isopropyl- §§ 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,5,6,9,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, (1R-(1.alpha.,4a.beta.,10a.alpha.))- §§ 8,13-Abietadien-18-oic acid	513439	001945-53-5	44
60	36.184	0.04	D:\DATABASE\DEMO.L			
			Pimaric acid §§ 1-Phenanthrenecarboxylic acid, 7-ethenyl-1,2,3,4,4a,4b,5,6,7,9,10,10a-dodecahydro-1,4a,7-trimethyl-, [1R-(1.alpha.,4a.beta.,4b.alpha.,7.beta.,10a.alpha.)]- §§ Podocarp-8(14)-en-15-oic acid, 13.alpha.-methyl-13-vinyl- §§ D-pimaric acid	466434	000127-27-5	55
			Palustric acid §§ Podocarpa-8,13-dien-15-oic acid, 13-isopropyl- §§ 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,5,6,9,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, (1R-(1.alpha.,4a.beta.,10a.alpha.))- §§ 8,13-Abietadien-18-oic acid	513439	001945-53-5	47
			2-Pentene, 3-diethylboxyl-2-trimethylgermyl-	250283	999250-28-6	38
61	36.238	0.06	D:\DATABASE\DEMO.L			
			1H-NAPHTHO[2,3-C]PYRAN-5,10-DIONE, 3,4-DIHYDRO-7,9-DIMETHOXY-1,3-DIMETHYL-, CIS-(.+-.)- §§ (+,-)-CIS-7,9-DIMETHOXY-1,3-DIMETHYL-3,4,5,10-TETRAHYDRONAPHTHO[2,3-C]PYRAN-5,10-DIONE	513558	084018-43-9	90
			KAUR-16-EN-18-OIC ACID §§ KAUR-16-EN-18-OIC ACID, (4.BETA.)- §§ (-)-KAURNENOIC ACID §§ (4-BETA)-KAUR-16-EN-18-OIC ACID	168418	020316-84-1	53
			2-ACETYL-4,9-DIMETHOXY-7-METHYL-5H-FURO[3,2-G][1]-BENZOPYRAN-5-ONE	513538	092611-83-1	50
62	36.383	0.20	D:\DATABASE\DEMO.L			
			METHYL ABIETA-7,13-DIEN-18-OATE §§ 1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL)-, METHYL ESTER, [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A.ALPHA.)]- §§ ABALYN §§ ABIETIC ACID METHYL ESTER	258918	000127-25-3	95
			Methyl abietate §§ 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,4b,5,6,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, methyl ester, [1R	258889	000127-25-3	95

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Data File : WLM-200c-10prsan-2jm.D
Acq On    : 12 Oct 2019  10:27
Operator  :
Sample    :
Misc      :
ALS Vial  : 4   Sample Multiplier: 1

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Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e

Peak#     RT  Area%          Library/ID                  Ref#     CAS#   Qual
                -(1.alpha.,4a.beta.,4b.alpha.,10a.
                alpha.)]- §§ Podocarpa-7,13-dien-1
                5-oic acid, 13-isopropyl-, methyl
                ester §§ Abalyn
                METHYL ABIETA-7,13-DIEN-18-OATE §§ 480550 000127-25-3 90
                 1-PHENANTHRENECARBOXYLIC ACID, 1,
                2,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1
                ,4A-DIMETHYL-7-(1-METHYLETHYL)-, M
                ETHYL ESTER, [1R-(1.ALPHA.,4A.BETA
                .,4B.ALPHA.,10A.ALPHA.)]- §§ ABALY
                N §§ ABIETIC ACID METHYL ESTER

53   36.502  0.12 D:\DATABASE\DEMO.L
                Palustric acid §§ Podocarpa-8,13-d 513439 001945-53-5 50
                ien-15-oic acid, 13-isopropyl- §§
                1-Phenanthrenecarboxylic acid, 1,2
                ,3,4,4a,5,6,9,10,10a-decahydro-1,4
                a-dimethyl-7-(1-methylethyl)-, (1R
                -(1.alpha.,4a.beta.,10a.alpha.))-
                §§ 8,13-Abietadien-18-oic acid
                KAUR-16-EN-18-OIC ACID §§ KAUR-16- 168418 020316-84-1 49
                EN-18-OIC ACID, (4.BETA.)- §§ (-)-
                KAURNENOIC ACID §§ (4-BETA)-KAUR-1
                6-EN-18-OIC ACID
                1-PHENANTHRENECARBOXYLIC ACID, 7-E 466436 005835-26-7 48
                THENYL-1,2,3,4,4A,4B,5,6,7,8,10,10
                A-DODECAHYDRO-1,4A,7-TRIMETHYL-, [
                1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,7.
                ALPHA.,10A.ALPHA.)]- §§ ISOPIMARIC
                 ACID §§ PODOCARP-7-EN-15-OIC ACID
                , 13.BETA.-METHYL-13-VINYL-

54   36.605  0.32 D:\DATABASE\DEMO.L
                Phenol, 2,4-bis(1-phenylethyl)- §§ 504578 002769-94-0 94
                 2,4-Bis(1-phenylethyl)phenol #
                KAUR-16-EN-18-OIC ACID §§ KAUR-16- 168418 020316-84-1 90
                EN-18-OIC ACID, (4.BETA.)- §§ (-)-
                KAURNENOIC ACID §§ (4-BETA)-KAUR-1
                6-EN-18-OIC ACID
                Abietic acid §§ 1-Phenanthrenecarb 513378 000514-10-3 51
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid

55   36.751  0.50 D:\DATABASE\DEMO.L
                Abietic acid §§ 1-Phenanthrenecarb 513344 000514-10-3 70
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid
                3-ACETYL-1-METHYL-2-(1'-METHYL-1H- 513641 000000-00-0 55
                INDOL-2'-YL)-1H-INDOLE
                Abietic acid §§ 1-Phenanthrenecarb 513347 000514-10-3 55
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
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Operator  :
Sample    :
Misc      :
ALS Vial  : 4   Sample Multiplier: 1

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Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autointl.e

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                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid

6  36.978  0.57 D:\DATABASE\DEMO.L
                ABIETA-8,11,13-TRIEN-18-OIC ACID § 503106 999503-11-8 99
                § PODOCARPA-8,11,13-TRIEN-15-SAEUR
                E, 13-ISOPROPYL-
                1-PHENANTHRENECARBOXYLIC ACID, 1,2 503110 001740-19-8 99
                ,3,4,4A,9,10,10A-OCTAHYDRO-1,4A-DI
                METHYL-7-(1-METHYLETHYL)-, [1R-(1.
                ALPHA.,4A.BETA.,10A.ALPHA.)]- §§ (
                -)-DEHYDROABIETIC ACID §§ 1,2,3,4,
                4A,9,10,10A-OCTAHYDRO-1,4A-DIMETHY
                L-7-(1-METHYLETHYL)-1-PHENANTHRENE
                CARBOXYLIC ACID
                1-Phenanthrenecarboxylic acid, 1,2 503093 001740-19-8 99
                ,3,4,4a,9,10,10a-octahydro-1,4a-di
                methyl-7-(1-methylethyl)-, [1R-(1.
                alpha.,4a.beta.,10a.alpha.)]- §§ P
                odocarpa-8,11,13-trien-15-oic acid
                , 13-isopropyl- §§ Abieta-8,11,13-
                trien-18-oic acid §§ Abietic acid,
                 dehydro-

7  37.037  0.88 D:\DATABASE\DEMO.L
                ABIETA-8,11,13-TRIEN-18-OIC ACID § 503106 999503-11-8 93
                § PODOCARPA-8,11,13-TRIEN-15-SAEUR
                E, 13-ISOPROPYL-
                1-PHENANTHRENECARBOXYLIC ACID, 1,2 503110 001740-19-8 78
                ,3,4,4A,9,10,10A-OCTAHYDRO-1,4A-DI
                METHYL-7-(1-METHYLETHYL)-, [1R-(1.
                ALPHA.,4A.BETA.,10A.ALPHA.)]- §§ (
                -)-DEHYDROABIETIC ACID §§ 1,2,3,4,
                4A,9,10,10A-OCTAHYDRO-1,4A-DIMETHY
                L-7-(1-METHYLETHYL)-1-PHENANTHRENE
                CARBOXYLIC ACID
                1-Phenanthrenecarboxylic acid, 1,2 503093 001740-19-8 78
                ,3,4,4a,9,10,10a-octahydro-1,4a-di
                methyl-7-(1-methylethyl)-, [1R-(1.
                alpha.,4a.beta.,10a.alpha.)]- §§ P
                odocarpa-8,11,13-trien-15-oic acid
                , 13-isopropyl- §§ Abieta-8,11,13-
                trien-18-oic acid §§ Abietic acid,
                 dehydro-

8  37.231  0.31 D:\DATABASE\DEMO.L
                ABIETA-7,13-DIEN-18-OIC ACID §§ 1- 168419 000514-10-3 87
                PHENANTHRENECARBOXYLIC ACID, 1,2,3
                ,4,4A,4B,5,6,10,10A-DECAHYDRO- §§
                1-PHENANTHRENECARBOXYLIC ACID, 1,2
                ,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,
                4A-DIMETHYL-7-(1-METHYLETHYL)-, [1
                R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A
                .ALPHA.)]-
                1H-2,10A-ETHANOPHENANTHRENE, KAUR- 513651 006730-83-2 60
                16-EN-18-OIC ACID DERIV. §§ KAUR-1
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  Data File : WLM-200c-10prsan-2jm.D
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  Operator  :
  Sample    :
  Misc      :
  ALS Vial  : 4   Sample Multiplier: 1

  Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

  Unknown Spectrum:   Apex
  Integration Events: ChemStation Integrator - autointl.e

Pk#     RT  Area%          Library/ID                    Ref#     CAS#   Qual
                6-EN-18-OIC ACID §§ KAUR-16-EN-18-
                OIC ACID, (4.ALPHA.)- §§ (-)-ENT-K
                AUR-16-EN-19-OIC ACID
                ABIETA-7,13-DIEN-18-OIC ACID §§ 1- 168420 000514-10-3 53
                PHENANTHRENECARBOXYLIC ACID, 1,2,3
                ,4,4A,4B,5,6,10,10A-DECAHYDRO- §§
                1-PHENANTHRENECARBOXYLIC ACID, 1,2
                ,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,
                4A-DIMETHYL-7-(1-METHYLETHYL)-, [1
                R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A
                .ALPHA.)]-

 69  37.269  0.87 D:\DATABASE\DEMO.L
                ABIETA-7,13-DIEN-18-OIC ACID §§ 1- 168420 000514-10-3 70
                PHENANTHRENECARBOXYLIC ACID, 1,2,3
                ,4,4A,4B,5,6,10,10A-DECAHYDRO- §§
                1-PHENANTHRENECARBOXYLIC ACID, 1,2
                ,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,
                4A-DIMETHYL-7-(1-METHYLETHYL)-, [1
                R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A
                .ALPHA.)]-
                1H-2,10A-ETHANOPHENANTHRENE, KAUR- 513651 006730-83-2 64
                16-EN-18-OIC ACID DERIV. §§ KAUR-1
                6-EN-18-OIC ACID §§ KAUR-16-EN-18-
                OIC ACID, (4.ALPHA.)- §§ (-)-ENT-K
                AUR-16-EN-19-OIC ACID
                Abietic acid §§ 1-Phenanthrenecarb 513378 000514-10-3 55
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid

 70  37.691  2.75 D:\DATABASE\DEMO.L
                Abietic acid §§ 1-Phenanthrenecarb 513378 000514-10-3 99
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid
                Abietic acid §§ 1-Phenanthrenecarb 513347 000514-10-3 94
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid
                .beta.-Pimaric acid §§ .delta.6,8( 513374 000079-54-9 90
                14)-Abietadienoic acid §§ 1-Pimari
                c acid §§ 1-Sapietic acid

