Supporting Information

Non-antimicrobial and non-anticancer properties of ZnO nanoparticles biosynthesized using different plant parts of *Bixa orellana*

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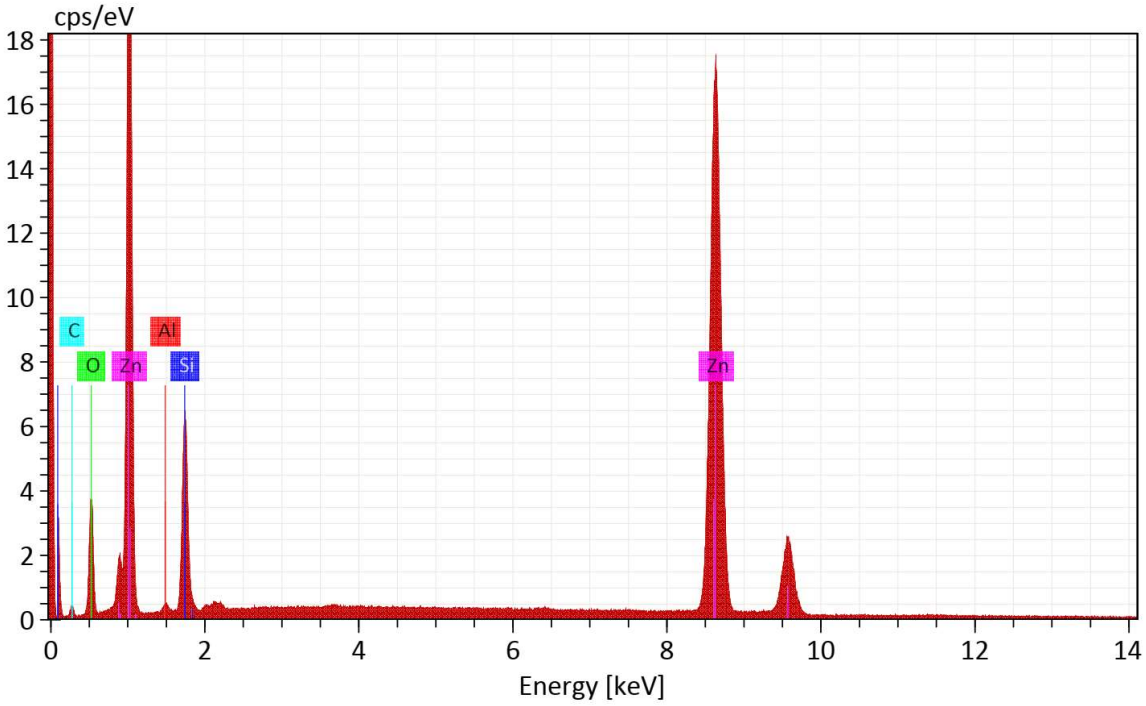
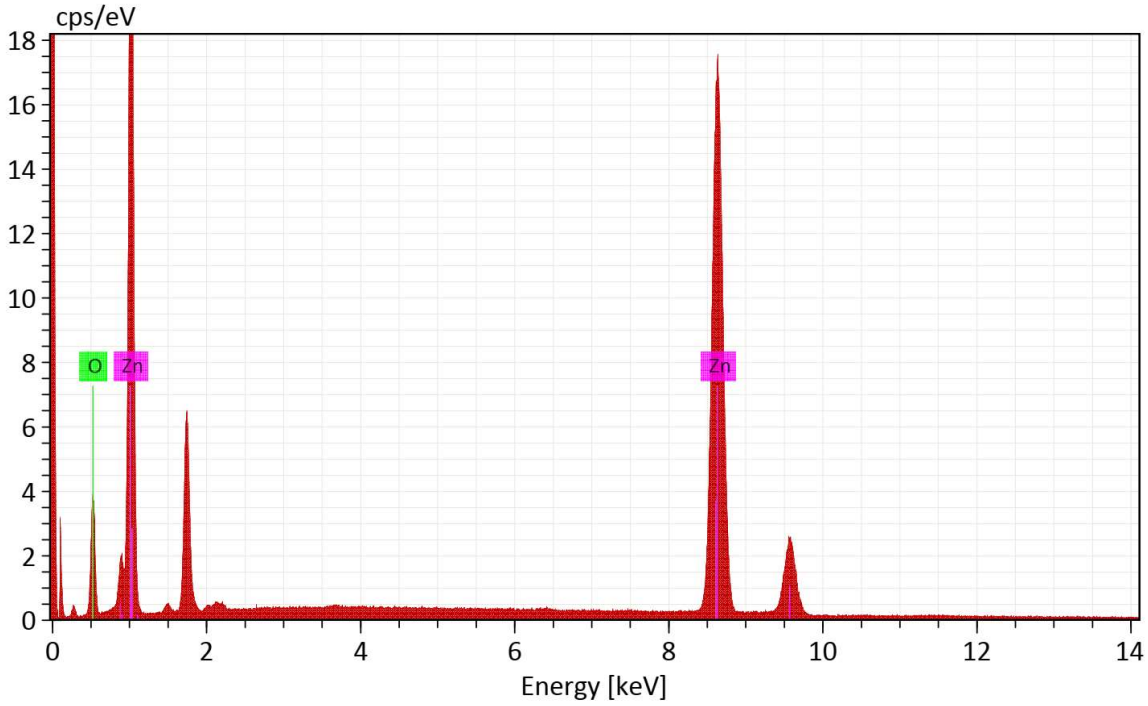
‡Saee Gharpure and Rachana Yadwade have equal contribution in this research.

(a)

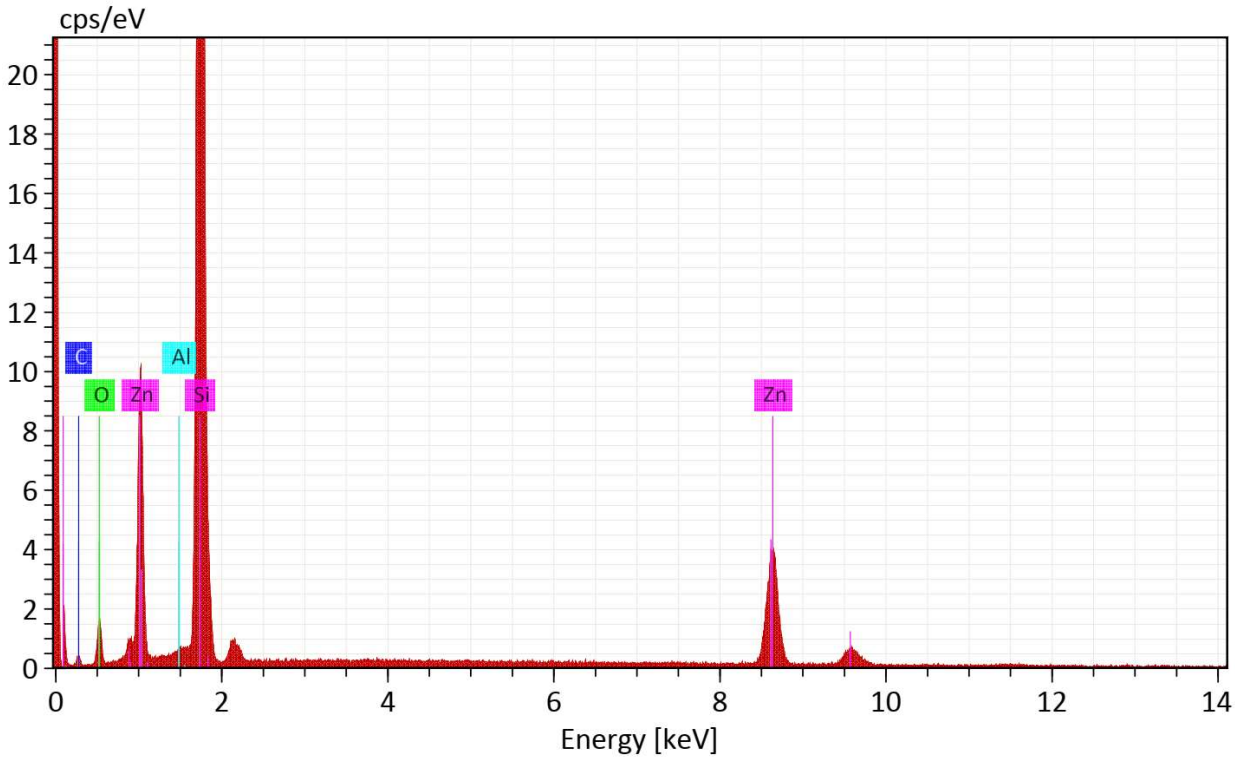


Element	At. No.	Netto	Mass [%]	Mass Norm. [%]	Atom [%]	abs. error [%] (1 sigma)	rel. error [%] (1 sigma)
Oxygen	8	24020	16.41	17.22	36.12	2.09	12.73
Zinc	30	336517	60.18	63.16	32.42	1.49	2.48
Carbon	6	2281	4.75	4.99	13.94	0.90	18.90
Aluminium	13	1637	0.58	0.61	0.76	0.06	10.49
Silicon	14	55810	13.36	14.02	16.76	0.62	4.67
		Sum	**95.28**	**100.00**	**100.00**		

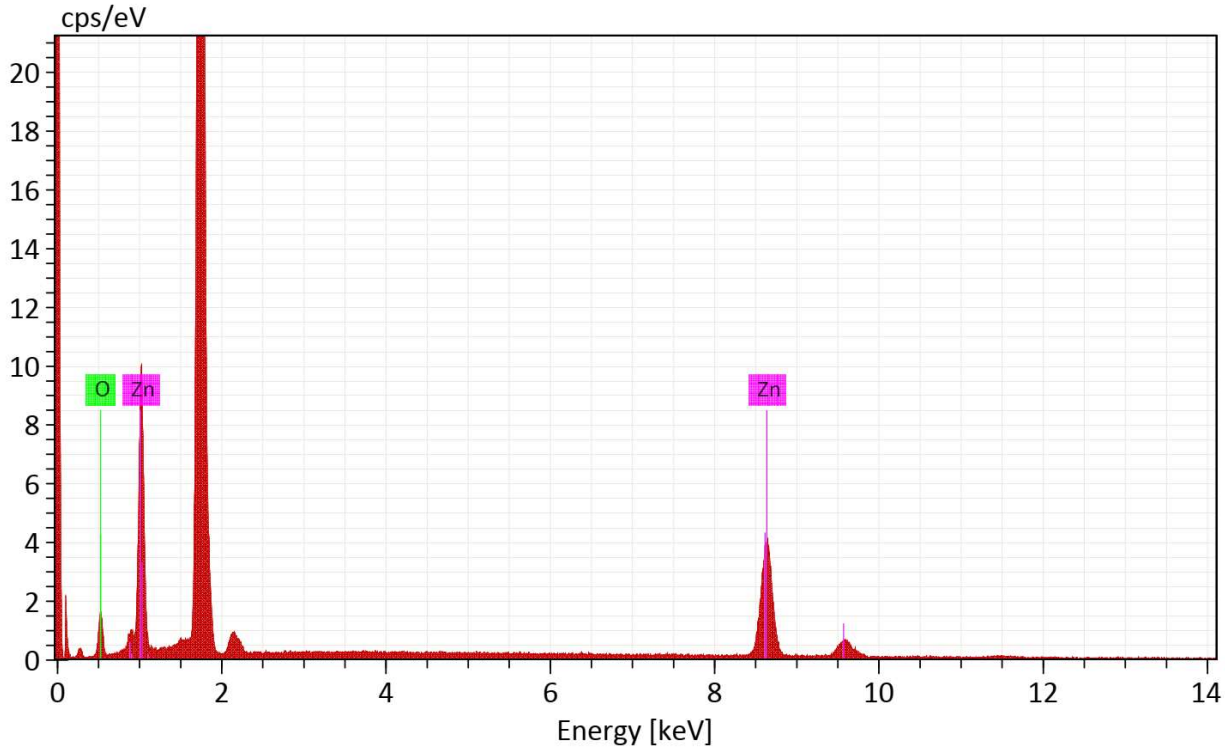


Element	At. No.	Netto	Mass [%]	Mass Norm. [%]	Atom [%]	abs. error [%] (1 sigma)	rel. error [%] (1 sigma)
Oxygen	8	23908	15.26	18.52	48.16	1.95	12.75
Zinc	30	336555	67.13	81.48	51.84	1.66	2.48
		Sum	**82.39**	**100.00**	**100.00**		

(b)

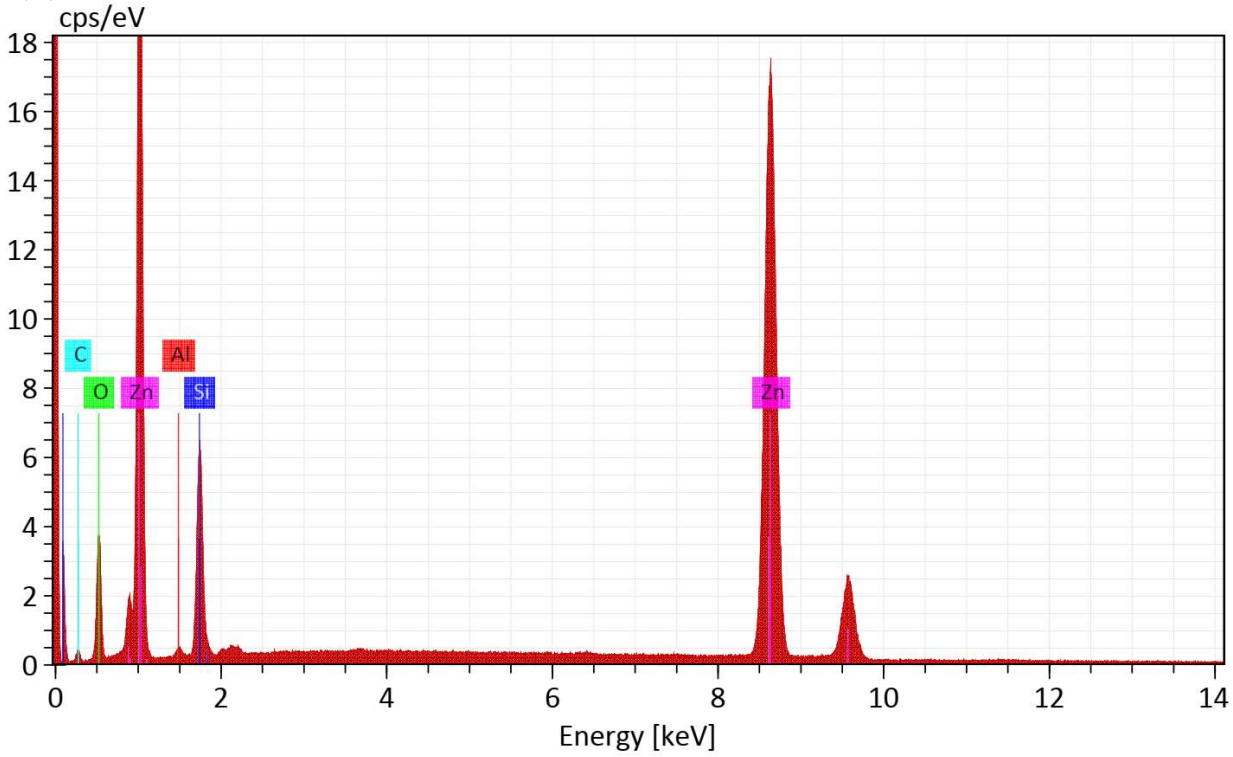


Element	At. No.	Netto	Mass [%]	Mass Norm. [%]	Atom [%]	abs. error [%] (1 sigma)	rel. error [%] (1 sigma)
Oxygen	8	5926	12.12	11.30	17.75	1.87	15.40
Zinc	30	44745	15.57	14.51	5.57	0.41	2.65
Carbon	6	1468	9.24	8.62	18.02	1.91	20.71
Silicon	14	373601	70.35	65.57	58.66	3.15	4.48
		Sum	**107.28**	**100.00**	**100.00**		

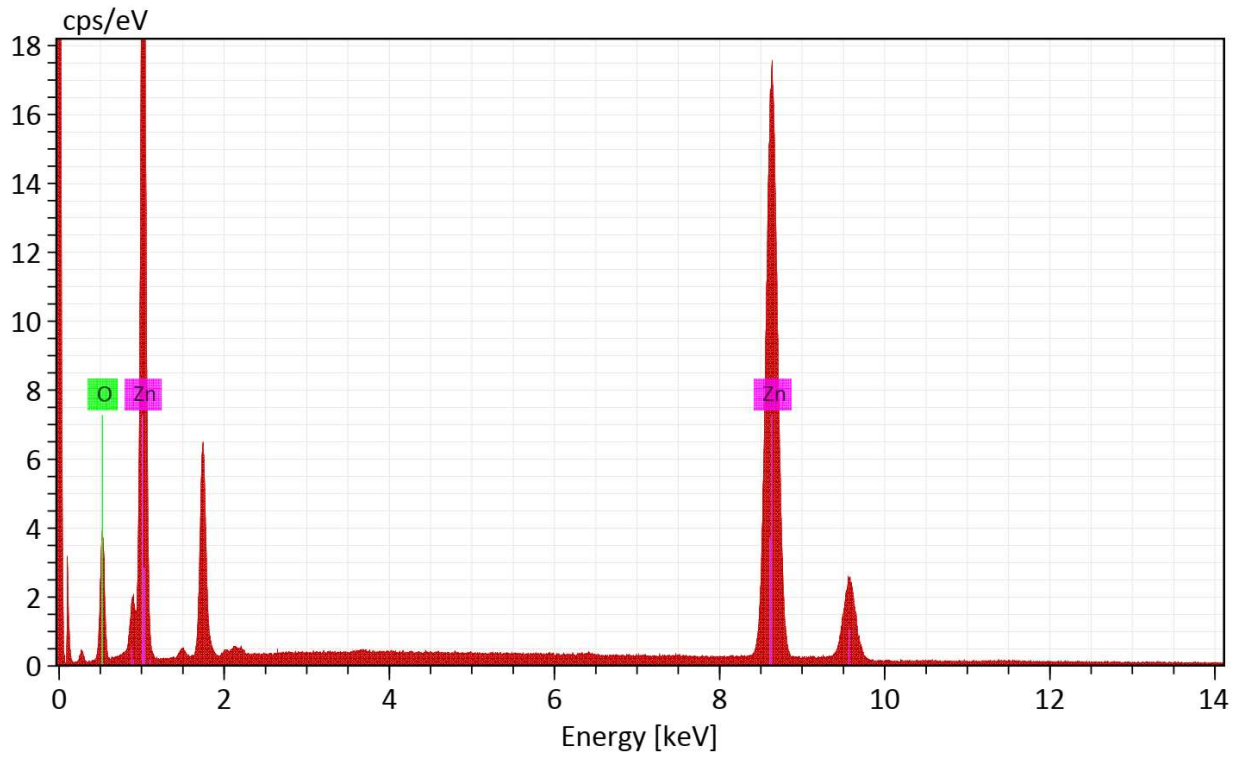


Element	At. No.	Netto	Mass [%]	Mass Norm. [%]	Atom [%]	abs. error [%] (1 sigma)	rel. error [%] (1 sigma)
Oxygen	8	5817	8.51	27.69	61.01	1.32	15.54
Zinc	30	44747	22.23	72.31	38.99	0.58	2.60
		Sum	**30.74**	**100.00**	**100.00**		

(c)



Element	At. No.	Netto	Mass [%]	Mass Norm. [%]	Atom [%]	abs. error [%] (1 sigma)	rel. error [%] (1 sigma)
Oxygen	8	24020	16.41	17.22	36.12	2.09	12.73
Zinc	30	336517	60.18	63.16	32.42	1.49	2.48
Carbon	6	2281	4.75	4.99	13.94	0.90	18.90
Aluminium	13	1637	0.58	0.61	0.76	0.06	10.49
Silicon	14	55810	13.36	14.02	16.76	0.62	4.67
		Sum	**95.28**	**100.00**	**100.00**		



Element	At. No.	Netto	Mass [%]	Mass Norm. [%]	Atom [%]	abs. error [%] (1 sigma)	rel. error [%] (1 sigma)
Oxygen	8	23908	15.26	18.52	48.16	1.95	12.75
Zinc	30	336555	67.13	81.48	51.84	1.66	2.48
		Sum	**82.39**	**100.00**	**100.00**		

Figure SI-1. EDS spectra of L-ZnO (a), S-ZnO (b) and Sc-ZnO (c) in auto mode as well as only for zinc and oxygen

(a)

Library Search

<< Target >>

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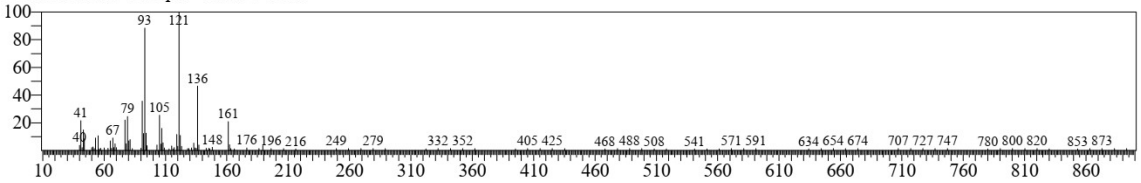
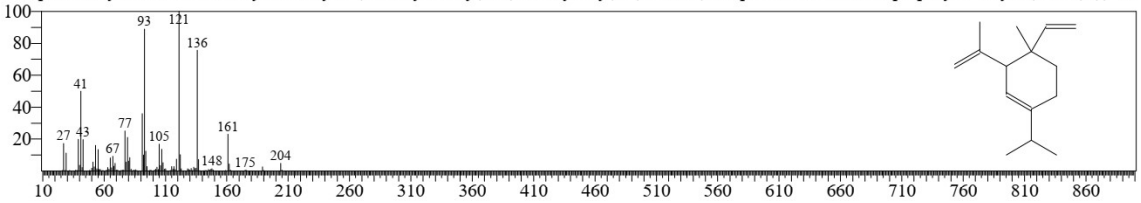


Hit#:1 Entry:46695 Library:NIST11.lib

SI:92 Formula:C15H24 CAS:20307-84-0 MolWeight:204 RetIndex:1377

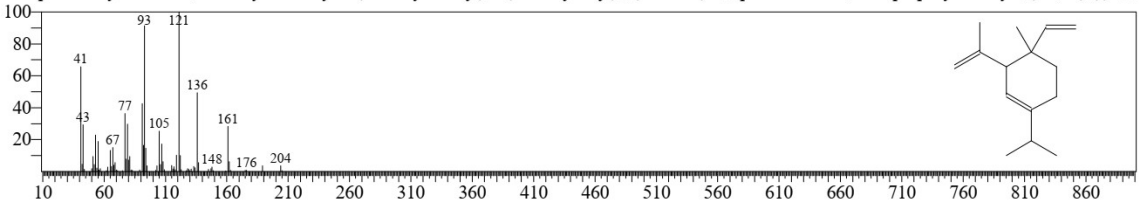
CompName:Cyclohexene, 4-ethenyl-4-methyl-3-(1-methylethenyl)-1-(1-methylethyl)-, (3R-trans)- $$ p-Menth-3-ene, 2-isopropenyl-1-vinyl-, (1S,2R)-(-)- $$



Hit#:2 Entry:18110 Library:NIST11s.lib

SI:91 Formula:C15H24 CAS:20307-84-0 MolWeight:204 RetIndex:1377

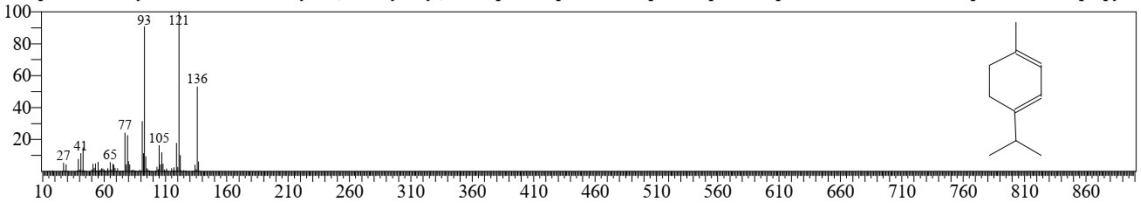
CompName:Cyclohexene, 4-ethenyl-4-methyl-3-(1-methylethenyl)-1-(1-methylethyl)-, (3R-trans)- $$ p-Menth-3-ene, 2-isopropenyl-1-vinyl-, (1S,2R)-(-)- $$



Hit#:3 Entry:6679 Library:NIST11s.lib

SI:90 Formula:C10H16 CAS:99-86-5 MolWeight:136 RetIndex:998

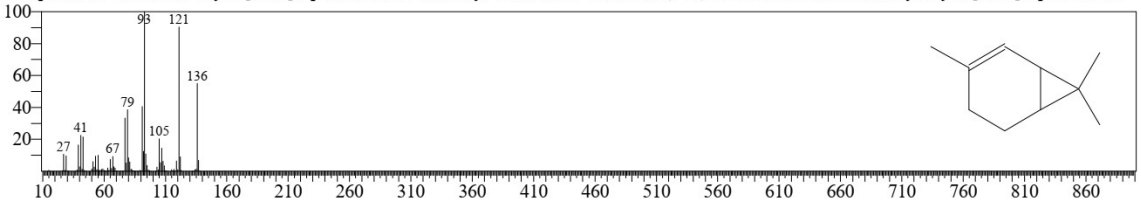
CompName:1,3-Cyclohexadiene, 1-methyl-4-(1-methylethyl)- $$ .alpha.-Terpinene $$ .alpha.-Terpinen $$ p-Mentha-1,3-diene $$ Terpilene $$ 1-Isopropyl-4



Hit#:4 Entry:9826 Library:NIST11.lib

SI:90 Formula:C10H16 CAS:554-61-0 MolWeight:136 RetIndex:948

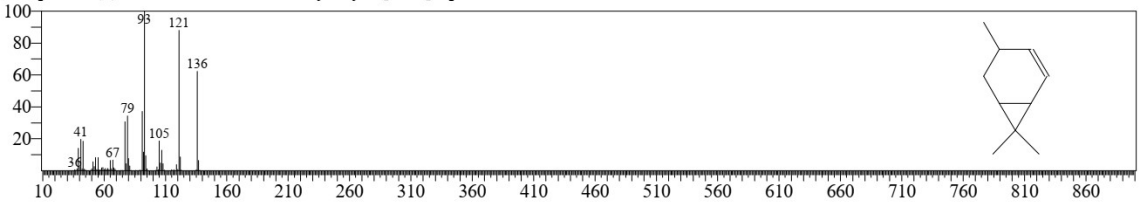
CompName:2-Carene $$ Bicyclo[4.1.0]hept-2-ene, 3,7,7-trimethyl- $$ .delta.-2-Carene $$ (.+/-.)-2-Carene $$ 3,7,7-Trimethylbicyclo[4.1.0]hept-2-ene $$



Hit#:5 Entry:9827 Library:NIST11.lib

SI:89 Formula:C10H16 CAS:29050-33-7 MolWeight:136 RetIndex:919

CompName:(+)-4-Carene $$ 4,7,7-Trimethylbicyclo[4.1.0]hept-2-ene # $$



Library Search

<< Target >>

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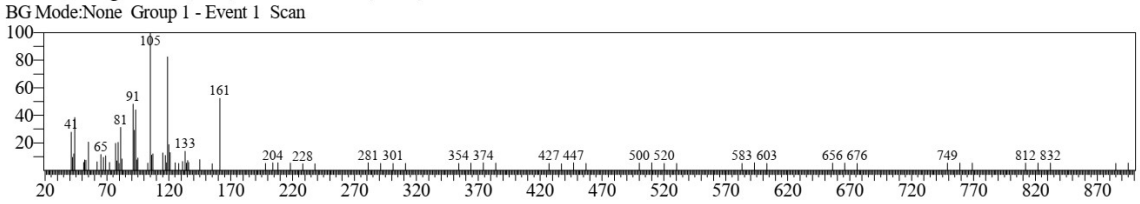
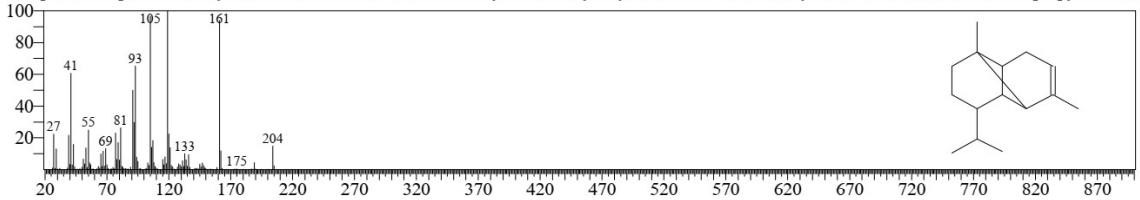


Hit#:1 Entry:18104 Library:NIST11s.lib

SI:83 Formula:C15H24 CAS:3856-25-5 MolWeight:204 RetIndex:1221

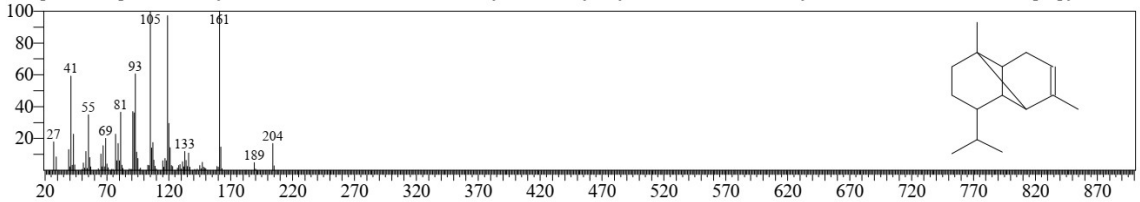
CompName:Copaene $$ Tricyclo[4.4.0.02,7]dec-3-ene, 1,3-dimethyl-8-(1-methylethyl)-, stereoisomer $$ Tricyclo[4.4.0.02,7]dec-3-ene, 8-isopropyl-1,3-din



Hit#:2 Entry:18133 Library:NIST11s.lib

SI:83 Formula:C15H24 CAS:3856-25-5 MolWeight:204 RetIndex:1221

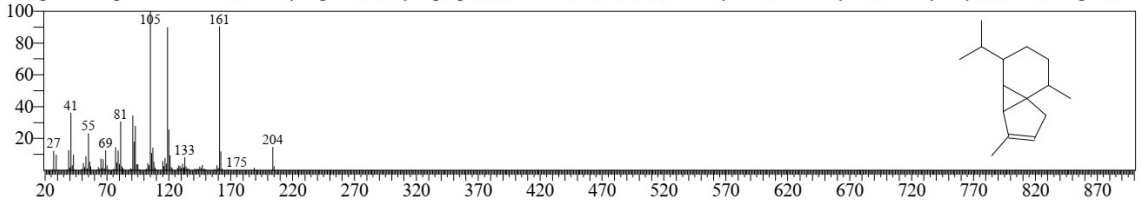
CompName:Copaene $$ Tricyclo[4.4.0.02,7]dec-3-ene, 1,3-dimethyl-8-(1-methylethyl)-, stereoisomer $$ Tricyclo[4.4.0.02,7]dec-3-ene, 8-isopropyl-1,3-din



Hit#:3 Entry:18090 Library:NIST11s.lib

SI:82 Formula:C15H24 CAS:17699-14-8 MolWeight:204 RetIndex:1344

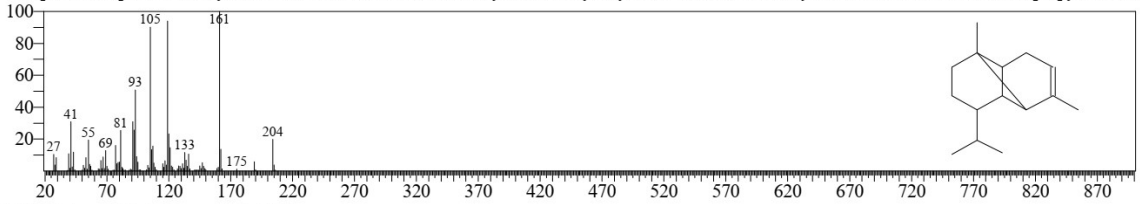
CompName:.alpha.-Cubebene $$ 1H-Cyclopenta[1,3]cyclopropa[1,2]benzene, 3a,3b,4,5,6,7-hexahydro-3,7-dimethyl-4-(1-methylethyl)-, [3aS-(3a.alpha.,3b.



Hit#:4 Entry:46736 Library:NIST11.lib

SI:81 Formula:C15H24 CAS:3856-25-5 MolWeight:204 RetIndex:1221

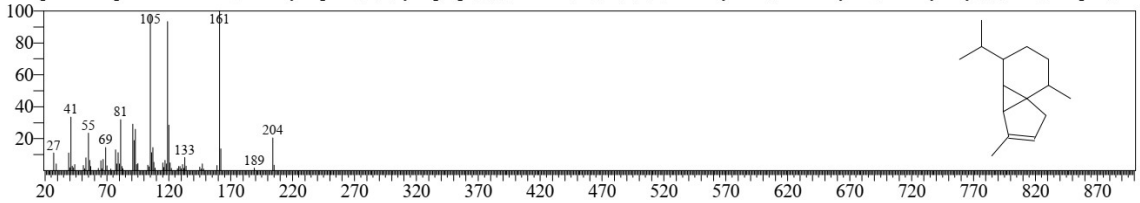
CompName:Copaene $$ Tricyclo[4.4.0.02,7]dec-3-ene, 1,3-dimethyl-8-(1-methylethyl)-, stereoisomer $$ Tricyclo[4.4.0.02,7]dec-3-ene, 8-isopropyl-1,3-din



Hit#:5 Entry:46726 Library:NIST11.lib

SI:81 Formula:C15H24 CAS:17699-14-8 MolWeight:204 RetIndex:1344

CompName:.alpha.-Cubebene $$ 1H-Cyclopenta[1,3]cyclopropa[1,2]benzene, 3a,3b,4,5,6,7-hexahydro-3,7-dimethyl-4-(1-methylethyl)-, [3aS-(3a.alpha.,3b.



Library Search

<< Target >>

Line#:1 R.Time:13.785(Scan#:2758) MassPeaks:55

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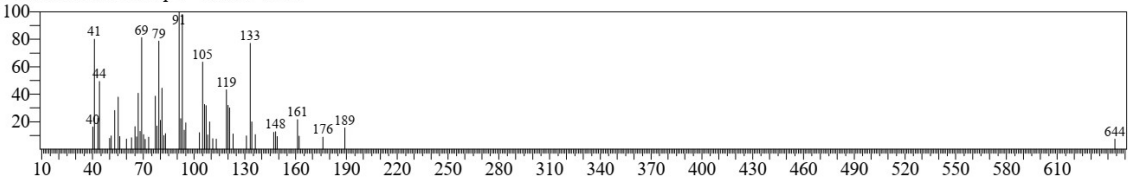
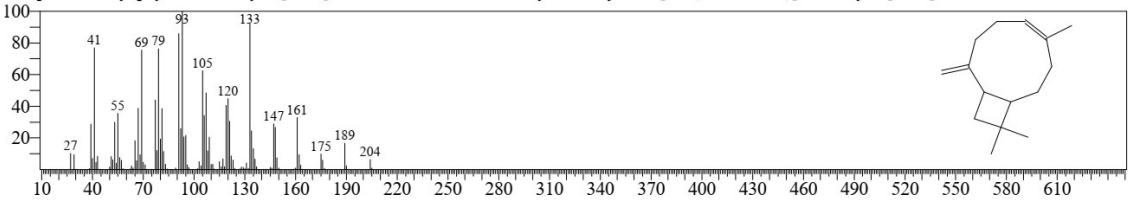


Hit#:1 Entry:46636 Library:NIST11.lib

SI:90 Formula:C15H24 CAS:87-44-5 MolWeight:204 RetIndex:1494

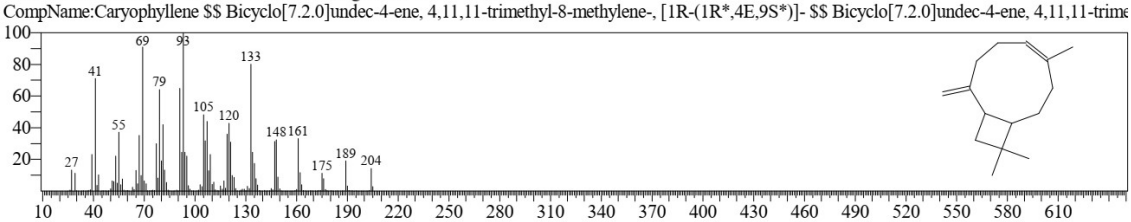
CompName:Caryophyllene $$ Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-, [1R-(1R*,4E,9S*)]- $$ Bicyclo[7.2.0]undec-4-ene, 4,11,11-trime



Hit#:2 Entry:18069 Library:NIST11s.lib

SI:87 Formula:C15H24 CAS:87-44-5 MolWeight:204 RetIndex:1494

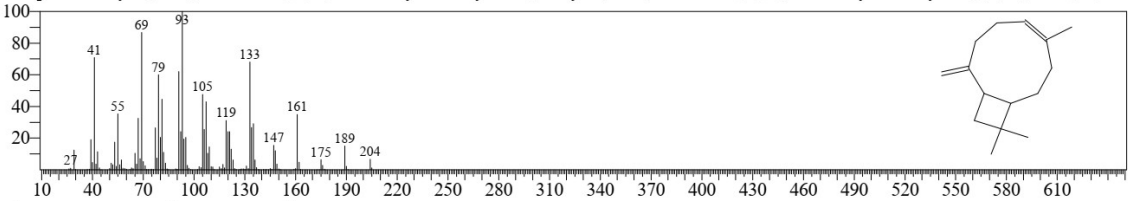
CompName:Caryophyllene $$ Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-, [1R-(1R*,4E,9S*)]- $$ Bicyclo[7.2.0]undec-4-ene, 4,11,11-trime



Hit#:3 Entry:18068 Library:NIST11s.lib

SI:87 Formula:C15H24 CAS:13877-93-5 MolWeight:204 RetIndex:1494

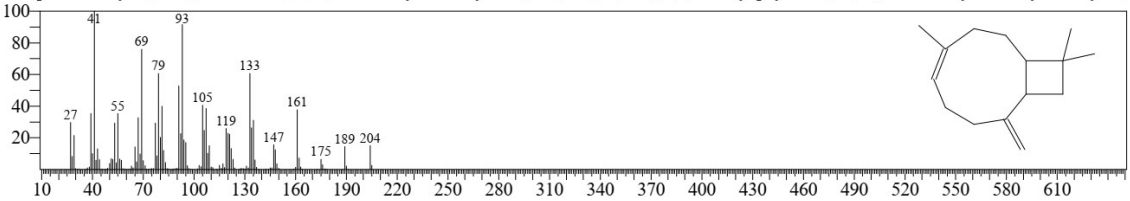
CompName:Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene- $$ Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-, (Z)- $$ cis-4,11,11-T