 71  38.366  0.09 D:\DATABASE\DEMO.L
                Abietic acid §§ 1-Phenanthrenecarb 513347 000514-10-3 93
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
```

Data Path : F:\DATA MS\daa\
Data File : WLM-200c-10psan-2jm.D
Acq On : 12 Oct 2019 10:27
Operator :
Sample :
Misc :
ALS Vial : 4 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid			
			Abietic acid $$ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid	513378	000514-10-3	92
			Abietic acid $$ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid	513344	000514-10-3	91
72	38.469	0.07	D:\DATABASE\DEMO.L			
			Abietic acid $$ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid	513378	000514-10-3	94
			Abietic acid $$ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid	513347	000514-10-3	93
			Abietic acid $$ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid	513344	000514-10-3	83
73	38.496	0.13	D:\DATABASE\DEMO.L			
			Abietic acid $$ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid	513347	000514-10-3	86
			Abietic acid $$ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- $$ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- $$ L-abietic acid	513344	000514-10-3	83
			Abietic acid $$ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet	513378	000514-10-3	78

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  Data Path : F:\DATA MS\daa\
  Data File : WLM-200c-10prsen-2jm.D
  Acq On    : 12 Oct 2019  10:27
  Operator  :
  Sample    :
  Misc      :
  ALS Vial  : 4   Sample Multiplier: 1

  Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

  Unknown Spectrum:   Apex
  Integration Events: ChemStation Integrator - autointl.e

Pk#     RT  Area%          Library/ID                  Ref#     CAS#   Qual
-------------------------------------------------------------------------------
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid

 74  38.820  0.07 D:\DATABASE\DEMO.L
                Abietic acid §§ 1-Phenanthrenecarb 513344 000514-10-3 78
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid
                Abietic acid §§ 1-Phenanthrenecarb 513378 000514-10-3 70
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid
                Abietic acid §§ 1-Phenanthrenecarb 513347 000514-10-3 64
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid

 75  39.003  0.14 D:\DATABASE\DEMO.L
                Abietic acid §§ 1-Phenanthrenecarb 513378 000514-10-3 84
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid
                Abietic acid §§ 1-Phenanthrenecarb 513347 000514-10-3 62
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid
                6-Hydroxy-7-isopropyl-1,4a-dimethy 513428 022595-48-8 46
                l-1,2,3,4,4a,9,10,10a-octahydro-1-
                phenanthrenemethanol, (1.alpha., 4
                a.beta., 10a.alpha)- §§ Abieta-8,1
                1,13-triene-12,18-diol #

 76  41.564  0.00 D:\DATABASE\DEMO.L
                ABIETA-7,13-DIEN-18-OIC ACID §§ 1- 168419 000514-10-3 60
                PHENANTHRENECARBOXYLIC ACID, 1,2,3
                ,4,4A,4B,5,6,10,10A-DECAHYDRO- §§
                1-PHENANTHRENECARBOXYLIC ACID, 1,2
                ,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,
                4A-DIMETHYL-7-(1-METHYLETHYL)-, [1
                R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A
                .ALPHA.)]-
                Abietic acid §§ 1-Phenanthrenecarb 513347 000514-10-3 55
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
```

Data Path : F:\DATA MS\daa\
Data File : WLM-200c-10prsan-2jm.D
Acq On : 12 Oct 2019 10:27
Operator :
Sample :
Misc :
ALS Vial : 4 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- §§ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- §§ L-abietic acid			
			Abietic acid §§ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m ethylethyl)-, [1R-(1.alpha.,4a.bet a.,4b.alpha.,10a.alpha.)]- §§ Podo carpa-7,13-dien-15-oic acid, 13-is opropyl- §§ L-abietic acid	513378	000514-10-3	50

Data Path : F:\DATA MS\daa\
Data File : WLM-200c-10prsan-3jm.D
Acq On : 10 Oct 2019 10:34
Operator :
Sample :
Misc :
ALS Vial : 1 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	1.962	6.68	D:\DATABASE\DEMO.L			
			Methyl Alcohol §§ Methanol §§ Carb inol §§ Methyl hydroxide	5073	000067-56-1	2
			METHANOL §§ HYDROXYMETHANE §§ ALCO HOL, METHYL §§ ALCOOL METHYLIQUE	5075	000067-56-1	2
			Methyl Alcohol §§ Methanol §§ Carb inol §§ Methyl hydroxide	5072	000067-56-1	2
2	2.135	0.14	D:\DATABASE\DEMO.L			
			Pentane, 2,4-dimethyl- §§ 2,4-Dime thylpentane	18750	000108-08-7	87
			PENTANE, 2,4-DIMETHYL- §§ 2,4-DIME THYLPENTANE §§ PENTANE, 2,4-DIMETH YL	19001	000108-08-7	83
			PENTANE, 2,4-DIMETHYL- §§ 2,4-DIME THYLPENTANE §§ PENTANE, 2,4-DIMETH YL	18833	000108-08-7	80
3	2.200	12.00	D:\DATABASE\DEMO.L			
			HEXANE, 3-METHYL- §§ 3-METHYLHEXAN E §§ 2-ETHYLPENTANE §§ HEXANE, 3-M ETHYL	18994	000589-34-4	64
			HEPTANE §§ ALIPHATIC HYDROCARBON § § DIPROPYL METHANE §§ DIPROPYLMETH ANE	18986	000142-82-5	62
			1-PENTANOL, 2-METHYL- §§ 2-METHYLP ENTAN-1-OL §§ (+-)-2-METHYL-1-PENT ANOL §§ (+-)-2-METHYLPENTANOL	19228	000105-30-6	59
4	2.243	4.59	D:\DATABASE\DEMO.L			
			Cyclopentane, 1,3-dimethyl-, cis- §§ cis-1,3-Dimethylcyclopentane §§ 1,3-Dimethylcyclopentane cis §§ 1 ,3-Dimethylcyclopentane #	62231	002532-58-3	91
			Cyclopentane, 1,3-dimethyl- §§ 1,3 -Dimethylcyclopentane	101343	002453-00-1	91
			1,3-DIMETHYLCYCLOPENTANE §§ CYCLOP ENTANE, 1,3-DIMETHYL-, CIS- §§ 1,3 -DIMETHYLCYCLOPENTANE (CIS) §§ 1,3 -DIMETHYLCYCLOPENTANE CIS	62286	002532-58-3	91
5	2.335	7.00	D:\DATABASE\DEMO.L			
			CYCLOHEXANE, METHYL- §§ METHYLCYCL OHEXANE §§ 1-METHYLCYCLOHEXANE §§ CYCLOHEXANE, METHYL	141469	000108-87-2	96
			CYCLOHEXANE, METHYL- §§ METHYLCYCL OHEXANE §§ 1-METHYLCYCLOHEXANE §§ CYCLOHEXANE, METHYL	141470	000108-87-2	95
			Cyclohexane, methyl- §§ Cyclohexyl methane §§ Hexahydrotoluene §§ Met hylcyclohexane	141386	000108-87-2	94
6	2.421	65.09	D:\DATABASE\DEMO.L			
			Toluene §§ Benzene, methyl §§ Meth acide §§ Methylbenzene	158579	000108-88-3	91
			BENZENE, METHYL- §§ METHYLBENZENE §§ TOLUENE §§ ANTISAL 1A	158622	000108-88-3	91
			BENZENE, METHYL- §§ METHYLBENZENE §§ TOLUENE §§ ANTISAL 1A	158625	000108-88-3	91

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Data Path : F:\DATA MS\daa\
Data File : WLM-200c-10prsan-3jm.D
Acq On    : 10 Oct 2019  10:34
Operator  :
Sample    :
Misc      :
ALS Vial  : 1   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e
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Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	1.962	6.68	D:\DATABASE\DEMO.L			
			Methyl Alcohol $$ Methanol $$ Carb inol $$ Methyl hydroxide	5073	000067-56-1	2
			METHANOL $$ HYDROXYMETHANE $$ ALCO HOL, METHYL $$ ALCOOL METHYLIQUE	5075	000067-56-1	2
			Methyl Alcohol $$ Methanol $$ Carb inol $$ Methyl hydroxide	5072	000067-56-1	2
2	2.135	0.14	D:\DATABASE\DEMO.L			
			Pentane, 2,4-dimethyl- $$ 2,4-Dime thylpentane	18750	000108-08-7	87
			PENTANE, 2,4-DIMETHYL- $$ 2,4-DIME THYLPENTANE $$ PENTANE, 2,4-DIMETH YL	19001	000108-08-7	83
			PENTANE, 2,4-DIMETHYL- $$ 2,4-DIME THYLPENTANE $$ PENTANE, 2,4-DIMETH YL	18833	000108-08-7	80
3	2.200	12.00	D:\DATABASE\DEMO.L			
			HEXANE, 3-METHYL- $$ 3-METHYLHEXAN E $$ 2-ETHYLPENTANE $$ HEXANE, 3-M ETHYL	18994	000589-34-4	64
			HEPTANE $$ ALIPHATIC HYDROCARBON $ $ DIPROPYL METHANE $$ DIPROPYLMETH ANE	18986	000142-82-5	62
			1-PENTANOL, 2-METHYL- $$ 2-METHYLP ENTAN-1-OL $$ (+-)-2-METHYL-1-PENT ANOL $$ (+-)-2-METHYLPENTANOL	19228	000105-30-6	59
4	2.243	4.59	D:\DATABASE\DEMO.L			
			Cyclopentane, 1,3-dimethyl-, cis- $$ cis-1,3-Dimethylcyclopentane $$ 1,3-Dimethylcyclopentane cis $$ 1 ,3-Dimethylcyclopentane #	62231	002532-58-3	91
			Cyclopentane, 1,3-dimethyl- $$ 1,3 -Dimethylcyclopentane	101343	002453-00-1	91
			1,3-DIMETHYLCYCLOPENTANE $$ CYCLOP ENTANE, 1,3-DIMETHYL-, CIS- $$ 1,3 -DIMETHYLCYCLOPENTANE (CIS) $$ 1,3 -DIMETHYLCYCLOPENTANE CIS	62286	002532-58-3	91
5	2.335	7.00	D:\DATABASE\DEMO.L			
			CYCLOHEXANE, METHYL- $$ METHYLCYCL OHEXANE $$ 1-METHYLCYCLOHEXANE $$ CYCLOHEXANE, METHYL	141469	000108-87-2	96
			CYCLOHEXANE, METHYL- $$ METHYLCYCL OHEXANE $$ 1-METHYLCYCLOHEXANE $$ CYCLOHEXANE, METHYL	141470	000108-87-2	95
			Cyclohexane, methyl- $$ Cyclohexyl methane $$ Hexahydrotoluene $$ Met hylcyclohexane	141386	000108-87-2	94
6	2.421	65.09	D:\DATABASE\DEMO.L			
			Toluene $$ Benzene, methyl $$ Meth acide $$ Methylbenzene	158579	000108-88-3	91
			BENZENE, METHYL- $$ METHYLBENZENE $$ TOLUENE $$ ANTISAL 1A	158622	000108-88-3	91
			BENZENE, METHYL- $$ METHYLBENZENE $$ TOLUENE $$ ANTISAL 1A	158625	000108-88-3	91

```
Data Path : F:\DATA MS\daa\
Data File : WLM-200c-10prsan-3jm.D
Acq On    : 10 Oct 2019  10:34
Operator  :
Sample    :
Misc      :
ALS Vial  : 1   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e
```

#	RT	Area%	Library/ID	Ref#	CAS#	Qual
7	2.745	0.89	D:\DATABASE\DEMO.L			
			Cyclohexane, ethyl- $$ Ethylcycloh	141508	001678-91-7	93
			exane			
			CYCLOHEXANE, ETHYL- $$ ETHYLCYCLOH	141561	001678-91-7	93
			EXANE $$ ETHYL CYCLOHEXANE $$ ETHY			
			LCYCLOHEXAN			
			Cyclohexane, ethyl- $$ Ethylcycloh	141506	001678-91-7	93
			exane			
8	30.544	0.06	D:\DATABASE\DEMO.L			
			2-Ethylthio-5-chloro-pyrimidin-4(3	402529	106146-79-6	42
			H)-one $$ 5-Chloro-2-(ethylsulfany			
			l)-4(3H)-pyrimidinone #			
			5-(2-Methoxy-phenyl)-2H-pyrazol-3-	402490	999402-49-4	41
			ol			
			METHYL 5-((Z)-[5-((Z)-((5Z)-5-[(2-	402636	070067-95-7	38
			CYANO-2,3,3-TRIMETHYL-3,4-DIHYDRO-			
			2H-PYRROL-5-YL)METHYLENE]-4,4-DIME			
			THYLPYRROLIDINYLIDENE)METHYL)-3,4-			
			DIMETHYL-2H-PYRROL-2-YLIDENE]METHY			
			L)-3,4-DIMETHYL-1H-PYRROLE-2-C $$			
			6,10-DITHIASPIRO[4.5]DECAN-1-OL			
9	31.689	0.08	D:\DATABASE\DEMO.L			
			3-HYDROXY-2,2,5,8-TETRAMETHYL-2H-N	481954	018142-17-1	70
			APHTHO[1,8-BC]FURAN-6,7-DIONE $$ 2			
			H-NAPHTHO[1,8-BC]FURAN-6,7-DIONE,			
			3-HYDROXY-2,2,5,8-TETRAMETHYL-			
			1-METHOXY-6,6A,7,8-TETRAHYDRO-6,6-	481992	130799-45-0	64
			DIMETHYL-9H-DIBENZO[B,D]PYRAN-9-ON			
			2H-Naphtho[1,8-bc]furan-6,7-dione,	481807	018142-17-1	55
			3-hydroxy-2,2,5,8-tetramethyl- $$			
			3-Hydroxy-2,2,5,8-tetramethyl-2H-			
			naphtho[1,8-bc]furan-6,7-dione #			
10	31.981	0.07	D:\DATABASE\DEMO.L			
			1,1':2',1"-TERPHENYL, 4'-ETHYL- $$	482059	061875-99-8	91
			4-ETHYL-1,2-DIPHENYL-BENZENE $$ 4			
			-ETHYL-1,2-DIPHENYLBENZENE $$ O-TE			
			RPHENYL, 4'-ETHYL-			
			(+-)-(3S*,4AS*,9AS*)-7-HYDROXY-3,6	482050	000000-00-0	90
			,8,9,9-PENTAMETHYL-1,2,3,4,4A,9A-H			
			EXAHYDROFLURENE			
			DIBENZOFURAN, 1,3,4-TRIMETHOXY- $$	481959	088256-10-4	53
			1,3,4-TRIMETHOXYDIBENZOFURAN			
11	33.493	0.10	D:\DATABASE\DEMO.L			
			Phenanthrene, 7-ethenyl-1,2,3,4,4a	481092	055255-56-6	92
			,5,6,7,8,9,10,10a-dodecahydro-1,1,			
			4a,7-tetramethyl- $$ Pimara-8,15-d			
			iene #			
			KAURA-5,16-DIEN-18-OL $$ KAURA-5,1	492904	023837-99-2	62
			6-DIEN-18(OR 19)-OL $$ KAURA-5,16-			
			DIEN-19-OL			
			PREGN-7-ENE, (5.ALPHA.)- $$ 5.ALPH	492909	063518-70-7	45
			A.-PREGN-7-ENE			
12	33.855	0.09	D:\DATABASE\DEMO.L			

Data Path : F:\DATA MS\daa\
Data File : WLM-200c-10prsan-3jm.D
Acq On : 10 Oct 2019 10:34
Operator :
Sample :
Misc :
ALS Vial : 1 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autointl.e

k#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			1-Methyl-10,18-bisnorabiata-8,11,13-triene	466158	999466-16-6	94
			10,13-DIMETHYL-4,5,6,7,8,9,10,11,12,13,14,15-DODECAHYDRO-1H-CYCLOPENTA[A]PHENANTHRENE §§ ANDROSTA-2,16-DIENE	466180	999466-18-8	90
			4-(N-METHYLAMINO)-6,7-(1,2,3,4-TETRAHYDRO-1,1,4,4-TETRAMETHYLBENZO)INDOLE	466219	000000-00-0	83
13	35.481	0.85	D:\DATABASE\DEMO.L			
			Xanthan-9-one, 1-hydroxy-3,5,8-trimethoxy- §§ 5,8-Dimethylbellidifolin §§ 1-Hydroxy-3,5,8-trimethoxyxanthan-9-one §§ 1-Hydroxy-3,5,8-trimethoxy-9H-xanthen-9-one #	504583	049599-09-9	68
			1-PHENANTHRENECARBOXYLIC ACID, 7-ETHENYL-1,2,3,4,4A,4B,5,6,7,8,10,10A-DODECAHYDRO-1,4A,7-TRIMETHYL-, [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,7.ALPHA.,10A.ALPHA.)]- §§ ISOPIMARIC ACID §§ PODOCARP-7-EN-15-OIC ACID, 13.BETA.-METHYL-13-VINYL-	466436	005835-26-7	50
			Androst-5-en-17-ol, 4,4-dimethyl-	513436	999513-44-9	48
14	35.670	0.10	D:\DATABASE\DEMO.L			
			Morphinan-6-one, 4,5-epoxy-3,14-dihydroxy-, (5.alpha.)-	504394	033522-95-1	44
			1H-Indole-3-carboxylic acid, 1-cyclopentyl-5-hydroxy-2-methyl-, ethyl ester	504368	999504-38-0	43
			PIMARA-8(14),15-DIEN-18-OIC ACID §§ 1-PHENANTHRENECARBOXYLIC ACID, 7-ETHENYL-1,2,3,4,4A,4B,5,6,7,9,10,10A-DODECAHYDRO-1,4A,7-TRIMETHYL-, [1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,7.BETA.,10A.ALPHA.)]- §§ (+)-PIMARIC ACID §§ .ALPHA.-PIMARIC ACID	504609	000127-27-5	30
15	35.751	0.17	D:\DATABASE\DEMO.L			
			DEHYDROABIETIC ACID	464556	000000-00-0	97
			1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methylethyl)-, methyl ester, [1R-(1.alpha.,4a.beta.,10a.alpha.)]- §§ Podocarpa-8,11,13-trien-15-oic acid, 13-isopropyl-, methyl ester §§ Methyl dehydroabietat	464538	001235-74-1	94
			METHYL ABIETA-8,11,13-TRIEN-18-OATE §§ 1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,9,10,10A-OCTAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL)-, METHYL ESTER, [1R-(1.ALPHA.,4A.BETA.,10A.ALPHA.)]- §§ DEHYDROABIETIC ACID METHYL ESTER §§ METHYL DEHYDROABIETATE	464550	001235-74-1	94
16	35.897	0.10	D:\DATABASE\DEMO.L			
			2-BUTYL-5-HEXYLINDANE §§ INDAN, 2-	398768	025446-32-6	62

Data Path : F:\DATA MS\daa\
Data File : WLM-200c-10pssn-3jm.D
Acq On : 10 Oct 2019 10:34
Operator :
Sample :
Misc :
ALS Vial : 1 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autointl.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			BUTYL-5-HEXYL- §§ 2-N-BUTYL-1-N-HE XYL-2,3-DIHYDROINDENE §§ 2-N-BUTYL -5-N-HEXYL-(2,3-DIHYDROINDENE)			
			Indan, 2-butyl-5-hexyl- §§ 2-n-But yl-5-n-hexyl-(2,3-dihydroindane) § § 2-n-Butyl-5-n-hexylindan §§ 2-Bu tyl-5-hexylindane #	398758	025446-32-6	62
			Pimaric acid §§ 1-Phenanthrenecarb oxylic acid, 7-ethenyl-1,2,3,4,4a, 4b,5,6,7,9,10,10a-dodecahydro-1,4a ,7-trimethyl-, [1R-(1.alpha.,4a.be ta.,4b.alpha.,7.beta.,10a.alpha.)] - §§ Podocarp-8(14)-en-15-oic acid , 13.alpha.-methyl-13-vinyl- §§ D- pimaric acid	466434	000127-27-5	46
17	36.383	0.03	D:\DATABASE\DEMO.L			
			Methyl abietate §§ 1-Phenanthrenec arboxylic acid, 1,2,3,4,4a,4b,5,6, 10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, methyl ester, [1R -(1.alpha.,4a.beta.,4b.alpha.,10a. alpha.)]- §§ Podocarpa-7,13-dien-1 5-oic acid, 13-isopropyl-, methyl ester §§ Abalyn	480547	000127-25-3	90
			METHYL ABIETA-7,13-DIEN-18-OATE §§ 1-PHENANTHRENECARBOXYLIC ACID, 1, 2,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1 ,4A-DIMETHYL-7-(1-METHYLETHYL)-, M ETHYL ESTER, [1R-(1.ALPHA.,4A.BETA .,4B.ALPHA.,10A.ALPHA.)]- §§ ABALY N §§ ABIETIC ACID METHYL ESTER	480550	000127-25-3	90
			Methyl abietate §§ 1-Phenanthrenec arboxylic acid, 1,2,3,4,4a,4b,5,6, 10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, methyl ester, [1R -(1.alpha.,4a.beta.,4b.alpha.,10a. alpha.)]- §§ Podocarpa-7,13-dien-1 5-oic acid, 13-isopropyl-, methyl ester §§ Abalyn	258889	000127-25-3	84
18	36.599	0.05	D:\DATABASE\DEMO.L			
			Phenol, 2,4-bis(1-phenylethyl)- §§ 2,4-Bis(1-phenylethyl)phenol #	504578	002769-94-0	89
			KAUR-16-EN-18-OIC ACID §§ KAUR-16- EN-18-OIC ACID, (4.BETA.)- §§ (-)- KAURNENOIC ACID §§ (4-BETA)-KAUR-1 6-EN-18-OIC ACID	168418	020316-84-1	55
			3-ACETYL-1-METHYL-2-(1'-METHYL-1H- INDOL-2'-YL)-1H-INDOLE	513641	000000-00-0	53
19	36.745	0.10	D:\DATABASE\DEMO.L			
			1H-NAPHTHO[2,3-C]PYRAN-5,10-DIONE, 3,4-DIHYDRO-7,9-DIMETHOXY-1,3-DIM ETHYL-, CIS-(.+-.)- §§ (+,-)-CIS-7 ,9-DIMETHOXY-1,3-DIMETHYL-3,4,5,10 -TETRAHYDRONAPHTHO[2,3-C]PYRAN-5,1 0-DIONE	513558	084018-43-9	91
			1H-NAPHTHO[2,3-C]PYRAN-5,10-DIONE,	513557	084018-44-0	91

Data Path : F:\DATA MS\daa\
Data File : WLM-200c-10prsan-3jm.D
Acq On : 10 Oct 2019 10:34
Operator :
Sample :
Misc :
ALS Vial : 1 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			3,4-DIHYDRO-7,9-DIMETHOXY-1,3-DIM ETHYL-, TRANS-(.+-.)- §§ (+,-)-DEO XYQUINONE A DIMETHYL ETHER §§ (+,-)-TRANS-7,9-DIMETHOXY-1,3-DIMETHYL -3,4,5,10-TETRAHYDRONAPHTHO[2,3-C] PYRAN-5,10-DIONE			
			KAUR-16-EN-18-OIC ACID §§ KAUR-16- EN-18-OIC ACID, (4.BETA.)- §§ (-)- KAURNENOIC ACID §§ (4-BETA)-KAUR-1 6-EN-18-OIC ACID	168418	020316-84-1	64
20	36.972	0.21	D:\DATABASE\DEMO.L			
			ABIETA-8,11,13-TRIEN-18-OIC ACID § § PODOCARPA-8,11,13-TRIEN-15-SAEUR E, 13-ISOPROPYL-	503106	999503-11-8	99
			1-Phenanthrenecarboxylic acid, 1,2 ,3,4,4a,9,10,10a-octahydro-1,4a-di methyl-7-(1-methylethyl)-, [1R-(1. alpha.,4a.beta.,10a.alpha.)]- §§ P odocarpa-8,11,13-trien-15-oic acid , 13-isopropyl- §§ Abieta-8,11,13- trien-18-oic acid §§ Abietic acid, dehydro-	503093	001740-19-8	96
			1-PHENANTHRENECARBOXYLIC ACID, 1,2 ,3,4,4A,9,10,10A-OCTAHYDRO-1,4A-DI METHYL-7-(1-METHYLETHYL)-, [1R-(1. ALPHA.,4A.BETA.,10A.ALPHA.)]- §§ (-)-DEHYDROABIETIC ACID §§ 1,2,3,4, 4A,9,10,10A-OCTAHYDRO-1,4A-DIMETHY L-7-(1-METHYLETHYL)-1-PHENANTHRENE CARBOXYLIC ACID	503110	001740-19-8	96
21	37.031	0.41	D:\DATABASE\DEMO.L			
			1-Phenanthrenecarboxylic acid, 1,2 ,3,4,4a,9,10,10a-octahydro-1,4a-di methyl-7-(1-methylethyl)-, [1R-(1. alpha.,4a.beta.,10a.alpha.)]- §§ P odocarpa-8,11,13-trien-15-oic acid , 13-isopropyl- §§ Abieta-8,11,13- trien-18-oic acid §§ Abietic acid, dehydro-	503093	001740-19-8	70
			1-PHENANTHRENECARBOXYLIC ACID, 1,2 ,3,4,4A,9,10,10A-OCTAHYDRO-1,4A-DI METHYL-7-(1-METHYLETHYL)-, [1R-(1. ALPHA.,4A.BETA.,10A.ALPHA.)]- §§ (-)-DEHYDROABIETIC ACID §§ 1,2,3,4, 4A,9,10,10A-OCTAHYDRO-1,4A-DIMETHY L-7-(1-METHYLETHYL)-1-PHENANTHRENE CARBOXYLIC ACID	503110	001740-19-8	70
			FERROCENE, 1-ACETYL-1'-(TRIMETHYLS ILYL)- §§ KETONE, METHYL 1'-(TRIME THYLSILYL)FERROCENYL §§ 1-ACETYL-1 '-(TRIMETHYLSILYL)FERROCENE §§ 3,3 '-DIDEUTERIO-1-ACETYL-1'-(TRIMETHY LSILYL)FERROCENE	513500	033307-60-7	53
22	37.231	0.10	D:\DATABASE\DEMO.L			
			ABIETA-7,13-DIEN-18-OIC ACID §§ 1- PHENANTHRENECARBOXYLIC ACID, 1,2,3	168419	000514-10-3	91