Hit#:4 Entry:18035 Library:NIST11s.lib

SI:87 Formula:C15H24 CAS:118-65-0 MolWeight:204 RetIndex:1494

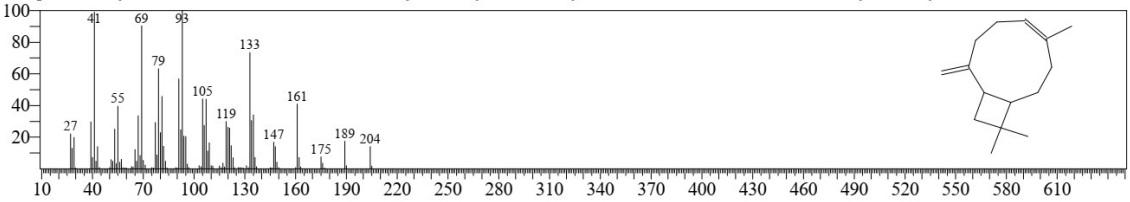
CompName:Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-,[1R-(1R*,4Z,9S*)]- $$ Isocaryophyllene $$ 4,11,11-Trimethyl-8-methylenebicyclo[



Hit#:5 Entry:46618 Library:NIST11.lib

SI:87 Formula:C15H24 CAS:13877-93-5 MolWeight:204 RetIndex:1494

CompName:Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene- $$ Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-, (Z)- $$ cis-4,11,11-T



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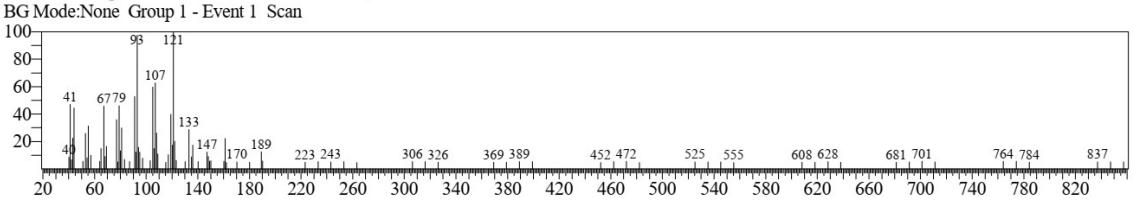
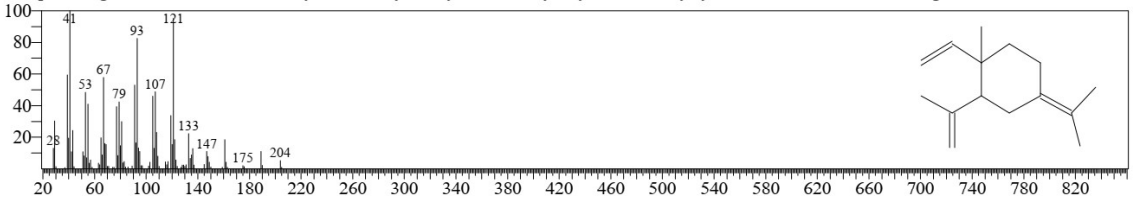


Hit#:1 Entry:18041 Library:NIST11s.lib

SI:89 Formula:C15H24 CAS:29873-99-2 MolWeight:204 RetIndex:1431

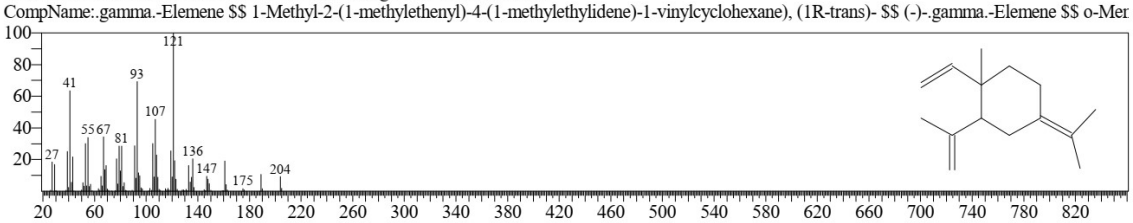
CompName:.gamma.-Elemene $$ 1-Methyl-2-(1-methylethenyl)-4-(1-methylethylidene)-1-vinylcyclohexane), (1R-trans)- $$ (-)-.gamma.-Elemene $$ o-Mer



Hit#:2 Entry:46692 Library:NIST11.lib

SI:87 Formula:C15H24 CAS:29873-99-2 MolWeight:204 RetIndex:1431

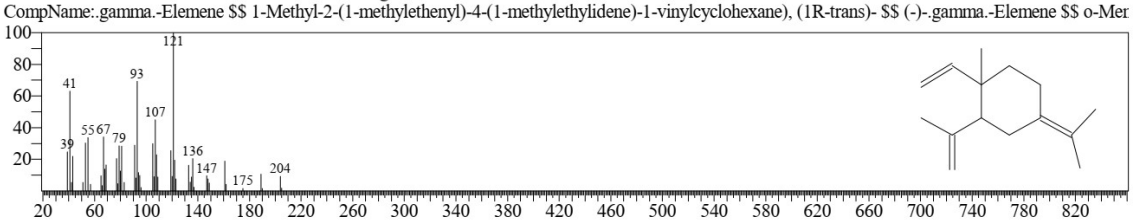
CompName:.gamma.-Elemene $$ 1-Methyl-2-(1-methylethenyl)-4-(1-methylethylidene)-1-vinylcyclohexane), (1R-trans)- $$ (-)-.gamma.-Elemene $$ o-Mer



Hit#:3 Entry:18109 Library:NIST11s.lib

SI:86 Formula:C15H24 CAS:29873-99-2 MolWeight:204 RetIndex:1431

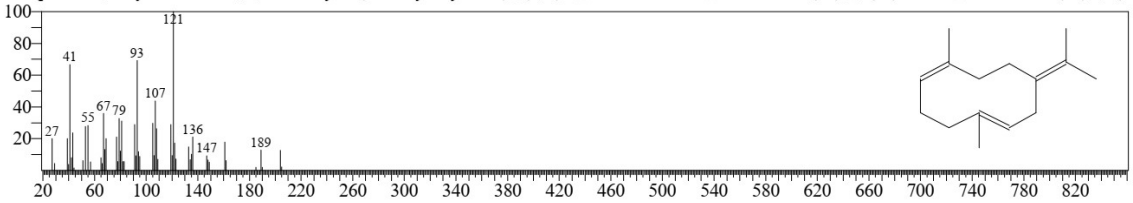
CompName:.gamma.-Elemene $$ 1-Methyl-2-(1-methylethenyl)-4-(1-methylethylidene)-1-vinylcyclohexane), (1R-trans)- $$ (-)-.gamma.-Elemene $$ o-Mer



Hit#:4 Entry:46693 Library:NIST11.lib

SI:86 Formula:C15H24 CAS:15423-57-1 MolWeight:204 RetIndex:1603

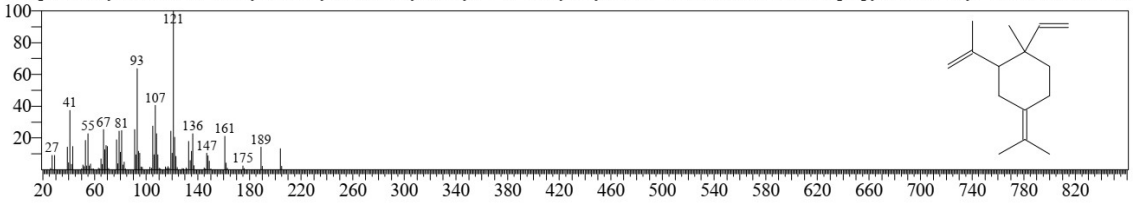
CompName:1,5-Cyclodecadiene, 1,5-dimethyl-8-(1-methylethylidene)-, (E,E)- $$ Germacrene B $$ Germacra-1(10),4,7(11)-triene $$ Germacra-1(10),4,7(1



Hit#:5 Entry:18111 Library:NIST11s.lib

SI:84 Formula:C15H24 CAS:3242-08-8 MolWeight:204 RetIndex:1431

CompName:Cyclohexane, 1-ethenyl-1-methyl-2-(1-methylethenyl)-4-(1-methylethylidene)- $$ o-Menth-8-ene, 4-isopropylidene-1-vinyl- $$ Elixene $$ 2-Isc



Library Search

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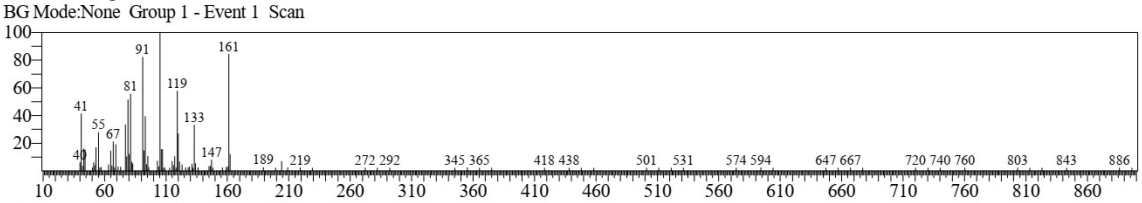
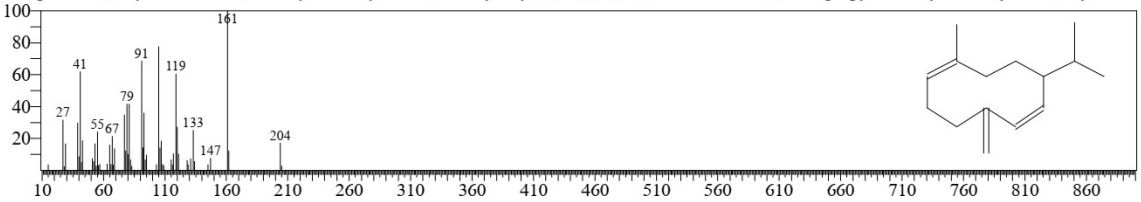


Hit#:1 Entry:46722 Library:NIST11.lib

SI:92 Formula:C15H24 CAS:23986-74-5 MolWeight:204 RetIndex:1515

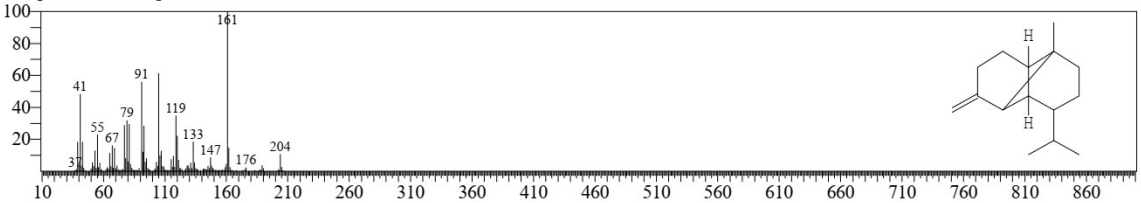
CompName:1,6-Cyclodecadiene, 1-methyl-5-methylene-8-(1-methylethyl)-, [S-(E,E)]- $$ Germacrene D $$ 8-Isopropyl-1-methyl-5-methylene-1,6-cyclodec



Hit#:2 Entry:46720 Library:NIST11.lib

SI:89 Formula:C15H24 CAS:0-00-0 MolWeight:204 RetIndex:1216

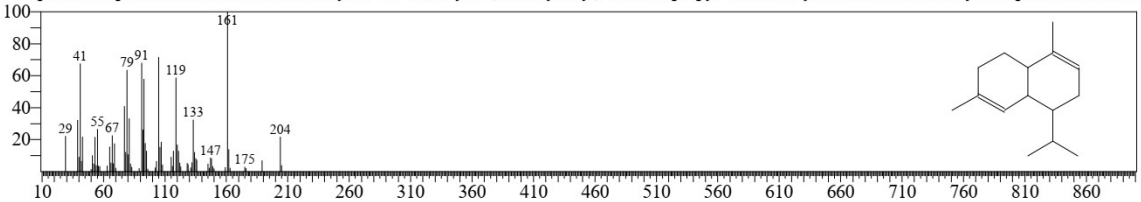
CompName:.beta.-copaene



Hit#:3 Entry:18130 Library:NIST11s.lib

SI:88 Formula:C15H24 CAS:483-75-0 MolWeight:204 RetIndex:1440

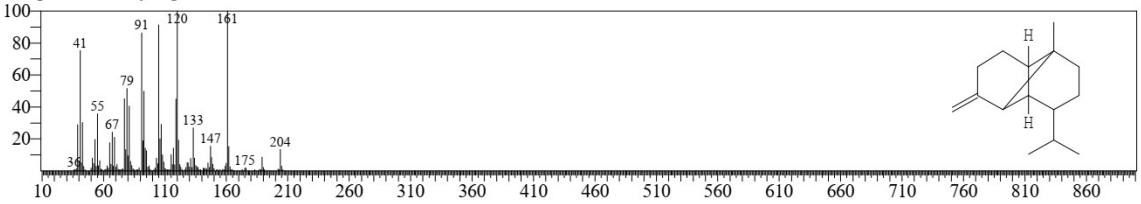
CompName:Naphthalene, 1,2,4a,5,6,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)- $$ 1-Isopropyl-4,7-dimethyl-1,2,4a,5,6,8a-hexahydronaphthalene # $$ 1



Hit#:4 Entry:46691 Library:NIST11.lib

SI:88 Formula:C15H24 CAS:0-00-0 MolWeight:204 RetIndex:1216

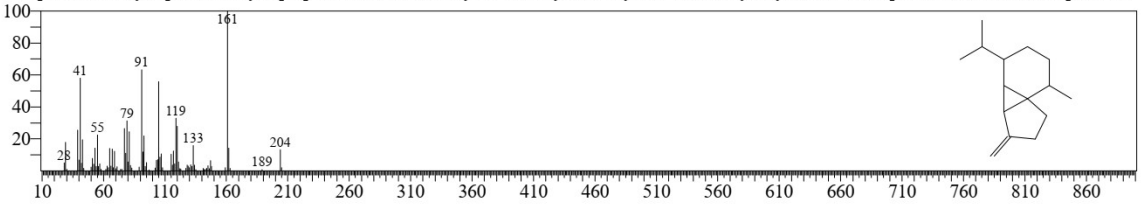
CompName:.beta.-ylangene



Hit#:5 Entry:18123 Library:NIST11s.lib

SI:88 Formula:C15H24 CAS:13744-15-5 MolWeight:204 RetIndex:1339

CompName:1H-Cyclopenta[1,3]cyclopropa[1,2]benzene, octahydro-7-methyl-3-methylene-4-(1-methylethyl)-, [3aS-(3a.alpha.,3b.beta.,4.beta.,7.alpha.,7aS*



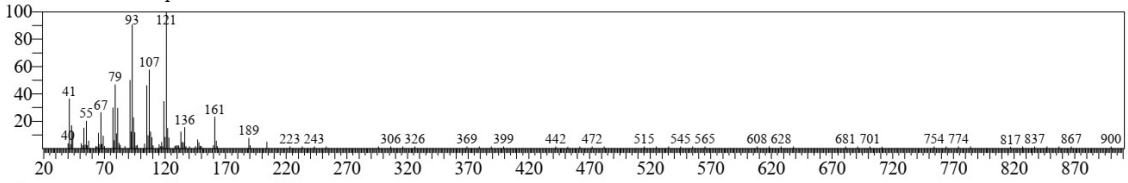
Library Search

<< Target >>

Line#:1 R.Time:14.800(Scan#:2961) MassPeaks:115

RawMode:Single 14.800(2961) BasePeak:121.15(10000)

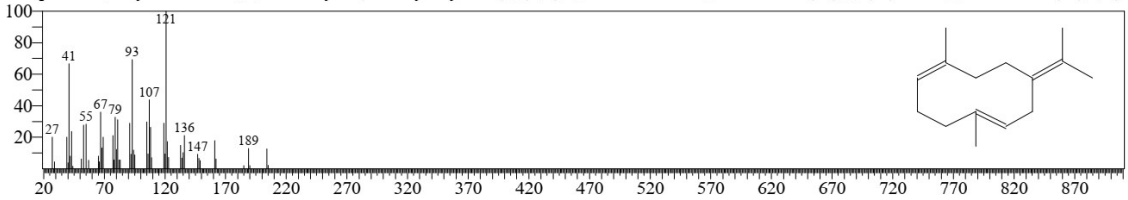
BG Mode:None Group 1 - Event 1 Scan



Hit#:1 Entry:46693 Library:NIST11.lib

SI:90 Formula:C15H24 CAS:15423-57-1 MolWeight:204 RetIndex:1603

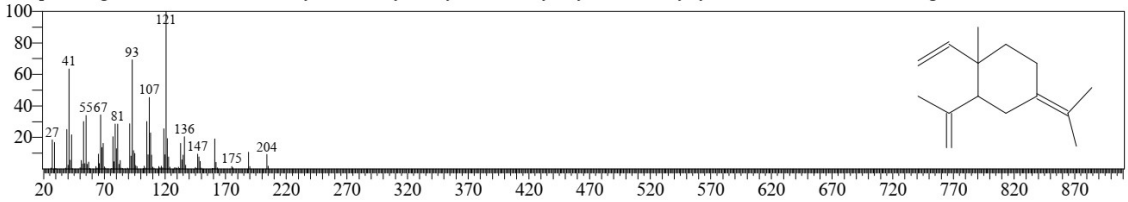
CompName:1,5-Cyclodecadiene, 1,5-dimethyl-8-(1-methylethylidene)-, (E,E)- $$ Germacrene B $$ Germacra-1(10),4,7(11)-triene $$ Germacra-1(10),4,7(1



Hit#:2 Entry:46692 Library:NIST11.lib

SI:90 Formula:C15H24 CAS:29873-99-2 MolWeight:204 RetIndex:1431

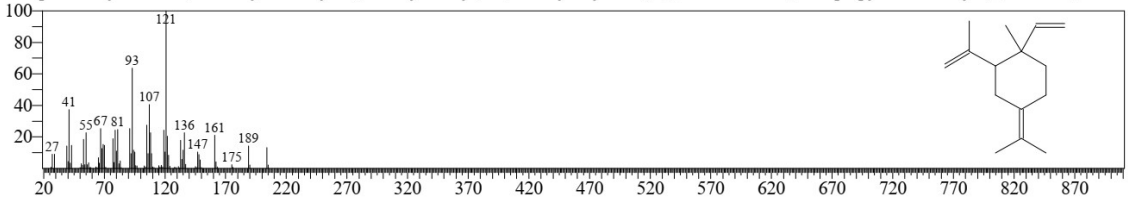
CompName:.gamma.-Elemene $$ 1-Methyl-2-(1-methylethenyl)-4-(1-methylethylidene)-1-vinylcyclohexane), (1R-trans)- $$ (-)-.gamma.-Elemene $$ o-Mer



Hit#:3 Entry:18111 Library:NIST11s.lib

SI:90 Formula:C15H24 CAS:3242-08-8 MolWeight:204 RetIndex:1431

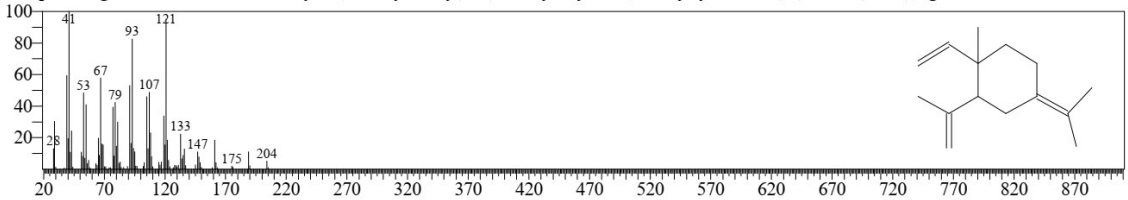
CompName:Cyclohexane, 1-ethenyl-1-methyl-2-(1-methylethenyl)-4-(1-methylethylidene)- $$ o-Menth-8-ene, 4-isopropylidene-1-vinyl- $$ Elixene $$ 2-Isc