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Data Path : F:\DATA MS\daa\
Data File : WLM-200c-10prsan-3jm.D
Acq On    : 10 Oct 2019  10:34
Operator  :
Sample    :
Misc      :
ALS Vial  : 1   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autointl.e

c#     RT  Area%          Library/ID                    Ref#     CAS#   Qual
                ,4,4A,4B,5,6,10,10A-DECAHYDRO- §§
                1-PHENANTHRENECARBOXYLIC ACID, 1,2
                ,3,4,4A,4B,5,6,10,10A-DECAHYDRO-1,
                4A-DIMETHYL-7-(1-METHYLETHYL)-, [1
                R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,10A
                .ALPHA.)]-
                ABIETA-8,11,13-TRIEN-18-OIC ACID § 503112 005155-70-4 91
                § 1-PHENANTHRENECARBOXYLIC ACID, 1
                ,2,3,4,4A,9,10,10A-OCTAHYDRO-1,4A-
                DIMETHYL-7-(1-METHYLETHYL)-, [1S-(
                1.ALPHA.,4A.ALPHA.,10A.BETA.)]- §§
                 13-ISOPROPYLPODOCARPA-8,11,13-TRI
                EN-16-OIC ACID §§ 4-EPIABIETIC ACI
                D, DEHYDRO-
                1-Phenanthrenecarboxylic acid, 1,2 503094 005155-70-4 91
                ,3,4,4a,9,10,10a-octahydro-1,4a-di
                methyl-7-(1-methylethyl)-, [1S-(1.
                alpha.,4a.alpha.,10a.beta.)]- §§ P
                odocarpa-8,11,13-trien-16-oic acid
                , 13-isopropyl- §§ Callitrisic aci
                d §§ 4-Epiabietic acid, dehydro-

23  37.669  1.09 D:\DATABASE\DEMO.L
                Abietic acid §§ 1-Phenanthrenecarb 513378 000514-10-3 99
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid
                Abietic acid §§ 1-Phenanthrenecarb 513344 000514-10-3 96
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid
                Abietic acid §§ 1-Phenanthrenecarb 513347 000514-10-3 94
                oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                10a-decahydro-1,4a-dimethyl-7-(1-m
                ethylethyl)-, [1R-(1.alpha.,4a.bet
                a.,4b.alpha.,10a.alpha.)]- §§ Podo
                carpa-7,13-dien-15-oic acid, 13-is
                opropyl- §§ L-abietic acid
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Data Path : P:\DATA MS\GAA\
Data File : WLM-200c-10pesen-4jm.D
Acq On : 12 Oct 2019 8:49
Operator :
Sample :
Misc :
ALS Vial : 2 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

k#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	1.962	6.25	D:\DATABASE\DEMO.L			
			Methyl Alcohol $$ Methanol $$ Carb inol $$ Methyl hydroxide	5073	000067-56-1	2
			METHANOL $$ HYDROXYMETHANE $$ ALCO HOL, METHYL $$ ALCOOL METHYLIQUE	5075	000067-56-1	2
			Methyl Alcohol $$ Methanol $$ Carb inol $$ Methyl hydroxide	5072	000067-56-1	2
2	2.135	0.16	D:\DATABASE\DEMO.L			
			Pentane, 2,4-dimethyl- $$ 2,4-Dime thylpentane	18750	000108-08-7	87
			PENTANE, 2,4-DIMETHYL- $$ 2,4-DIME THYLPENTANE $$ PENTANE, 2,4-DIMETH YL	63648	000108-08-7	83
			PENTANE, 2,4-DIMETHYL- $$ 2,4-DIME THYLPENTANE $$ PENTANE, 2,4-DIMETH YL	18833	000108-08-7	80
3	2.200	11.33	D:\DATABASE\DEMO.L			
			HEXANE, 3-METHYL- $$ 3-METHYLHEXAN E $$ 2-ETHYLPENTANE $$ HEXANE, 3-M ETHYL	18994	000589-34-4	64
			HEPTANE $$ ALIPHATIC HYDROCARBON $ $ DIPROPYL METHANE $$ DIPROPYLMETH ANE	18986	000142-82-5	58
			Hexane, 3-methyl- $$ 2-Ethylpentan e $$ 3-Methylhexane	18743	000589-34-4	58
4	2.243	4.40	D:\DATABASE\DEMO.L			
			1,3-DIMETHYLCYCLOPENTANE $$ CYCLOP ENTANE, 1,3-DIMETHYL-, CIS- $$ 1,3 -DIMETHYLCYCLOPENTANE (CIS) $$ 1,3 -DIMETHYLCYCLOPENTANE CIS	62286	002532-58-3	91
			Cyclopentane, 1,3-dimethyl- $$ 1,3 -Dimethylcyclopentane	101343	002453-00-1	91
			Cyclopentane, 1,3-dimethyl-, cis- $$ cis-1,3-Dimethylcyclopentane $$ 1,3-Dimethylcyclopentane cis $$ 1 ,3-Dimethylcyclopentane #	62231	002532-58-3	91
5	2.335	6.63	D:\DATABASE\DEMO.L			
			CYCLOHEXANE, METHYL- $$ METHYLCYCL OHEXANE $$ 1-METHYLCYCLOHEXANE $$ CYCLOHEXANE, METHYL	141469	000108-87-2	96
			CYCLOHEXANE, METHYL- $$ METHYLCYCL OHEXANE $$ 1-METHYLCYCLOHEXANE $$ CYCLOHEXANE, METHYL	141470	000108-87-2	95
			CYCLOHEXANE, METHYL- $$ METHYLCYCL OHEXANE $$ 1-METHYLCYCLOHEXANE $$ CYCLOHEXANE, METHYL	141467	000108-87-2	95
6	2.421	60.77	D:\DATABASE\DEMO.L			
			Toluene $$ Benzene, methyl $$ Meth acide $$ Methylbenzene	158580	000108-88-3	91
			Toluene $$ Benzene, methyl $$ Meth acide $$ Methylbenzene	158579	000108-88-3	91
			BENZENE, METHYL- $$ METHYLBENZENE $$ TOLUENE $$ ANTISAL 1A	158625	000108-88-3	91

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Data Path : F:\DATA MS\daa\
Data File : WLM-200c-1Cpraan-4jm.D
Acq On    : 12 Oct 2019   8:49
Operator  :
Sample    :
Misc      :
ALS Vial  : 2   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autointl.e

k#     RT  Areat%          Library/ID                    Ref#     CAS#   Qual
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 7   2.746  1.12 D:\DATABASE\DEMO.L
                 Cyclohexane, ethyl- $$ Ethylcycloh 141506 001678-91-7 93
                 exane
                 CYCLOHEXANE, ETHYL- $$ ETHYLCYCLOH 141561 001678-91-7 93
                 EXANE $$ ETHYL CYCLOHEXANE $$ ETHY
                 LCYCLOHEXAN
                 Cyclohexane, ethyl- $$ Ethylcycloh 141508 001678-91-7 93
                 exane

 8   2.870  0.57 D:\DATABASE\DEMO.L
                 1,3,5-Cycloheptatriene $$ Tropilid 158600 000544-25-2 81
                 ene $$ Cyclohepta-1,3,5-triene $$
                 Cycloheptatriene
                 BENZENE, METHYL- $$ METHYLBENZENE  158623 000108-88-3 81
                 $$ TOLUENE $$ ANTISAL 1A
                 1,3,5-CYCLOHEPTATRIENE $$ CYCLOHEP 158636 000544-25-2 76
                 TA-1,3,5-TRIENE $$ CYCLOHEPTATRIEN
                 E $$ CYCLOHEPTATRIENE [UN2603] [FL
                 AMMABLE LIQUID]

 9  17.304  0.02 D:\DATABASE\DEMO.L
                 2H-2,4a-Methanonaphthalene, 1,3,4, 350641 001135-66-6 98
                 5,6,7-hexahydro-1,1,5,5-tetramethy
                 l-, (2S)- $$ 2H-2,4a-Methanonaphth
                 alene, 1,3,4,5,6,7-hexahydro-1,1,5
                 ,5-tetramethyl-, (2S,4aR)-(-)- $$
                 Isolongifolene $$ (-)-Isolongifoli
                 ne
                 2H-2,4A-METHANONAPHTHALENE, 1,3,4, 350804 001135-66-6 98
                 5,6,7-HEXAHYDRO-1,1,5,5-TETRAMETHY
                 L-, (2S)- $$ (-)-ISOLONGIFOLENE $$
                  (-)-ISOLONGIFOLINE $$ (2S)-1,3,4,
                 5,6,7-HEXAHYDRO-1,1,5,5-TETRAMETHY
                 L-2H-2,4A-METHANONAPHTHALENE
                 2H-2,4a-Methanonaphthalene, 1,3,4, 350640 001135-66-6 97
                 5,6,7-hexahydro-1,1,5,5-tetramethy
                 l-, (2S)- $$ 2H-2,4a-Methanonaphth
                 alene, 1,3,4,5,6,7-hexahydro-1,1,5
                 ,5-tetramethyl-, (2S,4aR)-(-)- $$
                 Isolongifolene $$ (-)-Isolongifoli
                 ne

10  17.725  0.00 D:\DATABASE\DEMO.L
                 2-METHOXY-4-(METHOXYMETHYL)-6-METH   7347 063644-84-8  9
                 YLNICOTINONITRILE $$ PYRIDINE-3-CA
                 RBONITRILE, 2,4-DIMETHOXY-6-METHYL
                 Taurolidine $$ 2H-1,2,4-Thiadiazin   4983 019388-87-5  9
                 e, 4,4'-methylenebis[tetrahydro-,
                 1,1,1',1'-tetraoxide $$ 4,4'-Methy
                 lenebis(tetrahydro-1,2,4-thiadiazi
                 ne 1,1-dioxide) $$ Taurolin
                 4-BROMO-N-[(6-METHYL-2-PYRIDYL)AMI   7473 999007-47-4  4
                 NOMETHYL]PHTHALIMIDE $$ 5-BROMO-2-
                 {[(6-METHYL-2-PYRIDINYL)AMINO]METH
                 YL}-1H-ISOINDOLE-1,3(2H)-DIONE