Hit#:4 Entry:18041 Library:NIST11s.lib

SI:90 Formula:C15H24 CAS:29873-99-2 MolWeight:204 RetIndex:1431

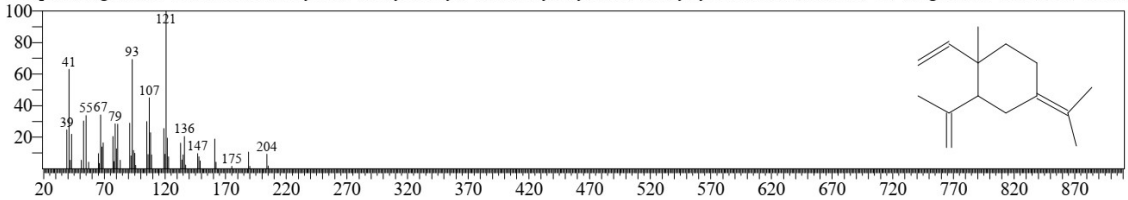
CompName:.gamma.-Elemene $$ 1-Methyl-2-(1-methylethenyl)-4-(1-methylethylidene)-1-vinylcyclohexane), (1R-trans)- $$ (-)-.gamma.-Elemene $$ o-Mer



Hit#:5 Entry:18109 Library:NIST11s.lib

SI:89 Formula:C15H24 CAS:29873-99-2 MolWeight:204 RetIndex:1431

CompName:.gamma.-Elemene $$ 1-Methyl-2-(1-methylethenyl)-4-(1-methylethylidene)-1-vinylcyclohexane), (1R-trans)- $$ (-)-.gamma.-Elemene $$ o-Mer



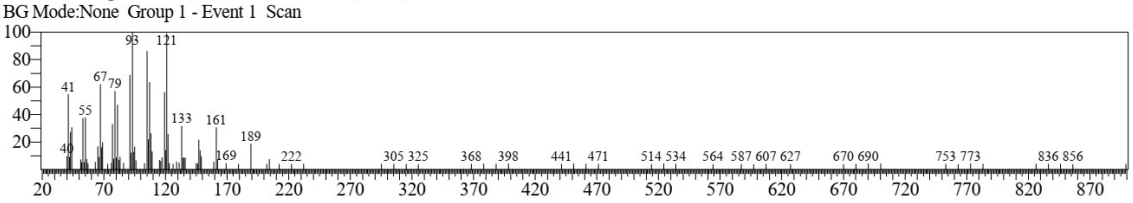
Library Search

<< Target >>

Line#:1 R.Time:15.605(Scan#:3122) MassPeaks:104

RawMode:Single 15.605(3122) BasePeak:93.10(10000)

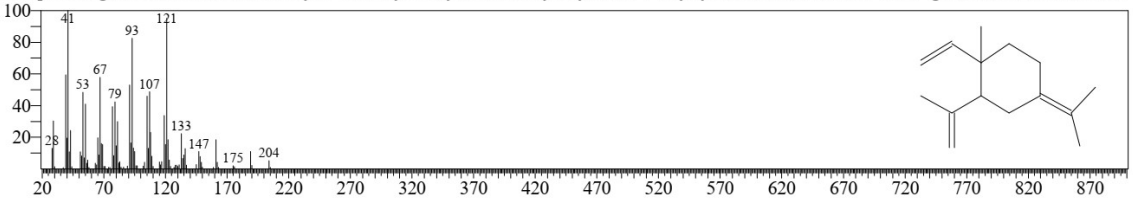
BG Mode:None Group 1 - Event 1 Scan



Hit#:1 Entry:18041 Library:NIST11s.lib

SI:89 Formula:C15H24 CAS:29873-99-2 MolWeight:204 RetIndex:1431

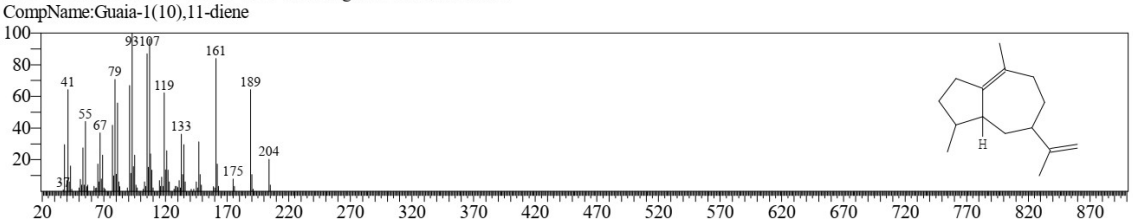
CompName:.gamma.-Elemene $$ 1-Methyl-2-(1-methylethenyl)-4-(1-methylethylidene)-1-vinylcyclohexane), (1R-trans)- $$ (-)-.gamma.-Elemene $$ o-Mer



Hit#:2 Entry:46631 Library:NIST11.lib

SI:88 Formula:C15H24 CAS:0-00-0 MolWeight:204 RetIndex:1490

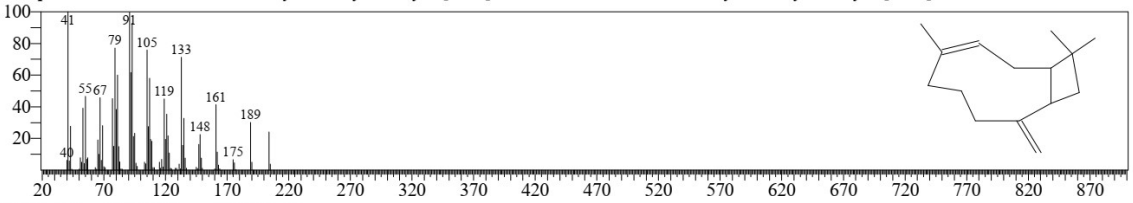
CompName:Guaia-1(10),11-diene



Hit#:3 Entry:46583 Library:NIST11.lib

SI:88 Formula:C15H24 CAS:0-00-0 MolWeight:204 RetIndex:1494

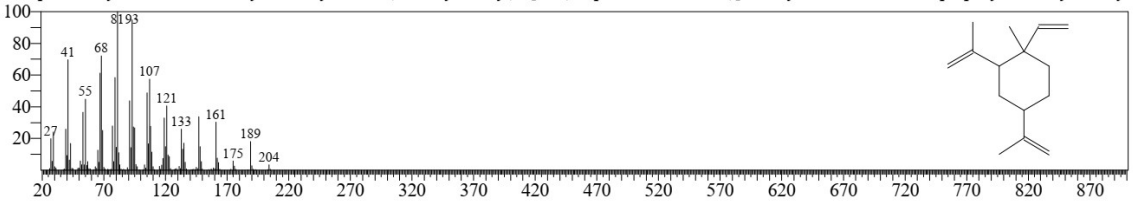
CompName:1R,3Z,9s-4,11,11-Trimethyl-8-methylenebicyclo[7.2.0]undec-3-ene $$ 4,11,11-Trimethyl-8-methylenebicyclo[7.2.0]undec-3-ene # $$



Hit#:4 Entry:18058 Library:NIST11s.lib

SI:87 Formula:C15H24 CAS:515-13-9 MolWeight:204 RetIndex:1398

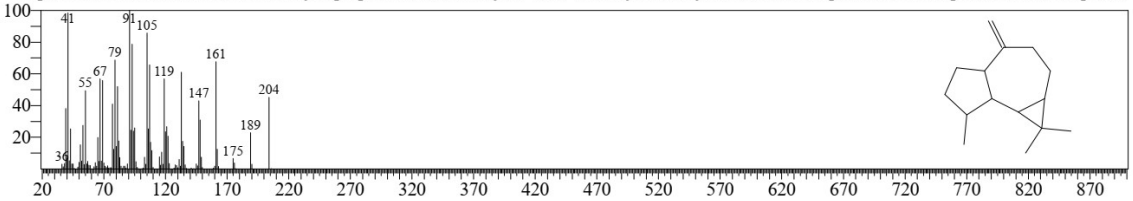
CompName:Cyclohexane, 1-ethenyl-1-methyl-2,4-bis(1-methylethenyl)-, [1S-(1.alpha.,2.beta.,4.beta.)]- $$ Cyclohexane, 2,4-diisopropenyl-1-methyl-1-vinyl



Hit#:5 Entry:18061 Library:NIST11s.lib

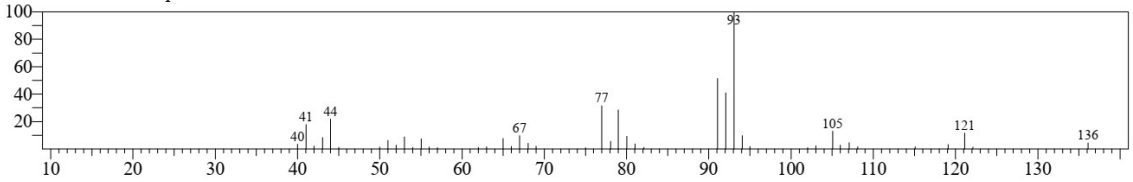
SI:87 Formula:C15H24 CAS:25246-27-9 MolWeight:204 RetIndex:1386

CompName:Alloaromadendrene $$ 1H-Cycloprop[e]azulene, decahydro-1,1,7-trimethyl-4-methylene-, [1aR-(1a.alpha.,4a.beta.,7.alpha.,7a.beta.,7b.alpha.)]-

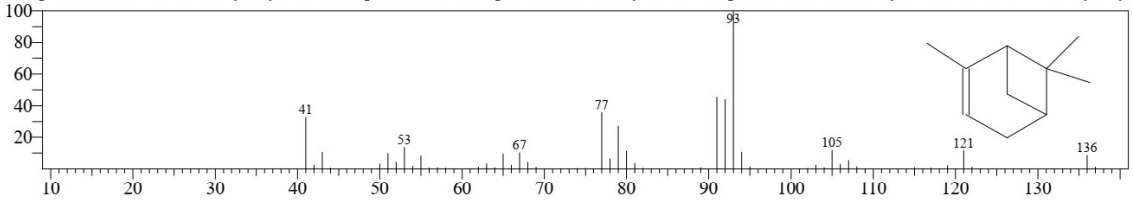


(b)

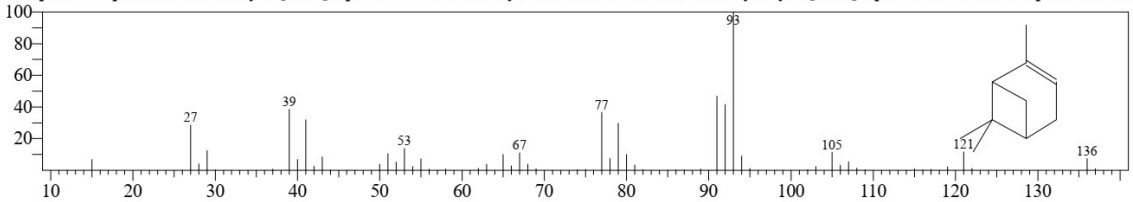
Library Search
<< Target >>
Line#:1 R.Time:6.170(Scan#:235) MassPeaks:44
RawMode:Single 6.170(235) BasePeak:93.05(10000)
BG Mode:None Group 1 - Event 1 Scan



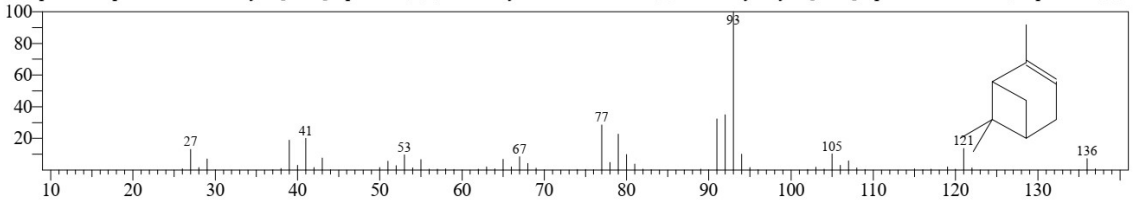
Hit#:1 Entry:6665 Library:NIST11s.lib
SI:94 Formula:C10H16 CAS:7785-70-8 MolWeight:136 RetIndex:948
CompName:(1R)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene $$ 1R-.alpha.-Pinene $$ Bicyclo[3.1.1]hept-2-ene, 2,6,6-trimethyl-, (1R)- $$ 2,6,6-Trimethylbicy



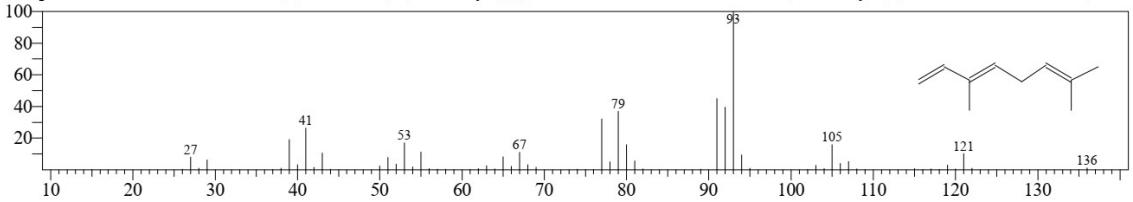
Hit#:2 Entry:9809 Library:NIST11.lib
SI:93 Formula:C10H16 CAS:80-56-8 MolWeight:136 RetIndex:948
CompName:.alpha.-Pinene $$ Bicyclo[3.1.1]hept-2-ene, 2,6,6-trimethyl- $$ 2-Pinene $$ 2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene $$ Pinene, .alpha. $$ 2,6,6



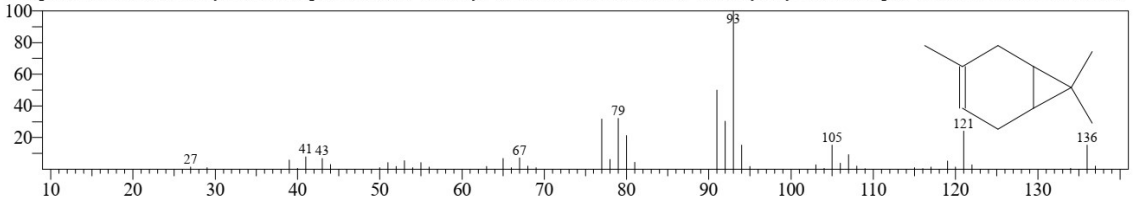
Hit#:3 Entry:6669 Library:NIST11s.lib
SI:93 Formula:C10H16 CAS:80-56-8 MolWeight:136 RetIndex:948
CompName:.alpha.-Pinene $$ Bicyclo[3.1.1]hept-2-ene, 2,6,6-trimethyl- $$ 2-Pinene $$ 2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene $$ Pinene, .alpha. $$ 2,6,6



Hit#:4 Entry:6664 Library:NIST11s.lib
SI:93 Formula:C10H16 CAS:3779-61-1 MolWeight:136 RetIndex:976
CompName:trans-.beta.-Ocimene $$ 1,3,6-Octatriene, 3,7-dimethyl-, (E)- $$ .beta.-trans-Ocimene $$ trans-3,7-Dimethyl-1,3,6-Octatriene $$ Ocimene, trans



Hit#:5 Entry:9807 Library:NIST11.lib
SI:92 Formula:C10H16 CAS:13466-78-9 MolWeight:136 RetIndex:948
CompName:3-Carene $$ Bicyclo[4.1.0]hept-3-ene, 3,7,7-trimethyl- $$ delta-3-Carene $$ 3,7,7-Trimethylbicyclo[4.1.0]hept-3-ene $$ .delta. 3-carene $$ 3,7



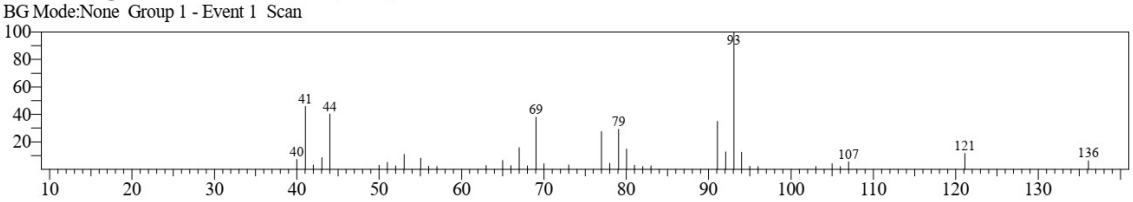
Library Search

<< Target >>

Line#:1 R.Time:7.000(Scan#:401) MassPeaks:39

RawMode:Single 7.000(401) BasePeak:93.05(10000)

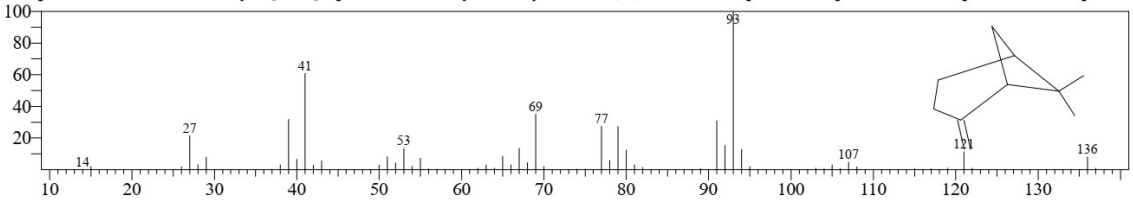
BG Mode:None Group 1 - Event 1 Scan



Hit#:1 Entry:9777 Library:NIST11.lib

SI:91 Formula:C10H16 CAS:127-91-3 MolWeight:136 RetIndex:943

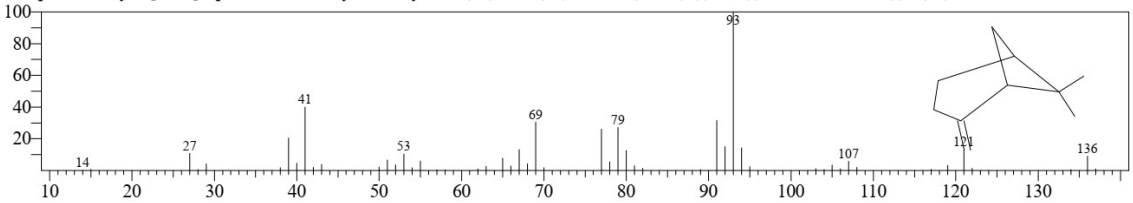
CompName:.beta.-Pinene $$ Bicyclo[3.1.1]heptane, 6,6-dimethyl-2-methylene- $$ 2(10)-Pinene $$ Nopinen $$ Nopinene $$ Pseudopinen $$ Pseudopinene



Hit#:2 Entry:6642 Library:NIST11s.lib

SI:90 Formula:C10H16 CAS:18172-67-3 MolWeight:136 RetIndex:943

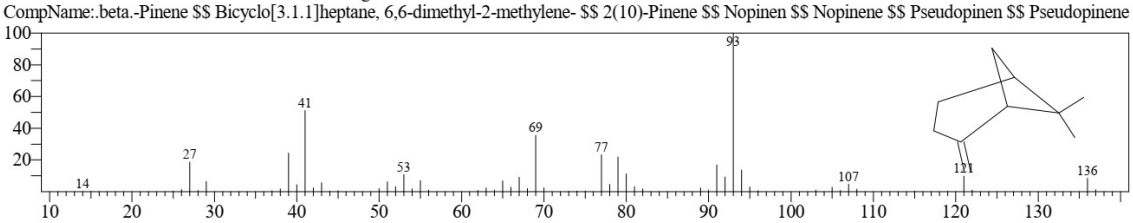
CompName:Bicyclo[3.1.1]heptane, 6,6-dimethyl-2-methylene-, (1S)- $$ 2(10)-Pinene, (1S,5S)-(-)- $$ (-)-.beta.-Pinene $$ (-)-2(10)-Pinene $$ L-.beta.-Pinen