11  30.215  0.04 D:\DATABASE\DEMO.L
                 4,7-Dimethoxy-2-methyl-1H-indene   402559 999402-56-3 47
                 METHYL 5-((Z)-[5-((Z)-((5Z)-5-[(2- 402636 070067-95-7 46
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Data Path : F:\DATA MS\daa\
Data File : WLM-200c-10prsan-4jm.D
Acq On    : 12 Oct 2019    8:49
Operator  :
Sample    :
Misc      :
ALS Vial  : 2   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e

k#     RT  Area%          Library/ID                  Ref#     CAS#   Qual
                CYANO-2,3,3-TRIMETHYL-3,4-DIHYDRO-
                2H-PYRROL-5-YL)METHYLENE]-4,4-DIME
                THYLPYRROLIDINYLIDENE)METHYL)-3,4-
                DIMETHYL-2H-PYRROL-2-YLIDENE]METHY
                L)-3,4-DIMETHYL-1H-PYRROLE-2-C $$
                6,10-DITHIASPIRO[4.5]DECAN-1-OL
                2-Ethylthio-5-chloro-pyrimidin-4(3 402529 106146-79-6 45
                H)-one $$ 5-Chloro-2-(ethylsulfany
                l)-4(3H)-pyrimidinone #

12  30.301  0.02 D:\DATABASE\DEMO.L
                ENT-PIMARA-8,15-DIENE               481166 021561-92-2 95
                1,1,4A-TRIMETHYL-6-METHYLENE-5-[(2 481156 005957-33-5 90
                E)-3-METHYL-2,4-PENTADIENYL]DECAHY
                DRONAPHTHALENE $$ NAPHTHALENE, DEC
                AHYDRO-1,1,4A-TRIMETHYL-6-METHYLEN
                E-5-(3-METHYL-2,4-PENTADIENYL)-, [
                4AS-(4A.ALPHA.,5.ALPHA.,8A.BETA.)]
                - $$ BIFORMEN $$ BIFORMENE
                Naphthalene, decahydro-1,1,4a-trim 481091 005957-33-5 90
                ethyl-6-methylene-5-(3-methyl-2,4-
                pentadienyl)-, [4aS-(4a.alpha.,5.a
                lpha.,8a.beta.)]- $$ Labda-8(20),1
                2,14-triene $$ Biformen $$ Biforme
                ne

13  30.544  0.07 D:\DATABASE\DEMO.L
                2-Ethylthio-5-chloro-pyrimidin-4(3 402529 106146-79-6 90
                H)-one $$ 5-Chloro-2-(ethylsulfany
                l)-4(3H)-pyrimidinone #
                METHYL 5-((Z)-[5-((Z)-((5Z)-5-[(2- 402636 070067-95-7 83
                CYANO-2,3,3-TRIMETHYL-3,4-DIHYDRO-
                2H-PYRROL-5-YL)METHYLENE]-4,4-DIME
                THYLPYRROLIDINYLIDENE)METHYL)-3,4-
                DIMETHYL-2H-PYRROL-2-YLIDENE]METHY
                L)-3,4-DIMETHYL-1H-PYRROLE-2-C $$
                6,10-DITHIASPIRO[4.5]DECAN-1-OL
                4-ISOPROPYLIDENE-2-ADAMANTANONE     402783 000000-00-0 49

14  30.755  0.01 D:\DATABASE\DEMO.L
                6-ETHYL-2-METHYL-4,6-DIHYDRO-2H-[1   7414 334023-40-4 38
                ,4]OXAZINO[3,2-C]QUINOLINE-3,5-DIO
                NE $$ 6-ETHYL-2-METHYL-2H-1-OXA-4,
                6-PHENANTHROLINE-3,5(4H,6H)-DIONE
                $$ 6-ETHYL-2-METHYL-6,10B-DIHYDRO-
                2H-[1,4]OXAZINO[3,2-C]QUINOLINE-3,
                5-DIONE
                (+-)METHYL HERITOL                    484 000000-00-0 14
                4-(METHOXYMETHYL)-6-METHYL-2-PHENO   7413 332057-36-0 12
                XYNICOTINONITRILE $$ PYRIDINE-3-CA
                RBONITRILE, 4-METHOXYMETHYL-6-METH
                YL-2-PHENOXY-

15  30.868  0.03 D:\DATABASE\DEMO.L
                3-Phenyl-4-azafluorene $$ 2-Phenyl 467987 033777-97-8 64
                -5H-indeno[1,2-b]pyridine #
                5-METHYLBENZO[C]ACRIDINE $$ BENZ[C 468083 003519-87-7 64
                ]ACRIDINE, 5-METHYL- $$ 5-METHYLBE
                NZ(C)ACRIDINE $$ 5-METHYLBENZO(C)A
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Data Path : F:\DATA MS\daa\
Data File : WLM-200c-10prsan-4jm.D
Acq On : 12 Oct 2019 8:49
Operator :
Sample :
Misc :
ALS Vial : 2 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autointl.e

k#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			CRIDINE			
			1,6-Ditritylfructose triacetate	469118	999469-12-6	64
16	30.944	0.00	D:\DATABASE\DEMO.L			
			6-ETHYL-2-METHYL-4,6-DIHYDRO-2H-[1,4]OXAZINO[3,2-C]QUINOLINE-3,5-DIONE §§ 6-ETHYL-2-METHYL-2H-1-OXA-4,6-PHENANTHROLINE-3,5(4H,6H)-DIONE §§ 6-ETHYL-2-METHYL-6,10B-DIHYDRO-2H-[1,4]OXAZINO[3,2-C]QUINOLINE-3,5-DIONE	7414	334023-40-4	43
			4-(METHOXYMETHYL)-6-METHYL-2-PHENOXYNICOTINONITRILE §§ PYRIDINE-3-CARBONITRILE, 4-METHOXYMETHYL-6-METHYL-2-PHENOXY-	7413	332057-36-0	27
			2,2,3,3,4,4,5,5-OCTAFLUORO-N-(3-METHOXYPHENYL)PENTANAMIDE §§ PENTANAMIDE, 2,2,3,3,4,4,5,5-OCTAFLUORO-N-(3-METHOXYPHENYL)-	7474	339166-43-7	10
17	31.084	0.01	D:\DATABASE\DEMO.L			
			4-(METHOXYMETHYL)-6-METHYL-2-PHENOXYNICOTINONITRILE §§ PYRIDINE-3-CARBONITRILE, 4-METHOXYMETHYL-6-METHYL-2-PHENOXY-	7413	332057-36-0	25
			(+-)METHYL HERITOL	484	000000-00-0	14
			2-METHOXY-4-(METHOXYMETHYL)-6-METHYLNICOTINONITRILE §§ PYRIDINE-3-CARBONITRILE, 2,4-DIMETHOXY-6-METHYL	7347	063644-84-8	9
18	31.192	0.05	D:\DATABASE\DEMO.L			
			5-METHYLBENZO[C]ACRIDINE §§ BENZ[C]ACRIDINE, 5-METHYL- §§ 5-METHYLBENZ(C)ACRIDINE §§ 5-METHYLBENZO(C)ACRIDINE	468083	003519-87-7	64
			10-METHYLBENZO[A]ACRIDINE §§ BENZ[A]ACRIDINE, 10-METHYL- §§ 10-METHYLBENZO(A)ACRIDINE	468080	003781-67-7	64
			3-Penten-2-one, 1,1,1,4-tetraphenyl §§ (3Z)-1,1,1,4-Tetraphenyl-3-penten-2-one #	468776	097991-11-2	64
19	31.306	0.01	D:\DATABASE\DEMO.L			
			6-ETHYL-2-METHYL-4,6-DIHYDRO-2H-[1,4]OXAZINO[3,2-C]QUINOLINE-3,5-DIONE §§ 6-ETHYL-2-METHYL-2H-1-OXA-4,6-PHENANTHROLINE-3,5(4H,6H)-DIONE §§ 6-ETHYL-2-METHYL-6,10B-DIHYDRO-2H-[1,4]OXAZINO[3,2-C]QUINOLINE-3,5-DIONE	7414	334023-40-4	10
			(+-)METHYL HERITOL	484	000000-00-0	8
20	31.684	0.10	D:\DATABASE\DEMO.L			
			3,4-DIHYDRO-7,12-DIMETHYLBENZ[A]ANTHRACENE	482069	000000-00-0	90
			(+-)-(3S*,4AS*,9AS*)-7-HYDROXY-3,6,8,9,9-PENTAMETHYL-1,2,3,4,4A,9A-HEXAHYDROFLURENE	482050	000000-00-0	90
			3-HYDROXY-2,2,5,8-TETRAMETHYL-2H-N	481954	018142-17-1	64

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Data File : WLM-200c-10prsan-4jm.D
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Sample    :
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Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#     RT  Area%          Library/ID                    Ref#     CAS#   Qual
                  APHTHO[1,8-BC]FURAN-6,7-DIONE §§ 2
                  H-NAPHTHO[1,8-BC]FURAN-6,7-DIONE,
                  3-HYDROXY-2,2,5,8-TETRAMETHYL-

21  31.835  0.01 D:\DATABASE\DEMO.L
                  1-Hexadecanamine §§ Hexadecylamine   4902 000143-27-1  9
                   §§ n-Cetylamine §§ n-Hexadecylami
                  ne
                  PHENOL, 2-SEC-BUTYL-4-(METHYLTHIO)    132 000000-00-0  4
                  -6-NITRO-
                  CYCLOPROPANECARBONYL CHLORIDE, 2,2   7425 005365-22-0  1
                  -DIBROMO-1-METHYL- §§ 2,2-DIBROMO-
                  1-METHYLCYCLOPROPANECARBONYL CHLOR
                  IDE

22  31.976  0.09 D:\DATABASE\DEMO.L
                  3,4-DIHYDRO-7,12-DIMETHYLBENZ[A]AN 482069 000000-00-0 90
                  THRACENE
                  (+-)-(3S*,4AS*,9AS*)-7-HYDROXY-3,6 482050 000000-00-0 90
                  ,8,9,9-PENTAMETHYL-1,2,3,4,4A,9A-H
                  EXAHYDROFLURENE
                  TETRAETHYLDICHLOROBENZENE          468172 000000-00-0 83

23  32.100  0.03 D:\DATABASE\DEMO.L
                  2(1H)-Phenanthrenone, 3,4,4a,9,10, 481103 055255-51-1 43
                  10a-hexahydro-7-methoxy-1,1,4a-tri
                  methyl- §§ 13-Methoxypodocarpa-8,1
                  1,13-trien-3-one #
                  Bis(acetylacetonato)cobalt §§ Coba 480942 014024-48-7 38
                  lt, bis(2,4-pentanedionato-O,O')-,
                   (T-4)- §§ Cobalt, bis(2,4-pentana
                  dionato)- §§ Acetylacetone cobalt(
                  II)
                  13-METHOXYPODOCARPA-8,11,13-TRIEN- 481146 055255-51-1 38
                  3-ONE §§ 2(1H)-PHENANTHRENONE, 3,4
                  ,4A,9,10,10A-HEXAHYDRO-7-METHOXY-1
                  ,1,4A-TRIMETHYL- §§ 7-METHOXY-1,1,
                  4A-TRIMETHYL-1,2,3,4,4A,9,10,10A-O
                  CTAHYDROPHENANTHREN-2-ONE

24  32.240  0.01 D:\DATABASE\DEMO.L
                  4-(METHOXYMETHYL)-6-METHYL-2-PHENO   7413 332057-36-0 32
                  XYNICOTINONITRILE §§ PYRIDINE-3-CA
                  RBONITRILE, 4-METHOXYMETHYL-6-METH
                  YL-2-PHENOXY-
                  Taurolidine §§ 2H-1,2,4-Thiadiazin   4983 019388-87-5 17
                  e, 4,4'-methylenebis[tetrahydro-,
                  1,1,1',1'-tetraoxide §§ 4,4'-Methy
                  lenebis(tetrahydro-1,2,4-thiadiazi
                  ne 1,1-dioxide) §§ Taurolin
                  1-Undecanamine §§ Undecylamine §§    4551 007307-55-3  9
                  n-Undecylamine §§ Hendecylamine

25  32.381  0.04 D:\DATABASE\DEMO.L
                  1-PHENYL-3-METHYL-4-(2-PROP-2-YL)- 419699 000000-00-0 53
                  5-ACETOXYPYRAZOLE
                  Pyrrolidin-2,5-dione, 3-ethylidene 419130 999419-13-6 52
                  -1-phenyl-
                  1-PHENYL-2-ACETYL-3-METHYL-5-(PROP 419698 000000-00-0 52
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Sample :
Misc :
ALS Vial : 2 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autointl.e