Hit#:3 Entry:6634 Library:NIST11s.lib

SI:89 Formula:C10H16 CAS:127-91-3 MolWeight:136 RetIndex:943

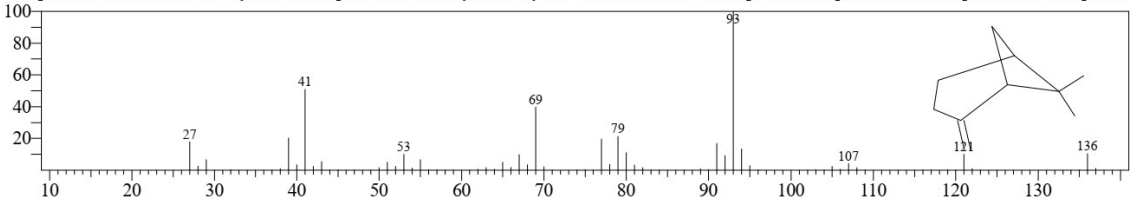
CompName:.beta.-Pinene $$ Bicyclo[3.1.1]heptane, 6,6-dimethyl-2-methylene- $$ 2(10)-Pinene $$ Nopinen $$ Nopinene $$ Pseudopinen $$ Pseudopinene



Hit#:4 Entry:6635 Library:NIST11s.lib

SI:89 Formula:C10H16 CAS:127-91-3 MolWeight:136 RetIndex:943

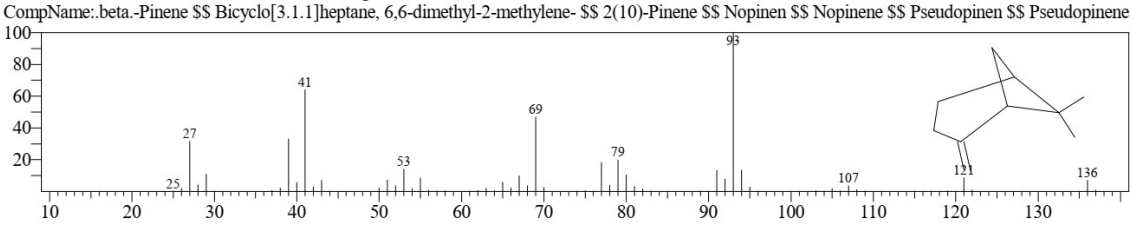
CompName:.beta.-Pinene $$ Bicyclo[3.1.1]heptane, 6,6-dimethyl-2-methylene- $$ 2(10)-Pinene $$ Nopinen $$ Nopinene $$ Pseudopinen $$ Pseudopinene



Hit#:5 Entry:6633 Library:NIST11s.lib

SI:88 Formula:C10H16 CAS:127-91-3 MolWeight:136 RetIndex:943

CompName:.beta.-Pinene $$ Bicyclo[3.1.1]heptane, 6,6-dimethyl-2-methylene- $$ 2(10)-Pinene $$ Nopinen $$ Nopinene $$ Pseudopinen $$ Pseudopinene



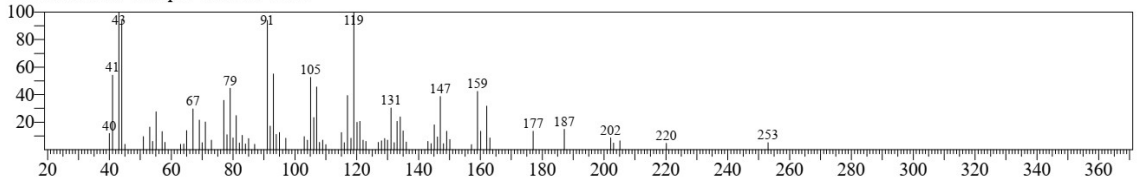
Library Search

<< Target >>

Line#:1 R.Time:19.800(Scan#:2961) MassPeaks:82

RawMode:Single 19.800(2961) BasePeak:119.05(10000)

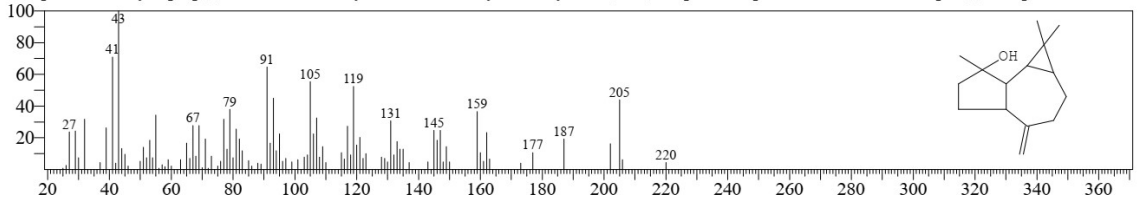
BG Mode:None Group 1 - Event 1 Scan



Hit#:1 Entry:20009 Library:NIST11s.lib

SI:87 Formula:C15H24O CAS:6750-60-3 MolWeight:220 RetIndex:1536

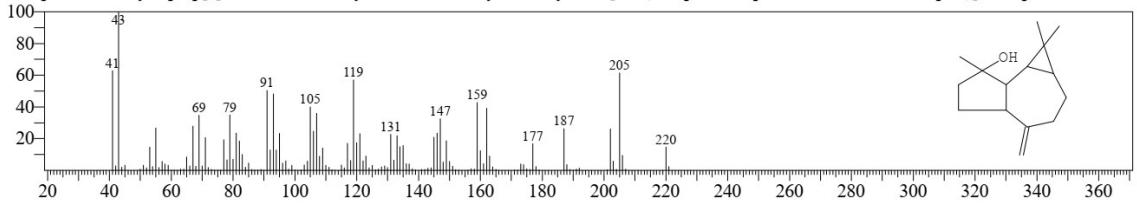
CompName:1H-Cycloprop[e]azulen-7-ol, decahydro-1,1,7-trimethyl-4-methylene-, [1ar-(1a.alpha.,4a.alpha.,7.beta.,7a.beta.,7b.alpha.)]- $$ Spathulenol $$ 1



Hit#:2 Entry:57738 Library:NIST11.lib

SI:82 Formula:C15H24O CAS:6750-60-3 MolWeight:220 RetIndex:1536

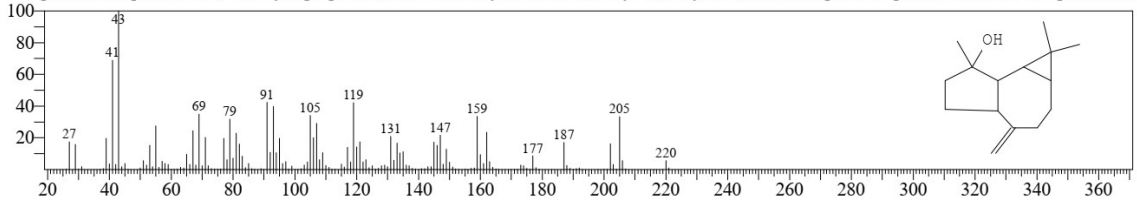
CompName:1H-Cycloprop[e]azulen-7-ol, decahydro-1,1,7-trimethyl-4-methylene-, [1ar-(1a.alpha.,4a.alpha.,7.beta.,7a.beta.,7b.alpha.)]- $$ Spathulenol $$ 1



Hit#:3 Entry:57734 Library:NIST11.lib

SI:81 Formula:C15H24O CAS:77171-55-2 MolWeight:220 RetIndex:1536

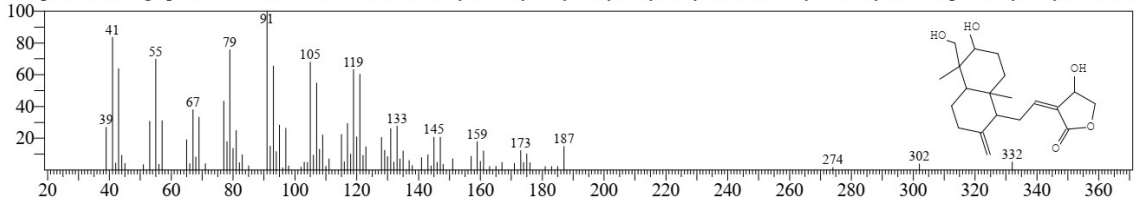
CompName:(-)-Spathulenol $$ 1H-Cycloprop[e]azulen-7-ol, decahydro-1,1,7-trimethyl-4-methylene-, [1aS-(1a.alpha.,4a.alpha.,7.beta.)] $$ Ent-Spathulenol



Hit#:4 Entry:155597 Library:NIST11.lib

SI:79 Formula:C20H30O5 CAS:5508-58-7 MolWeight:350 RetIndex:2944

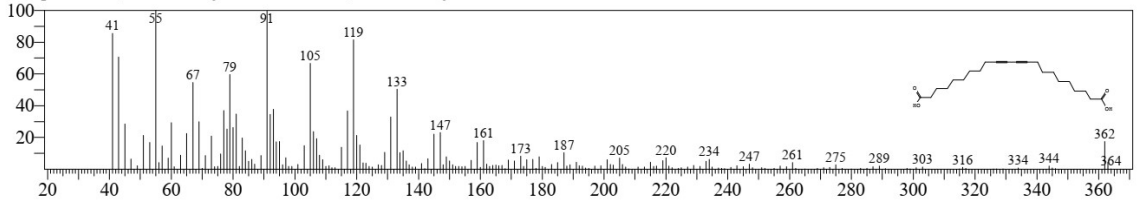
CompName:Andrographolide $$ 2(3H)-Furanone, 3-[2-[decahydro-6-hydroxy-5-(hydroxymethyl)-5,8a-dimethyl-2-methylene-1-naphthalenyl]ethylidene]dih



Hit#:5 Entry:163150 Library:NIST11.lib

SI:78 Formula:C22H34O4 CAS:28393-02-4 MolWeight:362 RetIndex:2956

CompName:10,12-Docasadiyndioic acid $$ 10,12-Docosadiynedioic acid # $$



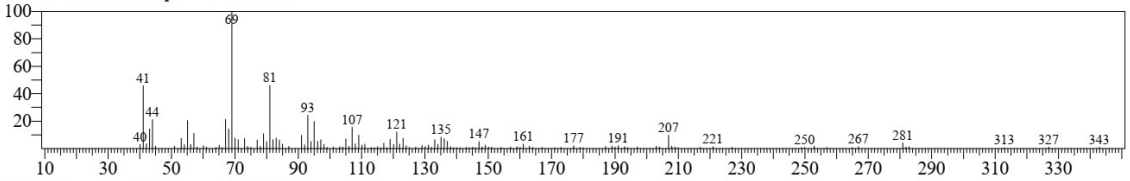
Library Search

<< Target >>

Line#:1 R.Time:25.615(Scan#:4124) MassPeaks:132

RawMode:Single 25.615(4124) BasePeak:69.05(10000)

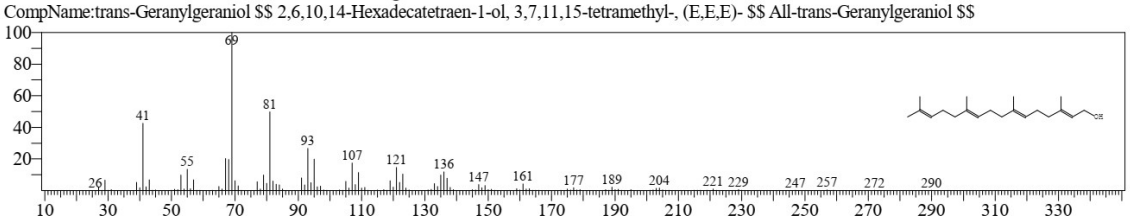
BG Mode:None Group 1 - Event 1 Scan



Hit#:1 Entry:110905 Library:NIST11.lib

SI:89 Formula:C20H34O CAS:24034-73-9 MolWeight:290 RetIndex:2192

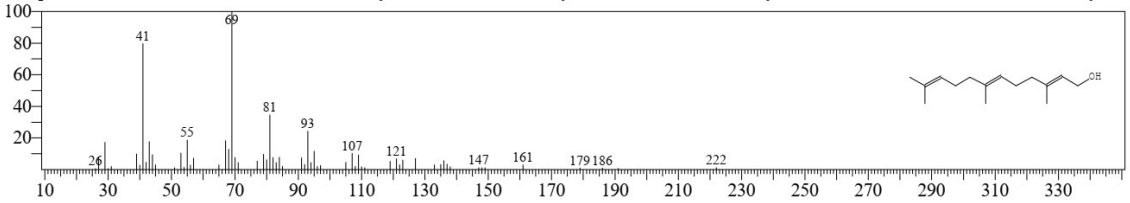
CompName:trans-Geranylgeraniol $$ 2,6,10,14-Hexadecatetraen-1-ol, 3,7,11,15-tetramethyl-, (E,E,E)- $$ All-trans-Geranylgeraniol $$



Hit#:2 Entry:20278 Library:NIST11s.lib

SI:88 Formula:C15H26O CAS:4602-84-0 MolWeight:222 RetIndex:1710

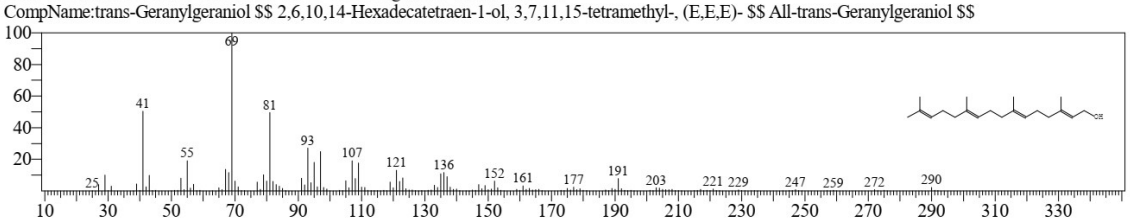
CompName:2,6,10-Dodecatrien-1-ol, 3,7,11-trimethyl- $$ Farnesol $$ Farnesyl alcohol $$ 3,7,11-Trimethyl-2,6,10-dodecatrien-1-ol $$ 3,7,11-Trimethyl-2,



Hit#:3 Entry:25623 Library:NIST11s.lib

SI:87 Formula:C20H34O CAS:24034-73-9 MolWeight:290 RetIndex:2192

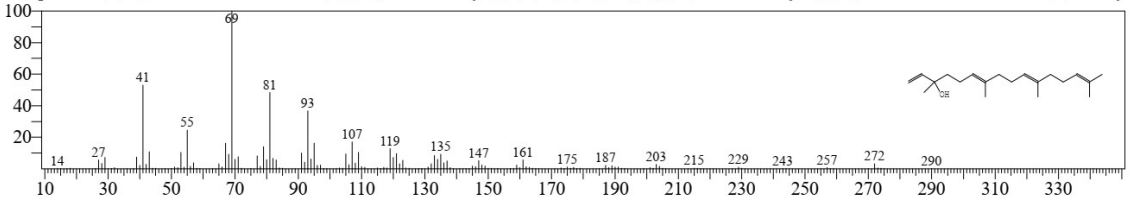
CompName:trans-Geranylgeraniol $$ 2,6,10,14-Hexadecatetraen-1-ol, 3,7,11,15-tetramethyl-, (E,E,E)- $$ All-trans-Geranylgeraniol $$



Hit#:4 Entry:110903 Library:NIST11.lib

SI:87 Formula:C20H34O CAS:1113-21-9 MolWeight:290 RetIndex:2046

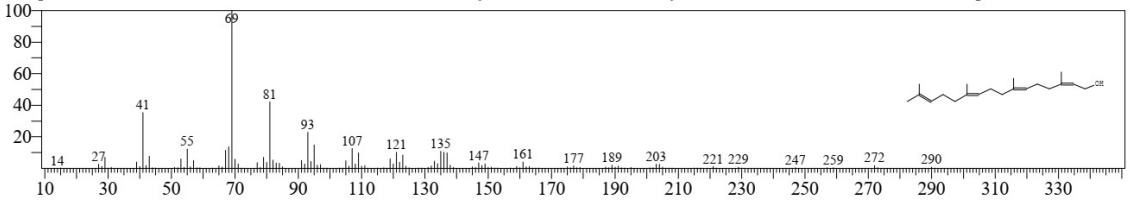
CompName:1,6,10,14-Hexadecatetraen-3-ol, 3,7,11,15-tetramethyl-, (E,E)- $$ (6E,10E)-3,7,11,15-Tetramethyl-1,6,10,14-hexadecatetraen-3-ol # $$ Gerany



Hit#:5 Entry:110904 Library:NIST11.lib

SI:87 Formula:C20H34O CAS:7614-21-3 MolWeight:290 RetIndex:2192

CompName:Hexadeca-2,6,10,14-tetraen-1-ol, 3,7,11,16-tetramethyl- $$ 3,7,11,15-Tetramethyl-2,6,10,14-hexadecatetraen-1-ol $$ Tetraprenol $$



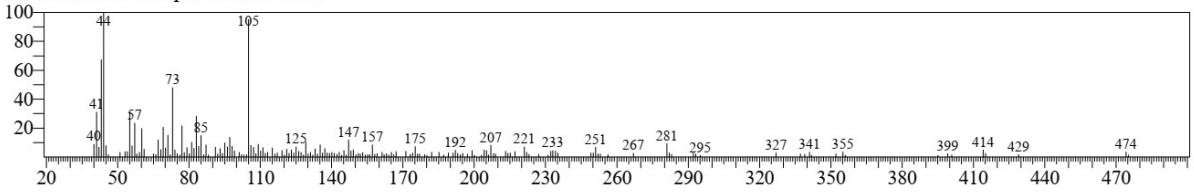
(c) Library Search

<< Target >>

Line#:1 R.Time:22.925(Scan#:3586) MassPeaks:183

RawMode:Single 22.925(3586) BasePeak:44.05(10000)

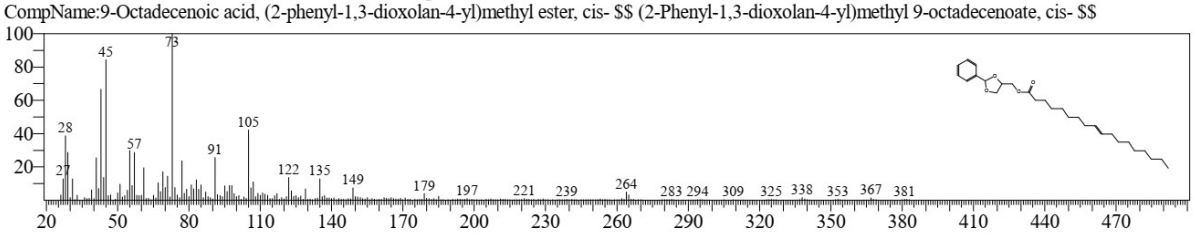
BG Mode:None Group 1 - Event 1 Scan



Hit#:1 Entry:195613 Library:NIST11.lib

SI:75 Formula:C28H44O4 CAS:56599-45-2 MolWeight:444 RetIndex:3238

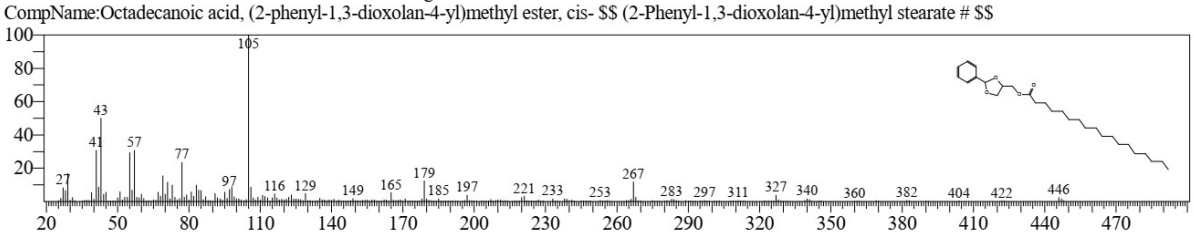
CompName:9-Octadecenoic acid, (2-phenyl-1,3-dioxolan-4-yl)methyl ester, cis- $$ (2-Phenyl-1,3-dioxolan-4-yl)methyl 9-octadecenoate, cis- $$



Hit#:2 Entry:196084 Library:NIST11.lib

SI:75 Formula:C28H46O4 CAS:56599-88-3 MolWeight:446 RetIndex:3230

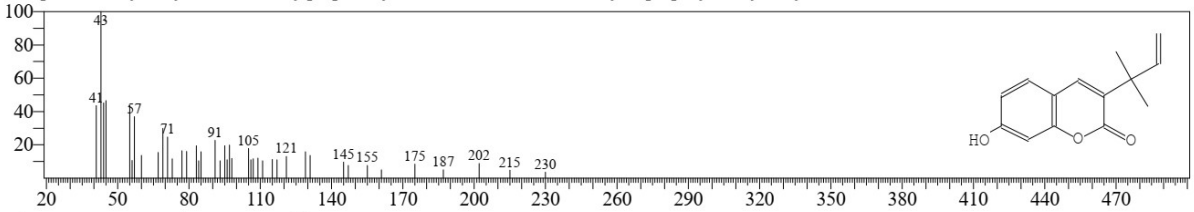
CompName:Octadecanoic acid, (2-phenyl-1,3-dioxolan-4-yl)methyl ester, cis- $$ (2-Phenyl-1,3-dioxolan-4-yl)methyl stearate # $$



Hit#:3 Entry:65115 Library:NIST11.lib

SI:75 Formula:C14H14O3 CAS:56881-08-4 MolWeight:230 RetIndex:1987

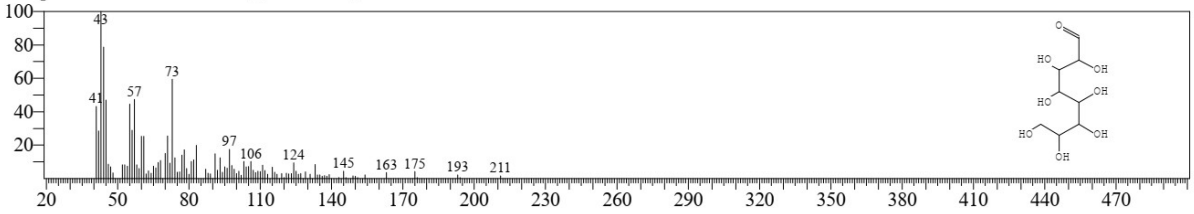
CompName:7-Hydroxy-3-(1,1-dimethylprop-2-enyl)coumarin $$ 3-(1,1-Dimethyl-2-propenyl)-7-hydroxy-2H-chromen-2-one # $$



Hit#:4 Entry:71579 Library:NIST11.lib

SI:71 Formula:C8H16O8 CAS:0-00-0 MolWeight:240 RetIndex:2221

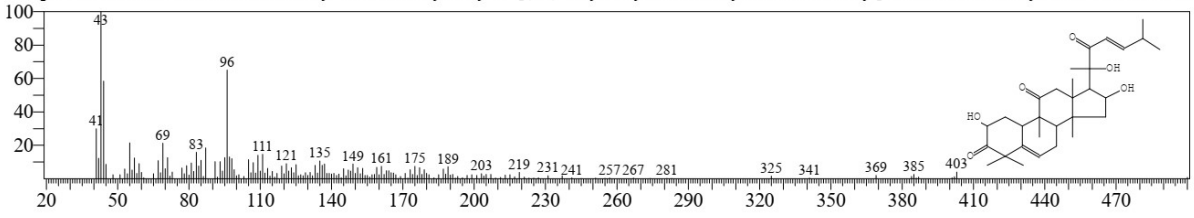
CompName:l-Gala-l-ido-octose $$ Octose # $$



Hit#:5 Entry:204708 Library:NIST11.lib

SI:70 Formula:C30H44O6 CAS:125596-54-5 MolWeight:500 RetIndex:3635

CompName:Cucurbitacin b, 25-desacetoxy- $$ 2,16-Dihydroxy-17-[(3E)-1-hydroxy-1,5-dimethyl-2-oxo-3-hexenyl]-4,4,9,14-tetramethylestr-5-ene-3,11-dio



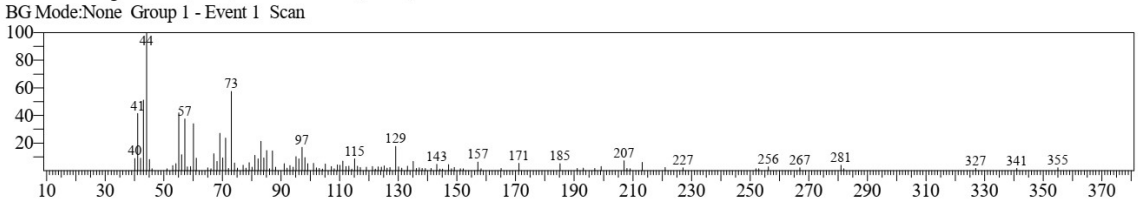
Library Search

<< Target >>

Line#:1 R.Time:23.640(Scan#:3729) MassPeaks:115

RawMode:Single 23.640(3729) BasePeak:44.05(10000)

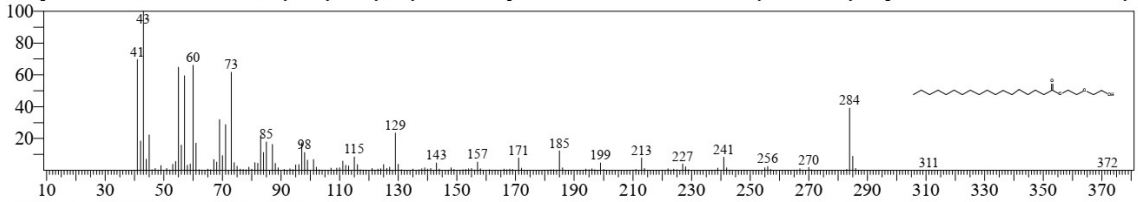
BG Mode:None Group 1 - Event 1 Scan



Hit#:1 Entry:169171 Library:NIST11.lib

SI:80 Formula:C22H44O4 CAS:106-11-6 MolWeight:372 RetIndex:2694

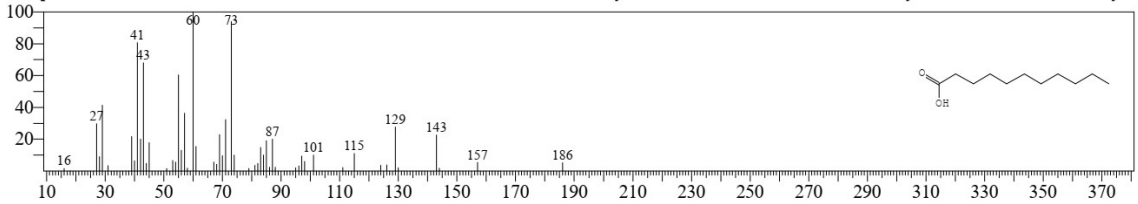
CompName:Octadecanoic acid, 2-(2-hydroxyethoxy)ethyl ester $$ Aqua Cera $$ Atlas G 2146 $$ Cerasynt $$ Cerasynt Special $$ Clindrol SDG $$ Diethyl



Hit#:2 Entry:15394 Library:NIST11s.lib

SI:80 Formula:C11H22O2 CAS:112-37-8 MolWeight:186 RetIndex:1471

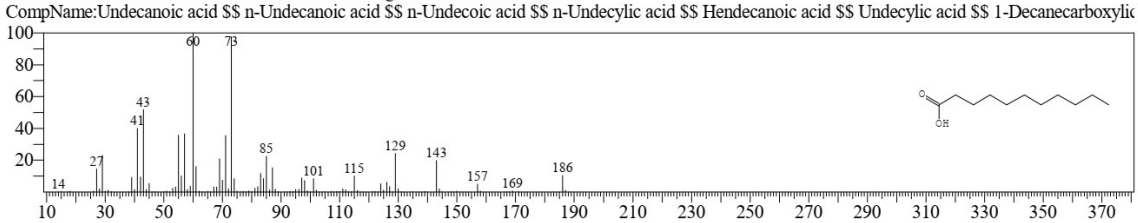
CompName:Undecanoic acid $$ n-Undecanoic acid $$ n-Undecoic acid $$ n-Undecylic acid $$ Hendecanoic acid $$ Undecylic acid $$ 1-Decanecarboxylic



Hit#:3 Entry:35174 Library:NIST11.lib

SI:79 Formula:C11H22O2 CAS:112-37-8 MolWeight:186 RetIndex:1471

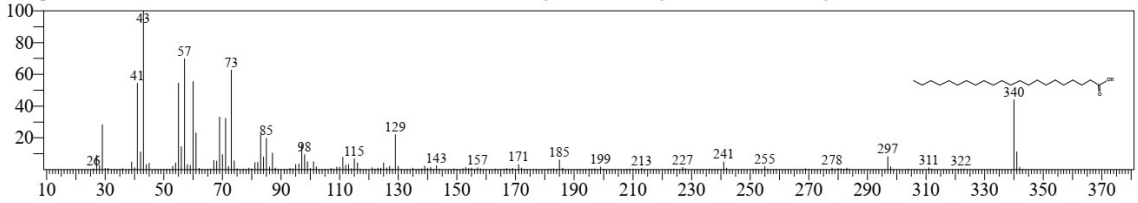
CompName:Undecanoic acid $$ n-Undecanoic acid $$ n-Undecoic acid $$ n-Undecylic acid $$ Hendecanoic acid $$ Undecylic acid $$ 1-Decanecarboxylic



Hit#:4 Entry:28080 Library:NIST11s.lib

SI:79 Formula:C22H44O2 CAS:112-85-6 MolWeight:340 RetIndex:2564

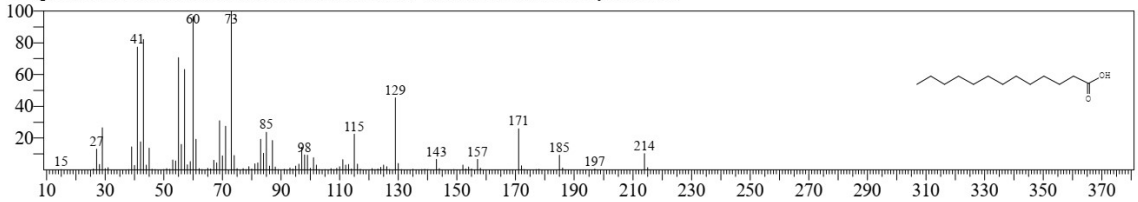
CompName:Docosanoic acid $$ n-Docosanoic acid $$ Behenic acid $$ Glycon B-70 $$ Hydrofol Acid 560 $$ Hydrofol 2022-55 $$ 1-Docosanoic acid $$



Hit#:5 Entry:53599 Library:NIST11.lib

SI:78 Formula:C13H26O2 CAS:638-53-9 MolWeight:214 RetIndex:1670

CompName:Tridecanoic acid $$ n-Tridecanoic acid $$ n-Tridecoic acid $$ Tridecylic acid $$



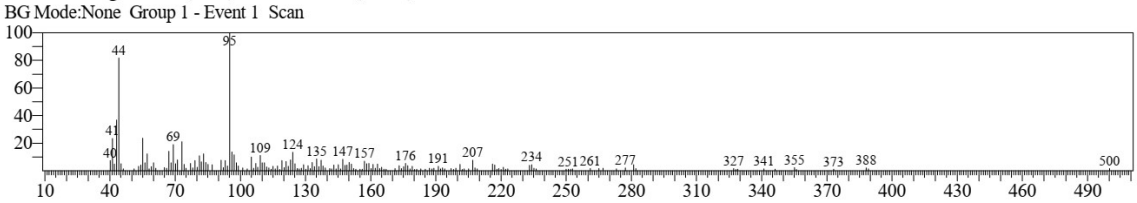
Library Search

<< Target >>

Line#:1 R.Time:23.935(Scan#:3788) MassPeaks:172

RawMode:Single 23.935(3788) BasePeak:95.05(10000)

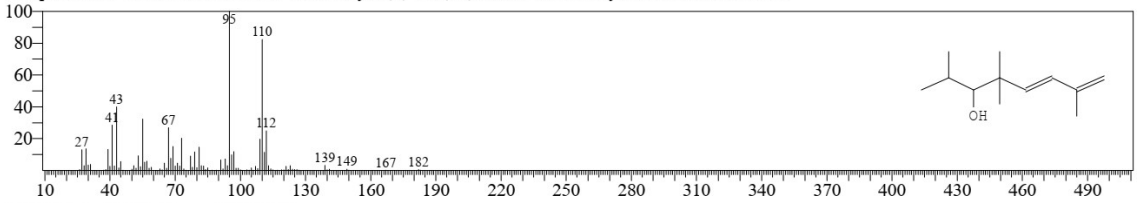
BG Mode:None Group 1 - Event 1 Scan



Hit#:1 Entry:32965 Library:NIST11.lib

SI:72 Formula:C12H22O CAS:77142-78-0 MolWeight:182 RetIndex:1203

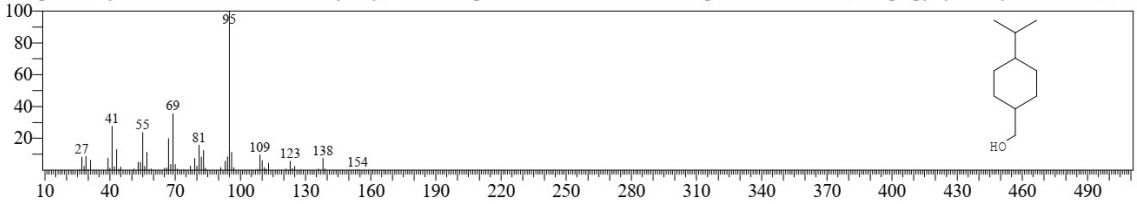
CompName:5,7-Octadien-3-ol, 2,4,4,7-tetramethyl-, (E)- $$ (5E)-2,4,4,7-Tetramethyl-5,7-octadien-3-ol # $$



Hit#:2 Entry:18695 Library:NIST11.lib

SI:72 Formula:C10H20O CAS:13674-19-6 MolWeight:156 RetIndex:1219

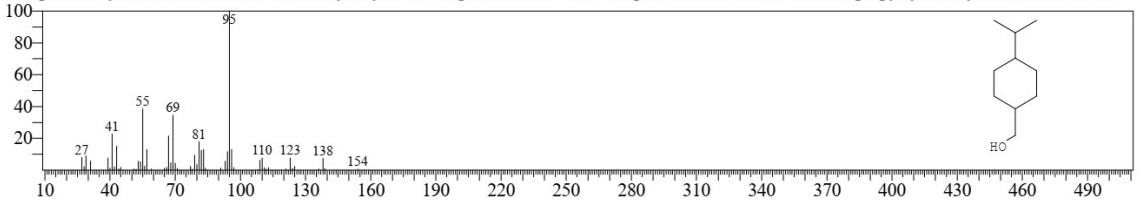
CompName:Cyclohexanemethanol, 4-(1-methylethyl)-, trans- $$ p-Menthan-7-ol, trans- $$ trans-p-Menthan-7-ol $$ (4-Isopropylcyclohexyl)methanol, (E)- $



Hit#:3 Entry:18690 Library:NIST11.lib

SI:71 Formula:C10H20O CAS:13828-37-0 MolWeight:156 RetIndex:1219

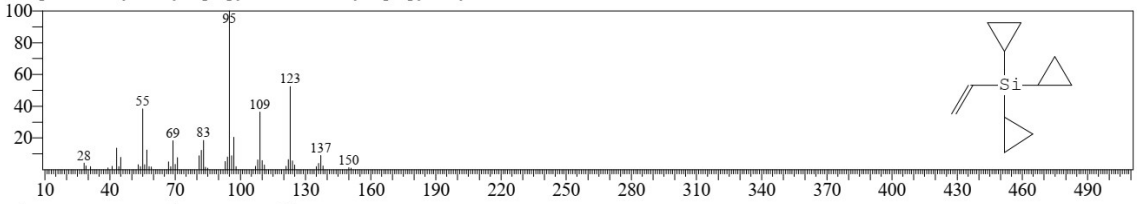
CompName:Cyclohexanemethanol, 4-(1-methylethyl)-, cis- $$ p-Menthan-7-ol, cis- $$ p-Methan-7-ol, (cis)- $$ (4-Isopropylcyclohexyl)methanol, (Z)- $$



Hit#:4 Entry:30371 Library:NIST11.lib

SI:71 Formula:C11H18Si CAS:0-00-0 MolWeight:178 RetIndex:1021

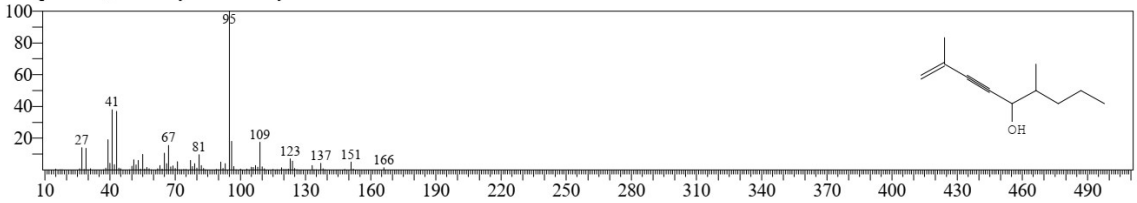
CompName:Vinyltris(cyclopropyl)silane $$ Tricyclopropyl(vinyl)silane # $$



Hit#:5 Entry:23615 Library:NIST11.lib

SI:71 Formula:C11H18O CAS:0-00-0 MolWeight:166 RetIndex:1197

CompName:2,6-Dimethyl-1-nonen-3-yn-5-ol



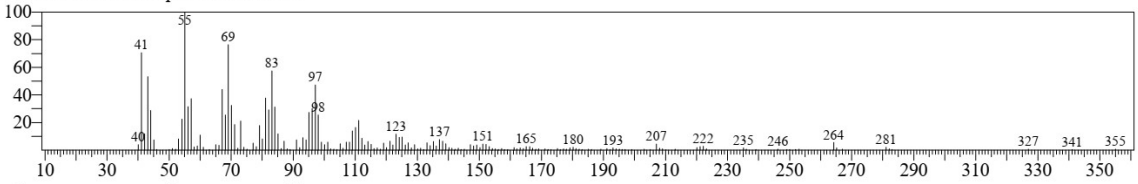
Library Search

<< Target >>

Line#:1 R.Time:24.900(Scan#:3981) MassPeaks:172

RawMode:Single 24.900(3981) BasePeak:55.10(10000)

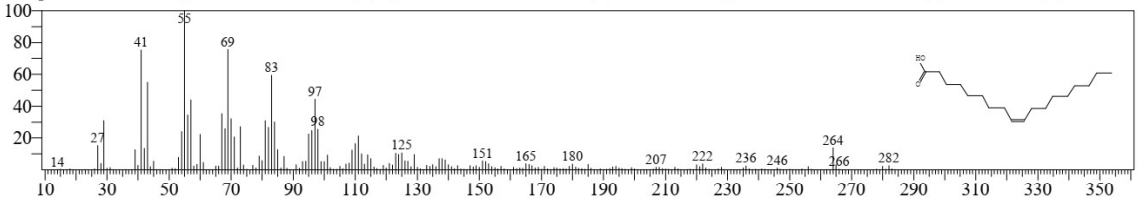
BG Mode:None Group 1 - Event 1 Scan



Hit#:1 Entry:25039 Library:NIST11s.lib

SI:92 Formula:C18H34O2 CAS:112-80-1 MolWeight:282 RetIndex:2175

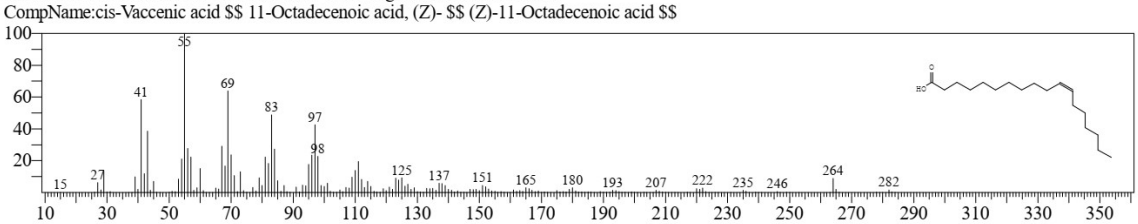
CompName:Oleic Acid $$ 9-Octadecenoic acid (Z)- $$ .DELTA.9-cis-Oleic acid $$ cis-Oleic Acid $$ cis-9-Octadecenoic Acid $$ Emersol 211 $$ Emersol