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			-2-YL)-2,5-DIHYDROPYRAZOLE-5-ONE			
26	32.581	0.01	D:\DATABASE\DEMO.L			
			4-(2-TOLUIDINO)-2(1H)-PYRIMIDINONE §§ 2(1H)-PYRIMIDINONE, 4-[(2-METHYLPHENYL)AMINO]- §§ 4-(2'-METHYLPHENYL)AMINO-1,2-DIHYDRO-1,3-DIAZINE-2-ONE §§ 4-(2-METHYLPHENYLAMINO)-PYRIMIDIN-2(1H)-ONE	419278	127970-29-0	46
			4-(2-Methylphenylamino)-pyrimidin-2(1H)-one §§ 4-(2-Tolylamino)cytosine §§ 4-(2-Toluidino)-2(1H)-pyrimidinone #	419189	127970-29-0	43
			1H-BENZIMIDAZOLE, 2-(4-THIAZOLYL)- §§ 1H-BENZIMIDAZOLE, 2- (4-THIAZOLYL)- §§ 2-(1,3-THIAZOL-4-YL)-1H-BENZIMIDAZOLE §§ 2-(1,3-THIAZOL-4-YL)BENZIMIDAZOLE	419260	000148-79-8	43
27	32.667	0.01	D:\DATABASE\DEMO.L			
			1-Hexadecanamine §§ Hexadecylamine §§ n-Cetylamine §§ n-Hexadecylamine	4902	000143-27-1	22
			1-Tetradecanamine §§ Tetradecylamine §§ Armeen 14 §§ Myristylamine	4815	002016-42-4	22
			1-Tetradecanamine §§ Tetradecylamine §§ Armeen 14 §§ Myristylamine	4817	002016-42-4	12
28	32.753	0.01	D:\DATABASE\DEMO.L			
			1-Hexadecanamine §§ Hexadecylamine §§ n-Cetylamine §§ n-Hexadecylamine	4902	000143-27-1	27
			4-BROMO-N-[(6-METHYL-2-PYRIDYL)AMINOMETHYL]PHTHALIMIDE §§ 5-BROMO-2-{[(6-METHYL-2-PYRIDINYL)AMINO]METHYL}-1H-ISOINDOLE-1,3(2H)-DIONE	7473	999007-47-4	14
			4-(METHOXYMETHYL)-6-METHYL-2-PHENOXYNICOTINONITRILE §§ PYRIDINE-3-CARBONITRILE, 4-METHOXYMETHYL-6-METHYL-2-PHENOXY-	7413	332057-36-0	10
29	32.975	0.01	D:\DATABASE\DEMO.L			
			4-(METHOXYMETHYL)-6-METHYL-2-PHENOXYNICOTINONITRILE §§ PYRIDINE-3-CARBONITRILE, 4-METHOXYMETHYL-6-METHYL-2-PHENOXY-	7413	332057-36-0	35
			1,12-DODECANEDIAMINE §§ DODECANE-1,12-DIAMINE §§ 1, 12-DIAMINODODECANE §§ 1, 12-DODECANEDIAMINE	4754	002783-17-7	9
			Tridecylamine §§ n-Tridecylamine §§ 1-Aminotridecane §§ 1-Tridecanamine	4735	002869-34-3	9
30	33.040	0.02	D:\DATABASE\DEMO.L			
			7-ETHYL-3-METHYL-2-NITRO-4-OXO-4,7-DIHYDROTHIENO[2,3-B]PYRIDINE-5-CARBOXYLIC ACID §§ THIENO[2,3-B]PYRIDINE-5-CARBOXILIC ACID,4,7-DIHYDRO-7-ETHYL-3-METHYL-2-NITRO-4-OXO-	7432	999007-43-3	10

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  Integration Events: ChemStation Integrator - autoint1.e

Pk#     RT  Area%          Library/ID                    Ref#     CAS#   Qual

                4-(METHOXYMETHYL)-6-METHYL-2-PHENO   7413 332057-36-0 10
                XYNICOTINONITRILE §§ PYRIDINE-3-CA
                RBONITRILE, 4-METHOXYMETHYL-6-METH
                YL-2-PHENOXY-
                Carbamic acid, (2-chloroethylidene   3171 005336-13-0  9
                )bis-, diethyl ester §§ Carbamic a
                cid, (2-chloroethylidene)di-, diet
                hyl ester

 31  33.132  0.02 D:\DATABASE\DEMO.L
                4,9(11)-Androstadiene-3,17-dione   502121 999502-13-3 48
                2-(2,4-DIMETHOXYPHENYL)-6-METHOXY-  502297 067685-23-8 30
                1-BENZOFURAN §§ BENZOFURAN, 2-(2,4
                -DIMETHOXYPHENYL)-6-METHOXY- §§ 2-
                (2',4'-DIMETHOXYPHENYL)-6-METHOXY-
                BENZOFURAN §§ 2-(2,4-DIMETHOXYPHEN
                YL)-6-METHOXYBENZOFURAN
                Tetracyclo[16.1.0.0(2,9).0(10,17)]  502080 999502-09-2 30
                nonadeca-2(9),10(17)-diene, 19,19-
                dimethyl-

 32  33.369  0.01 D:\DATABASE\DEMO.L
                4-(METHOXYMETHYL)-6-METHYL-2-PHENO   7413 332057-36-0 10
                XYNICOTINONITRILE §§ PYRIDINE-3-CA
                RBONITRILE, 4-METHOXYMETHYL-6-METH
                YL-2-PHENOXY-
                1-OCTADECANAMINE §§ OCTADECAN-1-AM   4965 000124-30-1 10
                INE §§ 1-AMINOOCTADECANE §§ 1-OCTA
                DECANAMIN
                1-Tetradecanamine §§ Tetradecylami   4817 002016-42-4 10
                ne §§ Armeen 14 §§ Myristylamine

 33  33.488  0.09 D:\DATABASE\DEMO.L
                Phenanthrene, 7-ethenyl-1,2,3,4,4a 481092 055255-56-6 93
                ,5,6,7,8,9,10,10a-dodecahydro-1,1,
                4a,7-tetramethyl- §§ Pimara-8,15-d
                iene #
                KAURA-5,16-DIEN-18-OL §§ KAURA-5,1 492904 023837-99-2 72
                6-DIEN-18(OR 19)-OL §§ KAURA-5,16-
                DIEN-19-OL
                Kaura-5,16-dien-18(or 19)-ol §§ Ka 492860 023837-99-2 50
                ura-5,16-dien-18-ol #

 34  33.688  0.02 D:\DATABASE\DEMO.L
                4-(N-METHYLAMINO)-6,7-(1,2,3,4-TET 466219 000000-00-0 53
                RAHYDRO-1,1,4,4-TETRAMETHYLBENZO)I
                NDOLE
                2(1H)-PHENANTHRENONE, 3,4,4A,9,10, 466277 016898-96-7 48
                10A-HEXAHYDRO-1,4A-DIMETHYL-7-(1-M
                ETHYLETHYL)-, [1S-(1.ALPHA.,4A.BET
                A.,10A.ALPHA.)]- §§ 18-NORABIETA-8
                ,11,13-TRIENE-3-ONE §§ 2(1H)-PHENA
                NTHRONE, 3,4,4A,9,10,10A-HEXAHYDRO
                -7-ISOPROPYL-1,4A-DIMETHYL-, (1S,4
                AS,10AS)-
                2-(4'-Methoxyphenyl)-2-(2'-methoxy 466153 155726-81-1 38
                phenyl)propane §§ 1-Methoxy-2-[1-(
                4-methoxyphenyl)-1-methylethyl]ben
                zene #
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Pk#     RT  Area%          Library/ID                    Ref#     CAS#   Qual
                trahydronaphthalene #

 39  34.547  0.05 D:\DATABASE\DEMO.L
                2H-1,4-BENZODIAZEPIN-2-ONE, 7-CHLO 481197 000604-75-1 38
                RO-1,3-DIHYDRO-3-HYDROXY-5-PHENYL-
                 §§ (+-)-OXAZEPAM §§ (RS)-OXAZEPAM
                 §§ 1,3-DIHYDRO-7-CHLORO-3-HYDROXY
                -5-PHENYL-2H-1,4-BENZODIAZEPIN-2-O
                NE
                2H-1,4-BENZODIAZEPIN-2-ONE, 7-CHLO 481198 000604-75-1 38
                RO-1,3-DIHYDRO-3-HYDROXY-5-PHENYL-
                 §§ (+-)-OXAZEPAM §§ (RS)-OXAZEPAM
                 §§ 1,3-DIHYDRO-7-CHLORO-3-HYDROXY
                -5-PHENYL-2H-1,4-BENZODIAZEPIN-2-O
                NE
                2H-1,4-BENZODIAZEPIN-2-ONE, 7-CHLO 481190 000604-75-1 38
                RO-1,3-DIHYDRO-3-HYDROXY-5-PHENYL-
                 §§ (+-)-OXAZEPAM §§ (RS)-OXAZEPAM
                 §§ 1,3-DIHYDRO-7-CHLORO-3-HYDROXY
                -5-PHENYL-2H-1,4-BENZODIAZEPIN-2-O
                NE

 40  34.720  0.02 D:\DATABASE\DEMO.L
                3H-[1]BENZOTHIENO[3,2-D]AZONINE-3-   7435 099659-20-8  9
                CARBONITRILE, 1,2,4,5,6,7-HEXAHYDR
                O-7-METHOXY- §§ 7-METHOXY-2,3,4,5,
                6,7-HEXAHYDRO-1H-[1]BENZOTHIENO[3,
                2-D]AZONINE-3-CARBONITRILE
                4-PENTENE(DITHIOIC) ACID, 2-ETHENY    730 107094-82-6  5
                L-3-METHYL-, METHYL ESTER, (R*,R*)
                - §§ METHYL 2-ETHENYL-3-METHYL-4-P
                ENTENEDITHIOATE
                3-TRIDEUTEROMETHOXY-4-METHYL-2(5H)   2514 000000-00-0  4
                -FURANONE

 41  34.785  0.01 D:\DATABASE\DEMO.L
                2-((E)-[((E)-2-([(E)-(2-HYDROXYPHE  45719 000094-91-7 43
                NYL)METHYLIDENE]AMINO)PROPYL)IMINO
                ]METHYL)PHENOL §§ .ALPHA.,.ALPHA.'
                -(1-METHYLETHYLENEDIIMINO)DI-ORTHO
                -CRESOL §§ .ALPHA.,.ALPHA.'-DIPROP
                YLENEDINITRILODI-O-CRESOL §§ ALPHA
                ,ALPHA'-(1-METHYLETHYLENEDIIMINO)D
                I-ORTHO-CRESOL
                MORPHINAN-3,14-DIOL, 4,5-EPOXY-17-  45786 006801-26-9 14
                METHYL-, (5.ALPHA.)- §§ 4,5.ALPHA.
                -EPOXY-17-METHYLMORPHINAN-3,14-DIO
                L §§ MORPHINAN-3,14-DIOL, 4,5-EPOX
                Y-17-METHYL-, (5ALPHA)-
                Morphinan-14-ol, 3-methoxy-17-meth  45783 001639-74-3 14
                yl- §§ (-)-14-Hydroxy-3-methoxy-17
                -methylmorphinan §§ 3-Methoxy-17-m
                ethylmorphinan-14-ol #