Hit#:2 Entry:104412 Library:NIST11.lib

SI:90 Formula:C18H34O2 CAS:506-17-2 MolWeight:282 RetIndex:2175

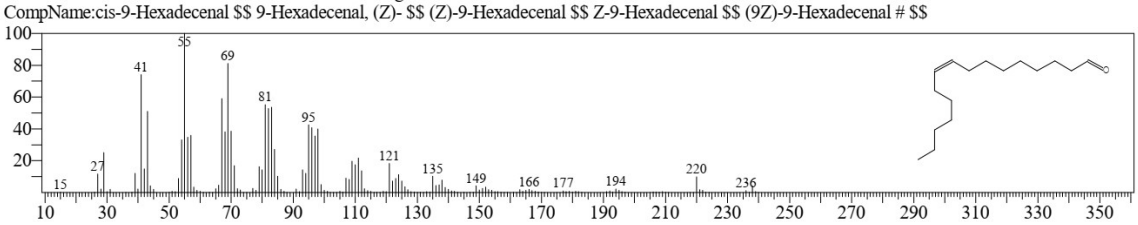
CompName:cis-Vaccenic acid $$ 11-Octadecenoic acid, (Z)- $$ (Z)-11-Octadecenoic acid $$



Hit#:3 Entry:70898 Library:NIST11.lib

SI:90 Formula:C16H30O CAS:56219-04-6 MolWeight:238 RetIndex:1808

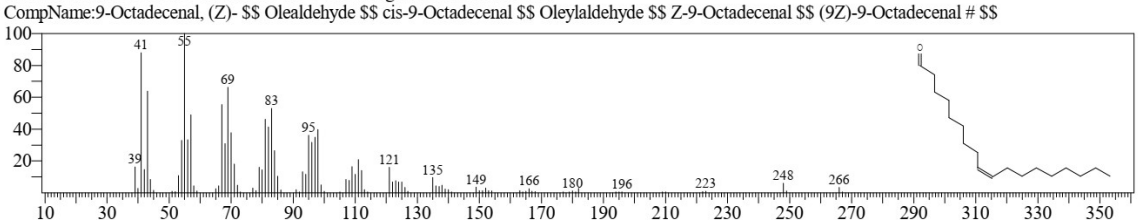
CompName:cis-9-Hexadecenal $$ 9-Hexadecenal, (Z)- $$ (Z)-9-Hexadecenal $$ Z-9-Hexadecenal $$ (9Z)-9-Hexadecenal # $$



Hit#:4 Entry:91949 Library:NIST11.lib

SI:90 Formula:C18H34O CAS:2423-10-1 MolWeight:266 RetIndex:2007

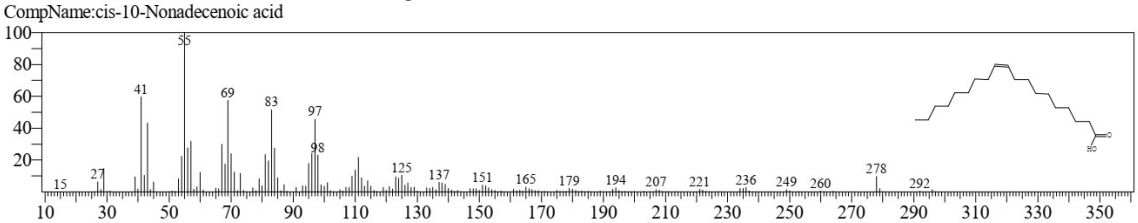
CompName:9-Octadecenal, (Z)- $$ Olealdehyde $$ cis-9-Octadecenal $$ Oleylaldehyde $$ Z-9-Octadecenal $$ (9Z)-9-Octadecenal # $$



Hit#:5 Entry:115406 Library:NIST11.lib

SI:90 Formula:C19H36O2 CAS:73033-09-7 MolWeight:296 RetIndex:2274

CompName:cis-10-Nonadecenoic acid



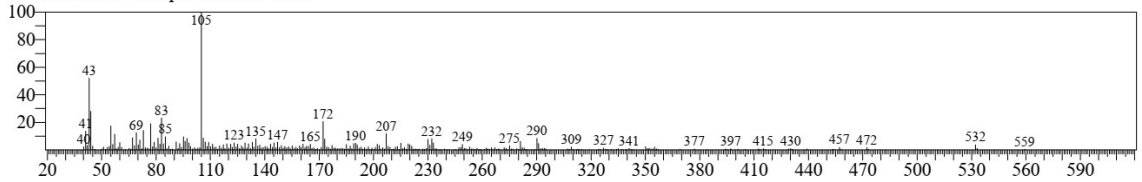
Library Search

<< Target >>

Line#:1 R.Time:26.860(Scan#:4373) MassPeaks:291

RawMode:Single 26.860(4373) BasePeak:105.05(10000)

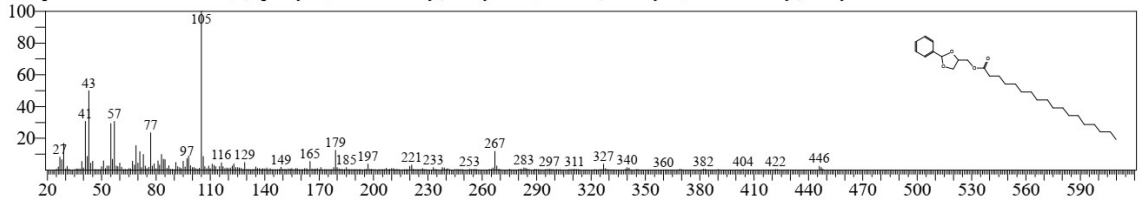
BG Mode:None Group 1 - Event 1 Scan



Hit#:1 Entry:196084 Library:NIST11.lib

SI:70 Formula:C28H46O4 CAS:56599-88-3 MolWeight:446 RetIndex:3230

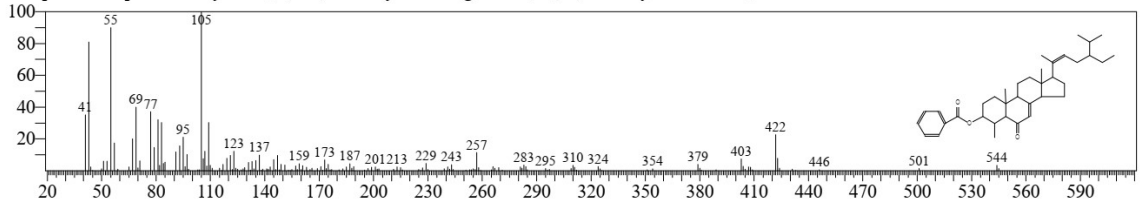
CompName:Octadecanoic acid, (2-phenyl-1,3-dioxolan-4-yl)methyl ester, cis- $$ (2-Phenyl-1,3-dioxolan-4-yl)methyl stearate # $$



Hit#:2 Entry:208114 Library:NIST11.lib

SI:68 Formula:C37H52O3 CAS:0-00-0 MolWeight:544 RetIndex:3726

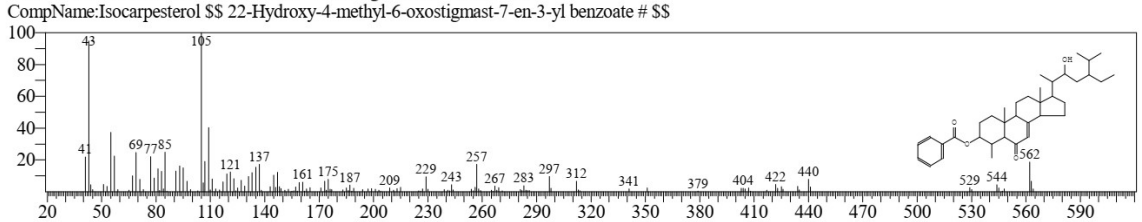
CompName:Carpesterol dehydrate $$ (20Z)-4-Methyl-6-oxostigmasta-7,20(22)-dien-3-yl benzoate # $$



Hit#:3 Entry:209017 Library:NIST11.lib

SI:67 Formula:C37H54O4 CAS:0-00-0 MolWeight:562 RetIndex:3839

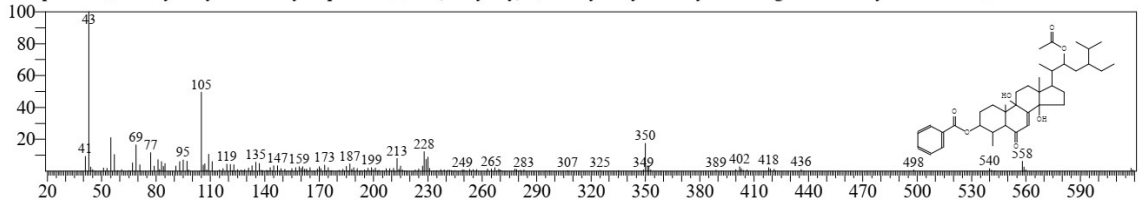
CompName:Isocarpesterol $$ 22-Hydroxy-4-methyl-6-oxostigmast-7-en-3-yl benzoate # $$



Hit#:4 Entry:211068 Library:NIST11.lib

SI:67 Formula:C39H56O7 CAS:0-00-0 MolWeight:636 RetIndex:4279

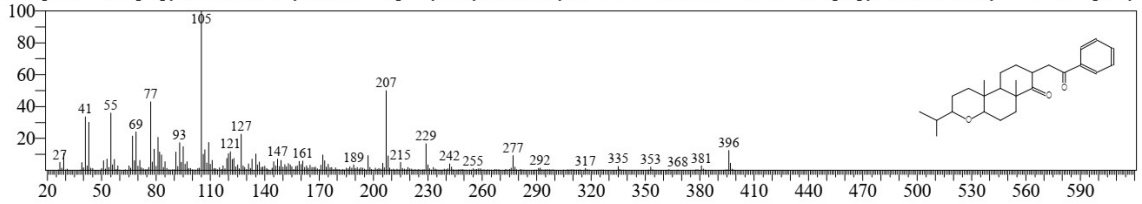
CompName:9,14-Dihydroxy-22-O-acetylcarpesterol $$ 22-(Acetyloxy)-9,14-dihydroxy-4-methyl-6-oxostigmast-7-en-3-yl benzoate # $$



Hit#:5 Entry:180829 Library:NIST11.lib

SI:66 Formula:C26H36O3 CAS:0-00-0 MolWeight:396 RetIndex:2956

CompName:3-Isopropyl-6a,10b-dimethyl-8-(2-oxo-2-phenyl-ethyl)-dodecahydro-benzo[f]chromen-7-one $$ 3-Isopropyl-6a,10b-dimethyl-8-(2-oxo-2-pheny



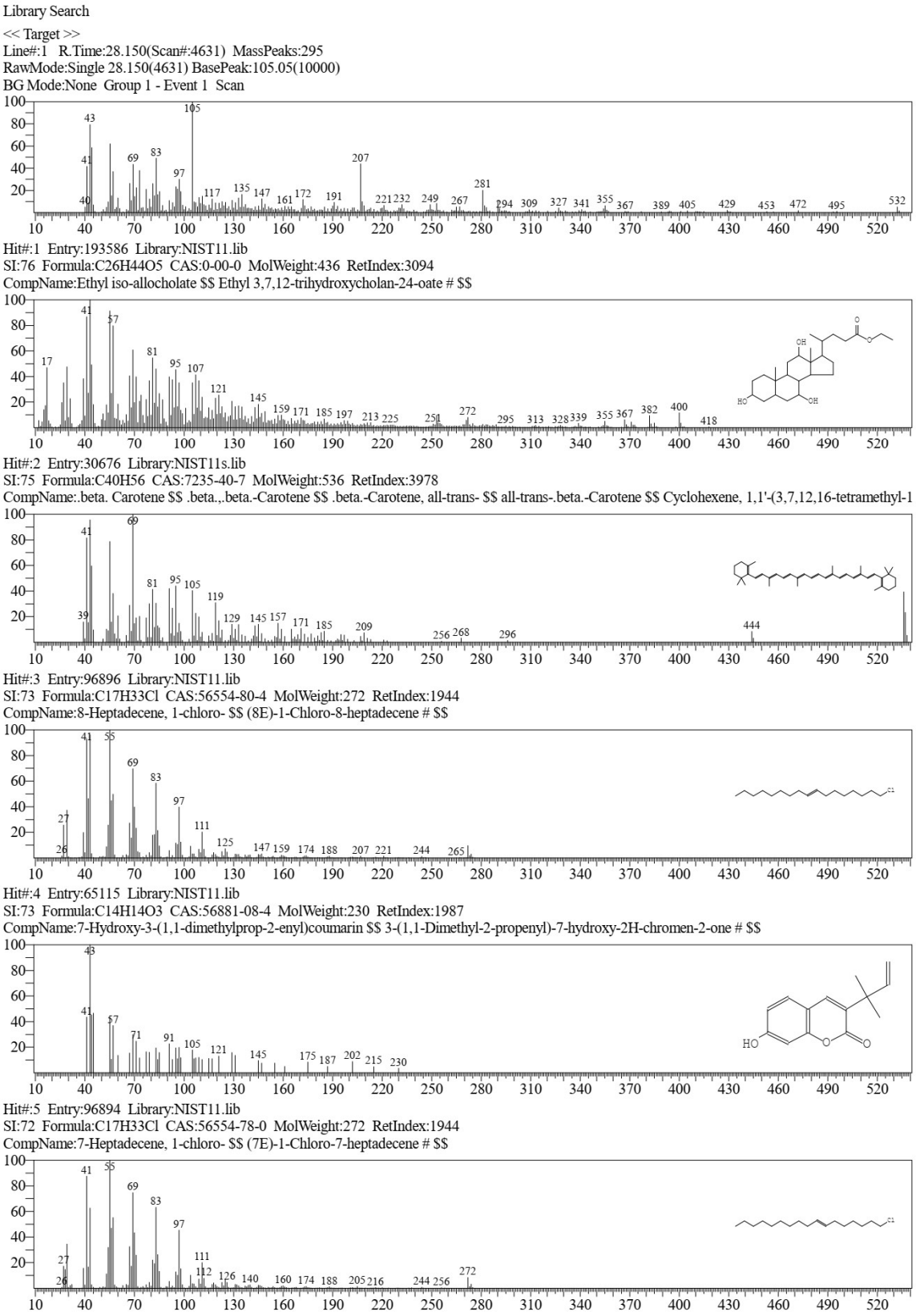


Figure SI-2. GC-MS analysis data of BL (a), BS (b) and BSc (c) extracts

(a)

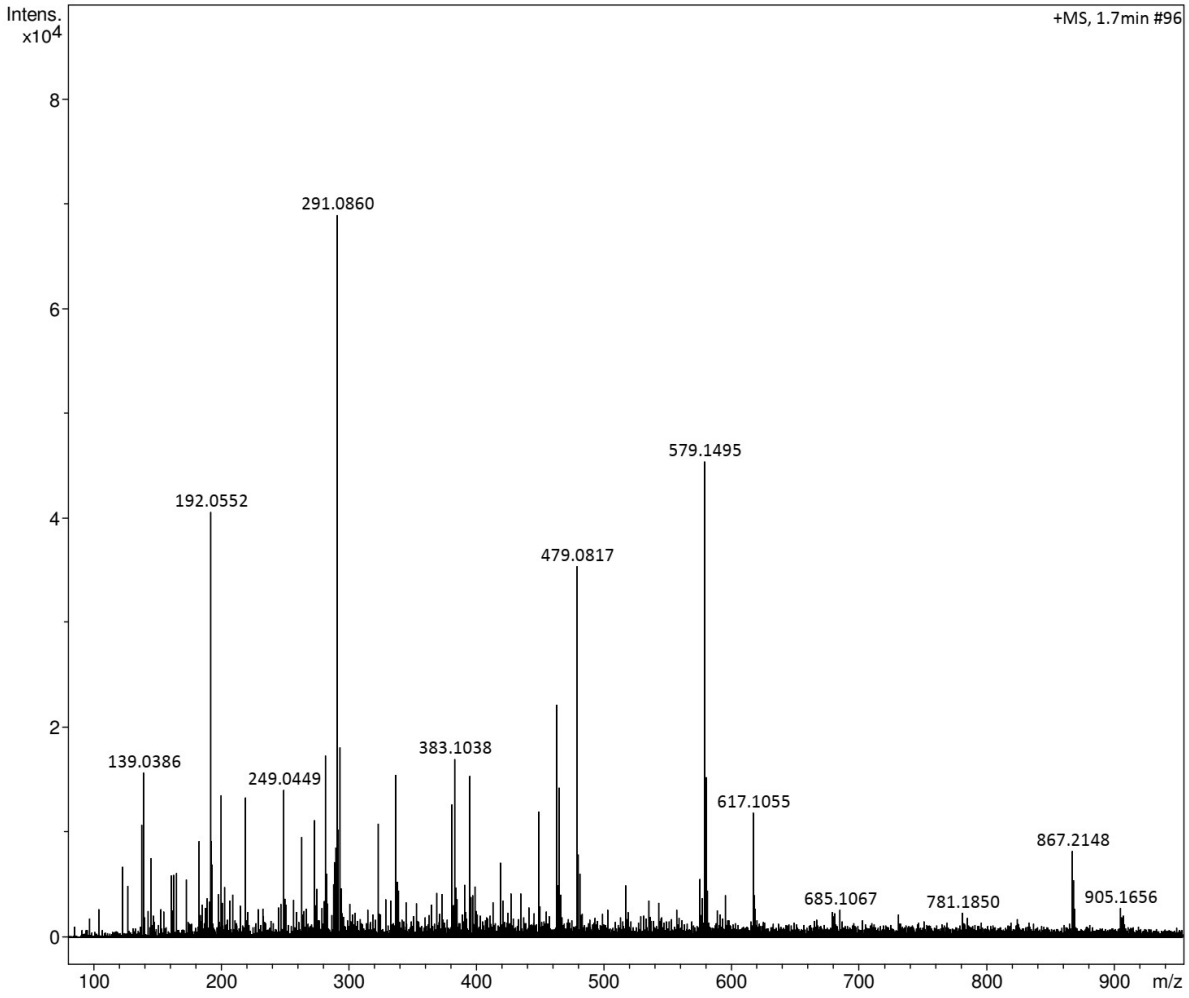
Savitribai Phule Pune University - Central Instrumentation Facility

Analysis Info

Analysis Name	D:\Data\2021\JULY\SPPU CAMPUS\DEPT OF CHEM\PROF. BALAPRASAD ANKAMWAR\BL_RB4_01_2899.d	Acquisition Date	7/28/2021 5:48:49 PM
Method	dlc_ms50-1500mz_10min_0.120ml flow_90b.m	Operator	CIF
Sample Name	BL	Instrument	impact HD 1819696.00184
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.7 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



(b)