 42  34.817  0.01 D:\DATABASE\DEMO.L
                2,4(1H,3H)-Pyrimidinedione, dihydr   4192 001635-26-3  9
                o-5-hydroxy- §§ 5-Hydroxydihydro-2
                ,4(1H,3H)-pyrimidinedione #
                5-HYDROXYDIHYDRO-2,4(1H,3H)-PYRIMI   4196 001635-26-3  9
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Data File : WLM-200c-10prsan-4jm.D
Acq On : 12 Oct 2019 8:49
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Sample :
Misc :
ALS Vial : 2 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			DIMEDIONE §§ 2,4(1H,3H)-PYRIMIDINE DIONE, DIHYDRO-5-HYDROXY- §§ 4,5-D IHYDRO-5-HYDROXY-URACIL			
			.beta.-Chloroethylurea §§ 2-Chloro ethylurea §§ N-(2-Chloroethyl)urea #	4104	006296-42-0	9
43	34.914	0.03	D:\DATABASE\DEMO.L			
			N-(5-Bromo-pyridin-2-yl)-3-phenyl- acrylamide §§ (2E)-N-(5-Bromo-2-py ridinyl)-3-phenyl-2-propenamide #	283383	328119-25-1	18
			1-ETHOXY-2-[(1E)-2-NITRO-1-PROPENY L]BENZENE §§ CIS-2-ETHOXY-.BETA.-M ETHYL-.BETA.-NITROSTYRENE §§ CIS-2 -ETHOXY-BETA-METHYL-BETA-NITROSTYR ENE §§ TRANS-2-ETHOXY-.BETA.-METHY L-.BETA.-NITROSTYRENE	282602	134040-21-4	15
			2,5-CYCLOHEXADIENE-1,4-DIONE, 3-HY DROXY-5-METHOXY-2-(1-OXO-3-PHENYL- 2-PROPENYL)- §§ 2-CINNAMOYL-3-HYDR OXY-5-METHOXY-1,4-BENZOQUINONE	283260	096960-60-0	14
44	35.022	0.03	D:\DATABASE\DEMO.L			
			(3,3-DIMETHOXYPROPYL)BENZENE §§ 1, 1-DIMETHOXY 3-PHENYLPROPANE §§ 1,1 -DIMETHOXY-3-PHENYLPROPANE §§ BENZ ENE, (3,3-DIMETHOXYPROPYL)-	122534	030076-98-3	58
			Benzene, (3,3-dimethoxypropyl)- §§ (3,3-Dimethoxypropyl)benzene #	122522	030076-98-3	58
			(3,3-DIMETHOXYPROPYL)BENZENE §§ 1, 1-DIMETHOXY 3-PHENYLPROPANE §§ 1,1 -DIMETHOXY-3-PHENYLPROPANE §§ BENZ ENE, (3,3-DIMETHOXYPROPYL)-	122536	030076-98-3	58
45	35.125	0.03	D:\DATABASE\DEMO.L			
			KAUR-16-EN-18-OIC ACID §§ KAUR-16- EN-18-OIC ACID, (4.BETA.)- §§ (-)- KAURNENOIC ACID §§ (4-BETA)-KAUR-1 6-EN-18-OIC ACID	168418	020316-84-1	42
			Benzonitrile, m-phenethyl- §§ 3-(2 -Phenylethyl)benzonitrile #	162409	034176-91-5	10
			3-(2-PHENYLETHYL)BENZONITRILE §§ B ENZONITRILE, M-PHENETHYL- §§ 1-(3- CYANOPHENYL)-2-PHENYLETHANE §§ M-C YANO-1,2-DIPHENYLETHANE	162420	034176-91-5	10
46	35.168	0.03	D:\DATABASE\DEMO.L			
			2-((E)-[((E)-2-([(E)-(2-HYDROXYPHE NYL)METHYLIDENE]AMINO)PROPYL)IMINO]METHYL)PHENOL §§ .ALPHA.,.ALPHA.' -(1-METHYLETHYLENEDIIMINO)DI-ORTHO -CRESOL §§ .ALPHA.,.ALPHA.'-DIPROP YLENEDINITRILODI-O-CRESOL §§ ALPHA ,ALPHA'-(1-METHYLETHYLENEDIIMINO)D I-ORTHO-CRESOL	45719	000094-91-7	25
			BUTYL 2-(METHYLAMINO)BENZOATE §§ A NTHRANILIC ACID, N-METHYL-, BUTYL ESTER §§ N-BUTYL O-METHYLAMINOBENZ OATE	209256	015236-34-7	14

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ata Path : F:\DATA MS\daa\
ata File : WLM-200c-10prsan-4jm.D
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isc      :
LS Vial  : 2   Sample Multiplier: 1

earch Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

nknown Spectrum:   Apex
ntegration Events: ChemStation Integrator - autointl.e

     RT  Area%          Library/ID                  Ref#     CAS#   Qual
                                                                      ____
              2-PROPEN-1-ONE, 3-[2-(ACETYLOXY)PH 212026 033777-37-6 12
              ENYL]-1-PHENYL- §§ 2-ACETOXYCHALCO
              NE

  35.303  0.04 D:\DATABASE\DEMO.L
              KAUR-16-EN-18-OIC ACID §§ KAUR-16- 168418 020316-84-1 49
              EN-18-OIC ACID, (4.BETA.)- §§ (-)-
              KAURNENOIC ACID §§ (4-BETA)-KAUR-1
              6-EN-18-OIC ACID
              Phenanthrene, 7-ethenyl-1,2,3,4,4a 165346 026549-04-2 23
              ,4b,5,6,7,8,10,10a-dodecahydro-4a,
              7-dimethyl-1-methylene-, [4aS-(4a.
              alpha.,4a.beta.,7.beta.,10a.beta.)
              ]- §§ 2,4b-Dimethyl-8-methylene-2-
              vinyl-1,2,3,4,4a,4b,5,6,7,8,8a,9-d
              odecahydrophenanthrene #
              2,4B-DIMETHYL-8-METHYLENE-2-VINYL- 165412 026549-04-2 23
              1,2,3,4,4A,4B,5,6,7,8,8A,9-DODECAH
              YDROPHENANTHRENE §§ PHENANTHRENE,
              7-ETHENYL-1,2,3,4,4A,4B,5,6,7,8,10
              ,10A-DODECAHYDRO-4A,7-DIMETHYL-1-M
              ETHYLENE-, [4AS-(4A.ALPHA.,4B.BETA
              .,7.BETA.,10A.BETA.)]-

  35.384  0.05 D:\DATABASE\DEMO.L
              Ketone, isopropylidenecyclopropyl  226907 029765-67-1 47
              methyl §§ 1-[2-(1-Methylethylidene
              )cyclopropyl]ethanone #
              p-Heptyloxyaniline §§ 4-n-Heptylox 228109 039905-44-7 46
              yaniline
              3-Aminophenyl-.beta.-phenylpropion 228628 999228-63-1 43
              ate

  35.481  1.07 D:\DATABASE\DEMO.L
              BENZ[A]ANTHRACENONE                513655 099707-96-7 83
              Xanthen-9-one, 1-hydroxy-3,5,8-tri 504583 049599-09-9 48
              methoxy- §§ 5,8-Dimethylbellidifol
              in §§ 1-Hydroxy-3,5,8-trimethoxyxa
              nthen-9-one §§ 1-Hydroxy-3,5,8-tri
              methoxy-9H-xanthen-9-one #
              PINE ROSIN MIXTURE                 504612 000000-00-0 38

  35.665  0.14 D:\DATABASE\DEMO.L
              1H-Indole-3-carboxylic acid, 1-cyc 504368 999504-38-0 43
              lopentyl-5-hydroxy-2-methyl-, ethy
              l ester
              1-PHENANTHRENECARBOXYLIC ACID, 7-E 466436 005835-26-7 35
              THENYL-1,2,3,4,4A,4B,5,6,7,8,10,10
              A-DODECAHYDRO-1,4A,7-TRIMETHYL-, [
              1R-(1.ALPHA.,4A.BETA.,4B.ALPHA.,7.
              ALPHA.,10A.ALPHA.)]- §§ ISOPIMARIC
               ACID §§ PODOCARP-7-EN-15-OIC ACID
              , 13.BETA.-METHYL-13-VINYL-
              Palustric acid §§ Podocarpa-8,13-d 513439 001945-53-5 35
              ien-15-oic acid, 13-isopropyl- §§
              1-Phenanthrenecarboxylic acid, 1,2
              ,3,4,4a,5,6,9,10,10a-decahydro-1,4
              a-dimethyl-7-(1-methylethyl)-, (1R
              -(1.alpha.,4a.beta.,10a.alpha.))-
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Data File : WLM-200c-10prean-4jm.D
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Operator  :
Sample    :
Misc      :
ALS Vial  : 2   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autointl.e

Peak#     RT  Area%          Library/ID                    Ref#     CAS#   Qual
                §§ 8,13-Abietadien-18-oic acid

51   35.752  0.26 D:\DATABASE\DEMO.L
                DEHYDROABIETIC ACID                     464556 000000-00-0 97
                METHYL ABIETA-8,11,13-TRIEN-18-OAT      464550 001235-74-1 96
                E §§ 1-PHENANTHRENECARBOXYLIC ACID
                , 1,2,3,4,4A,9,10,10A-OCTAHYDRO-1,
                4A-DIMETHYL-7-(1-METHYLETHYL)-, ME
                THYL ESTER, [1R-(1.ALPHA.,4A.BETA.
                ,10A.ALPHA.)]- §§ DEHYDROABIETIC A
                CID METHYL ESTER §§ METHYL DEHYDRO
                ABIETATE
                1-Phenanthrenecarboxylic acid, 1,2      464538 001235-74-1 96
                ,3,4,4a,9,10,10a-octahydro-1,4a-di
                methyl-7-(1-methylethyl)-, methyl
                ester, [1R-(1.alpha.,4a.beta.,10a.
                alpha.)]- §§ Podocarpa-8,11,13-tri
                en-15-oic acid, 13-isopropyl-, met
                hyl ester §§ Methyl dehydroabietat

52   35.897  0.19 D:\DATABASE\DEMO.L
                2-BUTYL-5-HEXYLINDANE §§ INDAN, 2-      398768 025446-32-6 55
                BUTYL-5-HEXYL- §§ 2-N-BUTYL-1-N-HE
                XYL-2,3-DIHYDROINDENE §§ 2-N-BUTYL
                -5-N-HEXYL-(2,3-DIHYDROINDENE)
                Indan, 2-butyl-5-hexyl- §§ 2-n-But      398758 025446-32-6 55
                yl-5-n-hexyl-(2,3-dihydroindene) §
                § 2-n-Butyl-5-n-hexylindan §§ 2-Bu
                tyl-5-hexylindane #
                1,1'-BIS(SPIRO[2.4]HEPTYLIDENE)         161353 000000-00-0 53

53   36.081  0.25 D:\DATABASE\DEMO.L
                1H-NAPHTHO[2,3-C]PYRAN-5,10-DIONE,      513558 084018-43-9 91
                 3,4-DIHYDRO-7,9-DIMETHOXY-1,3-DIM
                ETHYL-, CIS-(.+-.)- §§ (+,-)-CIS-7
                ,9-DIMETHOXY-1,3-DIMETHYL-3,4,5,10
                -TETRAHYDRONAPHTHO[2,3-C]PYRAN-5,1
                0-DIONE
                Pimaric acid §§ 1-Phenanthrenecarb      466434 000127-27-5 60
                oxylic acid, 7-ethenyl-1,2,3,4,4a,
                4b,5,6,7,9,10,10a-dodecahydro-1,4a
                ,7-trimethyl-, [1R-(1.alpha.,4a.be
                ta.,4b.alpha.,7.beta.,10a.alpha.)]
                - §§ Podocarp-8(14)-en-15-oic acid
                , 13.alpha.-methyl-13-vinyl- §§ D-
                pimaric acid
                Palustric acid §§ Podocarpa-8,13-d      513439 001945-53-5 49
                ien-15-oic acid, 13-isopropyl- §§
                1-Phenanthrenecarboxylic acid, 1,2
                ,3,4,4a,5,6,9,10,10a-decahydro-1,4
                a-dimethyl-7-(1-methylethyl)-, [1R
                -(1.alpha.,4a.beta.,10a.alpha.)]-
                §§ 8,13-Abietadien-18-oic acid

54   36.254  0.13 D:\DATABASE\DEMO.L
                1,4-DIHYDRO-9-ISOPROPYLIDENE-5,6,7      513581 000000-00-0 90
                ,8-TETRAMETHOXY-1,4-METHANONAPHTHA
                LENE
                Pimaric acid §§ 1-Phenanthrenecarb      504569 000127-27-5 55
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Data File : WLM-200c-10prean-4jm.D
Acq On : 12 Oct 2019 8:49
Operator :
Sample :
Misc :
ALS Vial : 2 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			oxylic acid, 7-ethenyl-1,2,3,4,4a, 4b,5,6,7,9,10,10a-dodecahydro-1,4a ,7-trimethyl-, [1R-(1.alpha.,4a.be ta.,4b.alpha.,7.beta.,10a.alpha.)] - §§ Podocarp-8(14)-en-15-oic acid , 13.alpha.-methyl-13-vinyl- §§ D- pimaric acid			
			Palustric acid §§ Podocarpa-8,13-d ien-15-oic acid, 13-isopropyl- §§ 1-Phenanthrenecarboxylic acid, 1,2 ,3,4,4a,5,6,9,10,10a-decahydro-1,4 a-dimethyl-7-(1-methylethyl)-, (1R -(1.alpha.,4a.beta.,10a.alpha.))- §§ 8,13-Abietadien-18-oic acid	513439	001945-53-5	46
55	36.378	0.16	D:\DATABASE\DEMO.L			
			17-NORKAUR-9(11)-EN-18-OIC ACID, 1 6-OXO-, METHYL ESTER, (4.ALPHA.)- §§ 16-OXO-17-NOR-9(11)-KAUREN-18-C ARBOXYLIC ACID-METHYLESTER §§ 1H-2 ,10A-ETHANOPHENANTHRENE, 17-NORKAU R-9(11)-EN-18-OIC ACID DERIV.	466510	063558-42-9	50
			Androst-2,16-diene	466169	999466-17-7	48
			10,13-DIMETHYL-4,5,6,7,8,9,10,11,1 2,13,14,15-DODECAHYDRO-1H-CYCLOPEN TA[A]PHENANTHRENE §§ ANDROSTA-2,16 -DIENE	466180	999466-18-8	48
56	36.497	0.13	D:\DATABASE\DEMO.L			
			1,4-DIHYDRO-9-ISOPROPYLIDENE-5,6,7 ,8-TETRAMETHOXY-1,4-METHANONAPHTHA LENE	513581	000000-00-0	90
			1H-NAPHTHO[2,3-C]PYRAN-5,10-DIONE, 3,4-DIHYDRO-7,9-DIMETHOXY-1,3-DIM ETHYL-, CIS-(.+-.)- §§ (+,-)-CIS-7 ,9-DIMETHOXY-1,3-DIMETHYL-3,4,5,10 -TETRAHYDRONAPHTHO[2,3-C]PYRAN-5,1 0-DIONE	513558	084018-43-9	72
			18-NOR-16-OXAANDROSTA-13(17),14-DI ENE-4-METHANOL, 4,8-DIMETHYL-, (4. BETA.,5.ALPHA.)- §§ PHENANTHRO[1,2 -C]FURAN, 18-NOR-16-OXAANDROSTA-13 (17),14-DIENE-4-METHANOL DERIV. §§ SPONGIA-13(16),14-DIEN-19-OL	513649	074804-02-7	49
57	36.600	0.29	D:\DATABASE\DEMO.L			
			O-HYDROGEN PERDEUTERIO HEXADECANOI C ACID	504545	039756-30-4	90
			KAUR-16-EN-18-OIC ACID §§ KAUR-16- EN-18-OIC ACID, (4.BETA.)- §§ (-)- KAURNENOIC ACID §§ (4-BETA)-KAUR-1 6-EN-18-OIC ACID	168418	020316-84-1	90
			Phenol, 2,4-bis(1-phenylethyl)- §§ 2,4-Bis(1-phenylethyl)phenol #	504578	002769-94-0	89
58	36.740	0.44	D:\DATABASE\DEMO.L			
			Abietic acid §§ 1-Phenanthrenecarb oxylic acid, 1,2,3,4,4a,4b,5,6,10, 10a-decahydro-1,4a-dimethyl-7-(1-m	513344	000514-10-3	70

Data Path : F:\DATA MS\daa\
Data File : WLM-200c-10prsan-4jm.D
Acq On : 12 Oct 2019 8:49
Operator :
Sample :
Misc :
ALS Vial : 2 Sample Multiplier: 1

Search Libraries: D:\DATABASE\DEMO.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autointl.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			ethylethyl)-, [1R-(1.alpha.,4a.beta.,4b.alpha.,10a.alpha.)]- §§ Podocarpa-7,13-dien-15-oic acid, 13-isopropyl- §§ L-abietic acid			
			Abietic acid §§ 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,4b,5,6,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1R-(1.alpha.,4a.beta.,4b.alpha.,10a.alpha.)]- §§ Podocarpa-7,13-dien-15-oic acid, 13-isopropyl- §§ L-abietic acid	513378	000514-10-3	55
			3-ACETYL-1-METHYL-2-(1'-METHYL-1H-INDOL-2'-YL)-1H-INDOLE	513641	000000-00-0	51
59	36.972	0.55	D:\DATABASE\DEMO.L			
			ABIETA-8,11,13-TRIEN-18-OIC ACID §§ PODOCARPA-8,11,13-TRIEN-15-SAEURE, 13-ISOPROPYL-	503106	999503-11-8	99
			1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,9,10,10A-OCTAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL)-, [1R-(1.ALPHA.,4A.BETA.,10A.ALPHA.)]- §§ (-)-DEHYDROABIETIC ACID §§ 1,2,3,4,4A,9,10,10A-OCTAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL)-1-PHENANTHRENECARBOXYLIC ACID	503110	001740-19-8	99
			1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1R-(1.alpha.,4a.beta.,10a.alpha.)]- §§ Podocarpa-8,11,13-trien-15-oic acid, 13-isopropyl- §§ Abieta-8,11,13-trien-18-oic acid §§ Abietic acid, dehydro-	503093	001740-19-8	99
60	37.032	0.77	D:\DATABASE\DEMO.L			
			ABIETA-8,11,13-TRIEN-18-OIC ACID §§ PODOCARPA-8,11,13-TRIEN-15-SAEURE, 13-ISOPROPYL-	503106	999503-11-8	94
			1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1R-(1.alpha.,4a.beta.,10a.alpha.)]- §§ Podocarpa-8,11,13-trien-15-oic acid, 13-isopropyl- §§ Abieta-8,11,13-trien-18-oic acid §§ Abietic acid, dehydro-	503093	001740-19-8	83
			Ethyl 4-hydroxy-7-trifluoromethyl-3-quinolinecarboxylate §§ 3-Quinolinecarboxylic acid, 4-hydroxy-7-(trifluoromethyl)-, ethyl ester	464415	000391-02-6	72
61	37.221	0.49	D:\DATABASE\DEMO.L			
			Abietic acid §§ 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,4b,5,6,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1R-(1.alpha.,4a.beta.,4b.alpha.,10a.alpha.)]- §§ Podocarpa-7,13-dien-15-oic acid, 13-is	513378	000514-10-3	93

Data Path : F:\DATA MS\daa\
Data File : WLM-200c-10prsan-4jm.D
Acq On : 12 Oct 2019 8:49
Operator :
Sample :
Misc :
ALS Vial : 2 Sample Multiplier: 1

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Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autointl.e

k#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			opropyl- §§ L-abietic acid			
			1-PHENANTHRENECARBOXYLIC ACID, 1,2	503110	001740-19-8	92
			,3,4,4A,9,10,10A-OCTAHYDRO-1,4A-DI			
			METHYL-7-(1-METHYLETHYL)-, [1R-(1.			
			ALPHA.,4A.BETA.,10A.ALPHA.)]- §§ (			
			-)-DEHYDROABIETIC ACID §§ 1,2,3,4,			
			4A,9,10,10A-OCTAHYDRO-1,4A-DIMETHY			
			L-7-(1-METHYLETHYL)-1-PHENANTHRENE			
			CARBOXYLIC ACID			
			1-Phenanthrenecarboxylic acid, 1,2	503093	001740-19-8	92
			,3,4,4a,9,10,10a-octahydro-1,4a-di			
			methyl-7-(1-methylethyl)-, [1R-(1.			
			alpha.,4a.beta.,10a.alpha.)]- §§ P			
			odocarpa-8,11,13-trien-15-oic acid			
			, 13-isopropyl- §§ Abieta-8,11,13-			
			trien-18-oic acid §§ Abietic acid,			
			dehydro-			
52	37.675	2.42	D:\DATABASE\DEMO.L			
			Abietic acid §§ 1-Phenanthrenecarb	513378	000514-10-3	99
			oxylic acid, 1,2,3,4,4a,4b,5,6,10,			
			10a-decahydro-1,4a-dimethyl-7-(1-m			
			ethylethyl)-, [1R-(1.alpha.,4a.bet			
			a.,4b.alpha.,10a.alpha.)]- §§ Podo			
			carpa-7,13-dien-15-oic acid, 13-is			
			opropyl- §§ L-abietic acid			
			Abietic acid §§ 1-Phenanthrenecarb	513344	000514-10-3	93
			oxylic acid, 1,2,3,4,4a,4b,5,6,10,			
			10a-decahydro-1,4a-dimethyl-7-(1-m			
			ethylethyl)-, [1R-(1.alpha.,4a.bet			
			a.,4b.alpha.,10a.alpha.)]- §§ Podo			
			carpa-7,13-dien-15-oic acid, 13-is			
			opropyl- §§ L-abietic acid			
			Abietic acid §§ 1-Phenanthrenecarb	513347	000514-10-3	90
			oxylic acid, 1,2,3,4,4a,4b,5,6,10,			
			10a-decahydro-1,4a-dimethyl-7-(1-m			
			ethylethyl)-, [1R-(1.alpha.,4a.bet			
			a.,4b.alpha.,10a.alpha.)]- §§ Podo			
			carpa-7,13-dien-15-oic acid, 13-is			
			opropyl- §§ L-abietic acid			
53	38.480	0.19	D:\DATABASE\DEMO.L			
			.beta.-Pimaric acid §§ .delta.6,8(	513374	000079-54-9	94
			14)-Abietadienoic acid §§ l-Pimari			
			c acid §§ l-Sapietic acid			
			Abietic acid §§ 1-Phenanthrenecarb	513378	000514-10-3	92
			oxylic acid, 1,2,3,4,4a,4b,5,6,10,			
			10a-decahydro-1,4a-dimethyl-7-(1-m			
			ethylethyl)-, [1R-(1.alpha.,4a.bet			
			a.,4b.alpha.,10a.alpha.)]- §§ Podo			
			carpa-7,13-dien-15-oic acid, 13-is			
			opropyl- §§ L-abietic acid			
			Abietic acid §§ 1-Phenanthrenecarb	513347	000514-10-3	86
			oxylic acid, 1,2,3,4,4a,4b,5,6,10,			
			10a-decahydro-1,4a-dimethyl-7-(1-m			
			ethylethyl)-, [1R-(1.alpha.,4a.bet			
			a.,4b.alpha.,10a.alpha.)]- §§ Podo			
			carpa-7,13-dien-15-oic acid, 13-is			
			opropyl- §§ L-abietic acid			

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Data Path : F:\DATA MS\daa\
Data File : WLM-200c-10prsan-4jm.D
Acq On    : 12 Oct 2019    8:49
Operator  :
Sample    :
Misc      :
ALS Vial  : 2   Sample Multiplier: 1

Search Libraries:   D:\DATABASE\DEMO.L                Minimum Quality:   0

Unknown Spectrum:   Apex
Integration Events: ChemStation Integrator - autointl.e

Pk#     RT  Area%          Library/ID                  Ref#     CAS#   Qual
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64  39.020  0.06 D:\DATABASE\DEMO.L
                 Abietic acid §§ 1-Phenanthrenecarb 513378 000514-10-3 84
                 oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                 10a-decahydro-1,4a-dimethyl-7-(1-m
                 ethylethyl)-, [1R-(1.alpha.,4a.bet
                 a.,4b.alpha.,10a.alpha.)]- §§ Podo
                 carpa-7,13-dien-15-oic acid, 13-is
                 opropyl- §§ L-abietic acid
                 Abietic acid §§ 1-Phenanthrenecarb 513344 000514-10-3 80
                 oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                 10a-decahydro-1,4a-dimethyl-7-(1-m
                 ethylethyl)-, [1R-(1.alpha.,4a.bet
                 a.,4b.alpha.,10a.alpha.)]- §§ Podo
                 carpa-7,13-dien-15-oic acid, 13-is
                 opropyl- §§ L-abietic acid
                 Abietic acid §§ 1-Phenanthrenecarb 513347 000514-10-3 70
                 oxylic acid, 1,2,3,4,4a,4b,5,6,10,
                 10a-decahydro-1,4a-dimethyl-7-(1-m
                 ethylethyl)-, [1R-(1.alpha.,4a.bet
                 a.,4b.alpha.,10a.alpha.)]- §§ Podo
                 carpa-7,13-dien-15-oic acid, 13-is
                 opropyl- §§ L-abietic acid
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Lampiran 7. Dokumentasi