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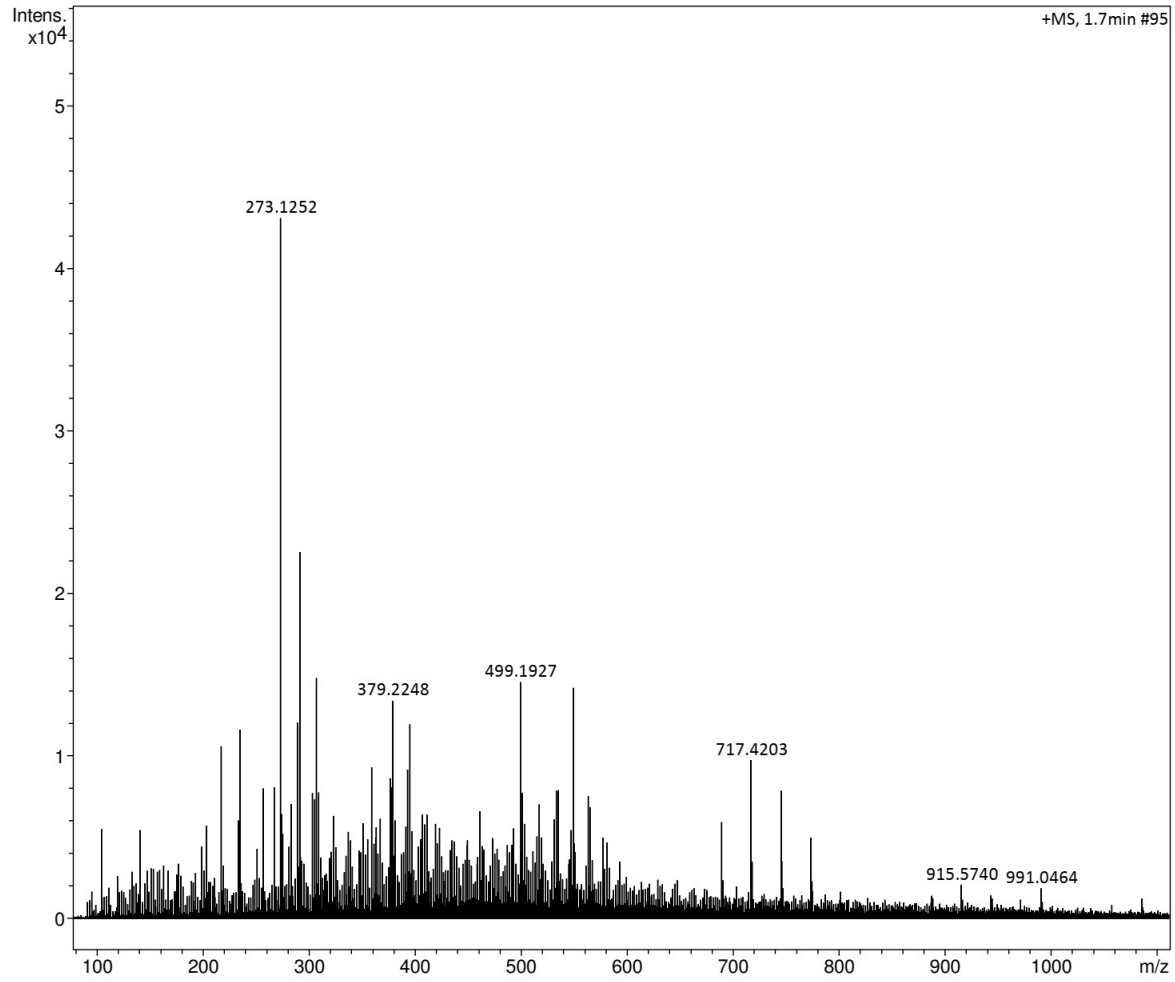
Analysis Info

Analysis Name	D:\Data\2021\JULY\SPPU CAMPUS\DEPT OF CHEM\PROF. BALAPRASAD ANKAMWAR\BS_RB3_01_2898.d	Acquisition Date	7/28/2021 5:38:11 PM
Method	dlc_ms50-1500mz_10min_0.120ml flow_90b.m	Operator	CIF
Sample Name	BS	Instrument	impact HD 1819696.00184
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.7 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



(c)

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Analysis Info

Analysis Name	D:\Data\2021\JULY\SPPU CAMPUS\DEPT OF CHEM\PROF. BALAPRASAD ANKAMWAR\BSh_RB2_01_2897.d	Acquisition Date	7/28/2021 5:27:31 PM
Method	dlc_ms50-1500mz_10min_0.120ml flow_90b.m	Operator	CIF
Sample Name	BSh	Instrument	impact HD 1819696.00184
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.7 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

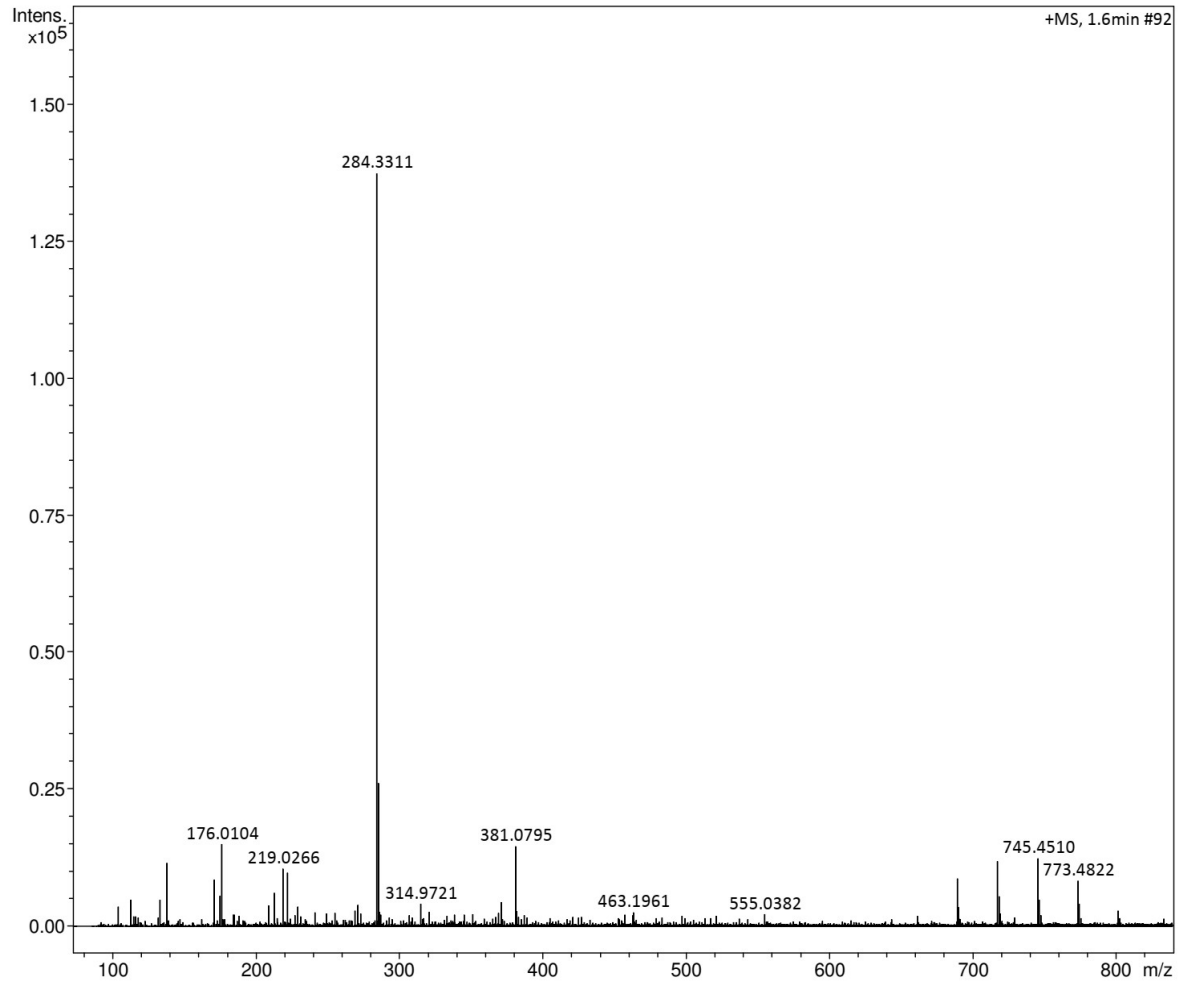
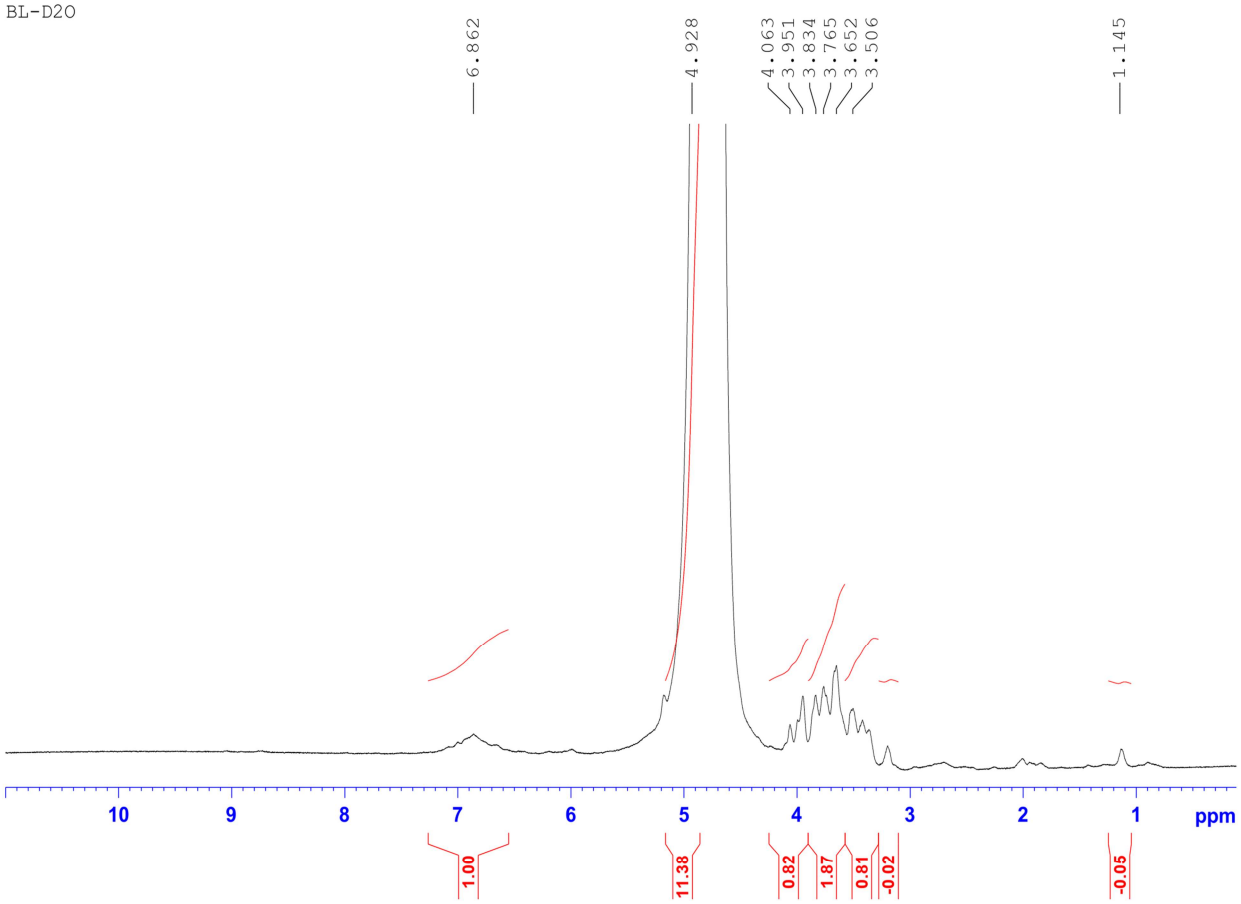
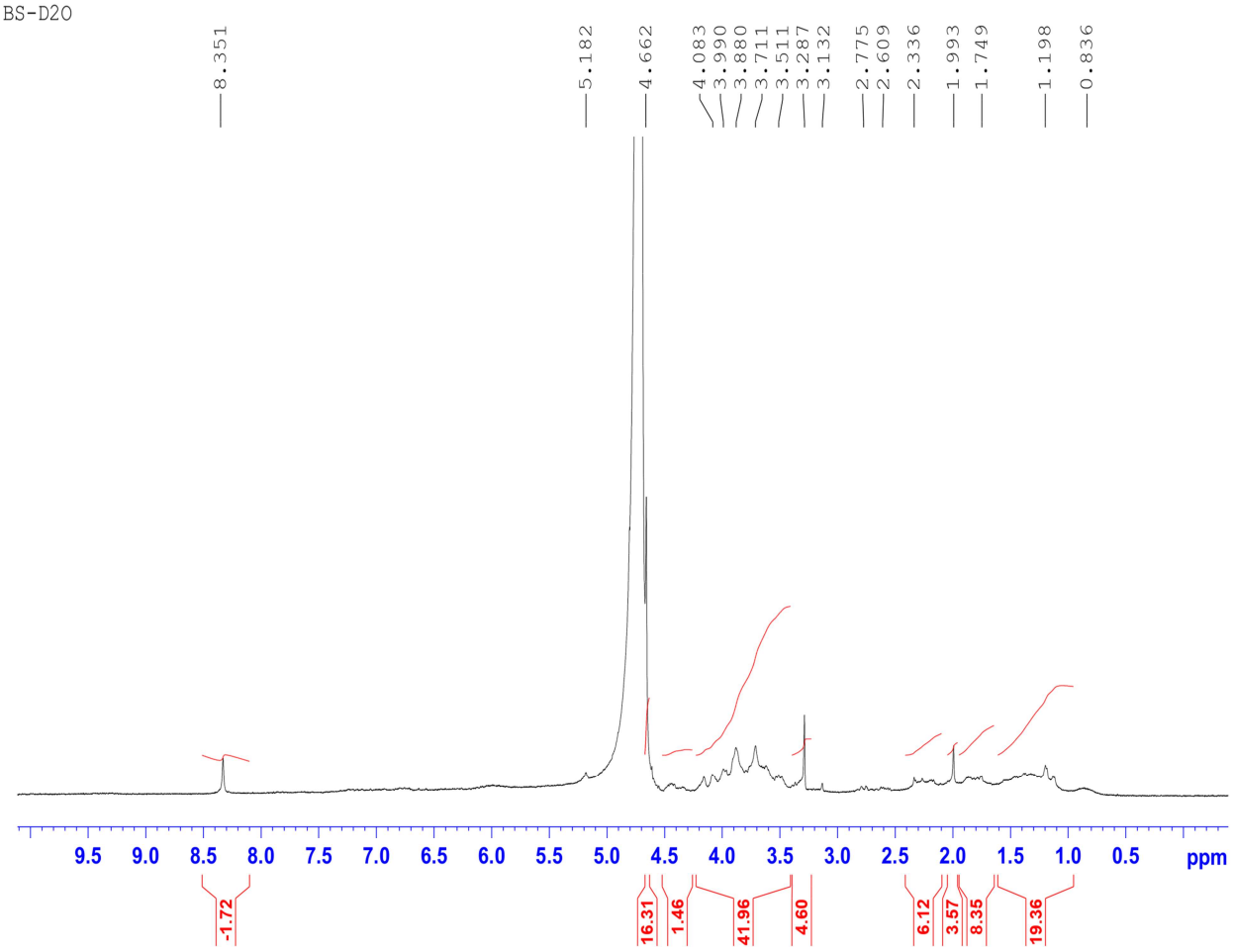


Figure SI-3. HR-MS spectra of BL (a), BS (b), BSc (c) extracts

(a) BL-D2O


6.862
4.928
4.063
3.951
3.834
3.765
3.652
3.506
1.145
10
9
8
7
6
5
4
3
2
1
ppm
1.00
11.38
0.82
1.87
0.81
-0.02
-0.05

(b) BS-D2O


8.351
5.182
4.662
4.083
3.990
3.880
3.711
3.511
3.287
3.132
2.775
2.609
2.336
1.993
1.749
1.198
0.836
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
-1.72
16.31
1.46
41.96
4.60
6.12
3.57
8.35
19.36

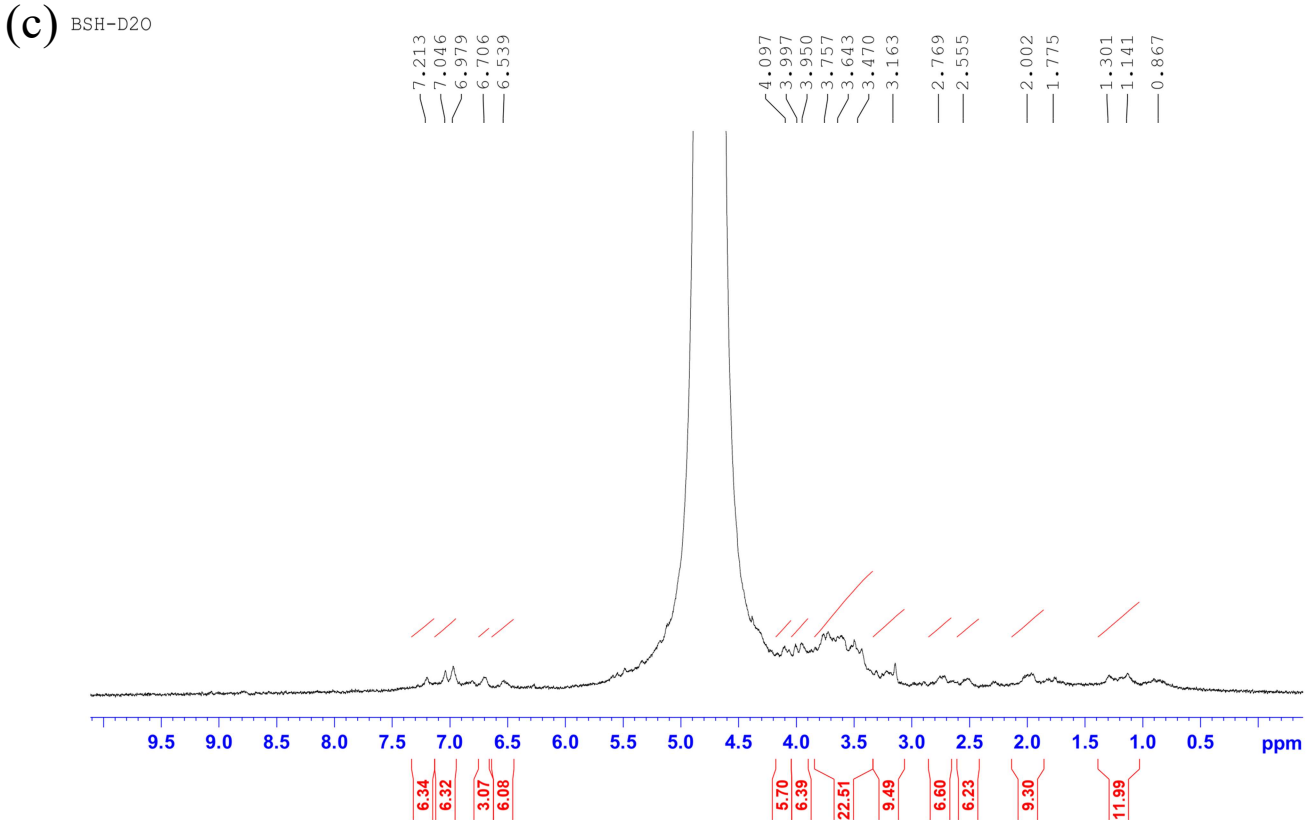


Figure SI-4. NMR spectra of BL (a), BS (b) and BSc (c) extracts