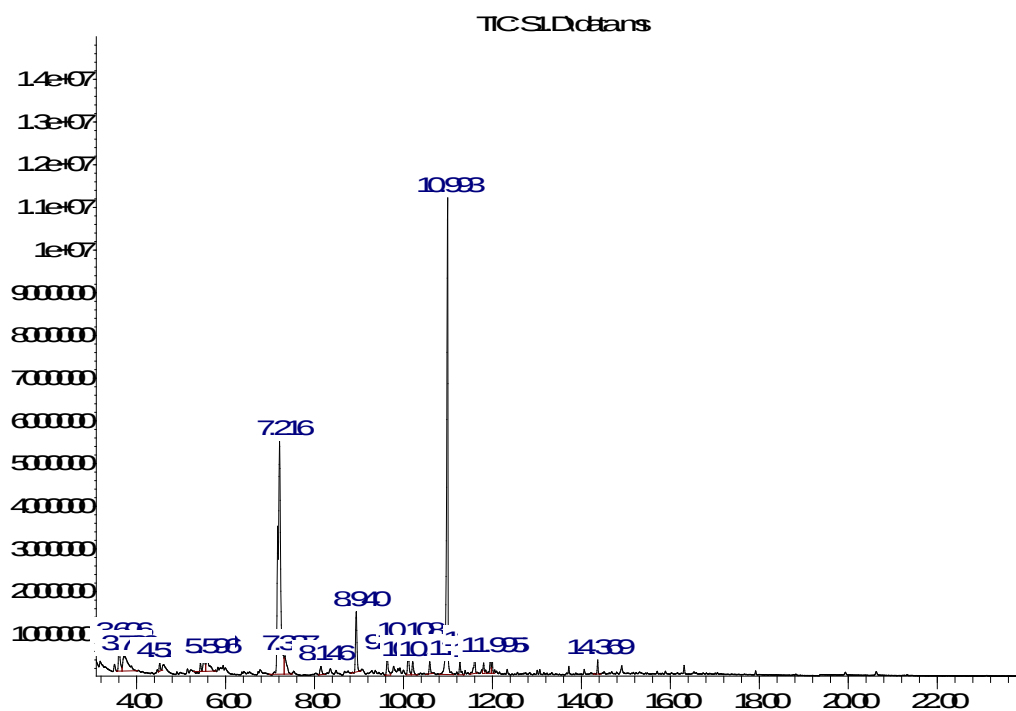


Abundance



Time-->

Library Search Report

Data Path : C:\msdchem\1\methods\scan.M\

Data File : S1.D

Acq On : 19 Nov 2024 14:34

Operator :

Sample : S1

Misc :

ALS Vial : 1 Sample Multiplier: 1

Search Libraries: C:\Database\NIST14.L

Minimum Quality: 90

Unknown Spectrum: Apex

Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	3.606	2.58	C:\Database\NIST14.L			
			Eucalyptol	27464	000470-82-6	59
			2-Heptyne	2864	001119-65-9	49
			3,8,11-Trioxatetracyclo[4.4.1.0(2,4).0(7,9)]undecane, (1.alpha.,2.beta.,4.beta.,6.alpha.,7.beta.,9.beta.)-	28353	050267-13-5	49
2	3.725	4.46	C:\Database\NIST14.L			
			Eucalyptol	27467	000470-82-6	56
			2-Heptyne	2864	001119-65-9	49
			2-Octyne	5996	002809-67-8	43
3	4.519	0.52	C:\Database\NIST14.L			
			2-Hepten-1-ol, (E)-	7621	033467-76-4	52
			(Z)-4-Decen-1-ol, trifluoroacetate	112948	1000352-33-5	38
			2-Octyne	5996	002809-67-8	38
4	5.437	0.15	C:\Database\NIST14.L			
			endo-Borneol	27489	000507-70-0	72
			Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, (1S-endo)-	27824	000464-45-9	72

			1,4-Pentadiene, 2,3,3-trimethyl-	6130 000756-02-5 64
5	5.521	1.54	C:\Database\NIST14.L	
			9-Azadispiro[3.1.3.0]nonane	10415 135763-48-3 64
			Cyclopentane, (3-methylbutylidene)	17366 053366-51-1 60
			Isoborneol	27470 000124-76-5 60
6	5.593	2.31	C:\Database\NIST14.L	
			Santolina epoxide	25854 060485-45-2 52
			2-Nonyne	10817 019447-29-1 49
			Bicyclo[4.1.0]heptane, 3,7,7-trime	17429 002778-68-9 49
			thyl-, [1S-(1.alpha.,3.beta.,6.alp	
			ha.)]-	
7	7.217	34.79	C:\Database\NIST14.L	
			Phenol, 2-methyl-5-(1-methylethyl)	24485 000499-75-2 81
			Phenol, 2-methyl-5-(1-methylethyl)	24486 000499-75-2 81
			3-Methyl-4-isopropylphenol	24408 003228-02-2 81
8	7.337	2.50	C:\Database\NIST14.L	
			3-Methyl-4-isopropylphenol	24408 003228-02-2 90
			Thymol	24338 000089-83-8 87
			Phenol, 2-ethyl-4,5-dimethyl-	24439 002219-78-5 87
9	8.146	0.82	C:\Database\NIST14.L	
			2-Undecenal	38128 002463-77-6 50
			9-Oxabicyclo[6.1.0]nonane, cis-	11674 004925-71-7 43

10-Undecenal 38132 000112-45-8 38

10 8.940 4.96 C:\Database\NIST14.L

Caryophyllene 68509 000087-44-5 70

1,3,6,10-Dodecatetraene, 3,7,11-tr 68667 026560-14-5 50

imethyl-, (Z,E)-

Caryophyllene 68512 000087-44-5 49

11 9.640 1.72 C:\Database\NIST14.L

Naphthalene, 1,2,4a,5,6,8a-hexahyd 68752 000483-75-0 98

ro-4,7-dimethyl-1-(1-methylethyl)-

.gamma.-Muurolene 68569 030021-74-0 98

.gamma.-Muurolene 68584 030021-74-0 98

12 10.107 2.30 C:\Database\NIST14.L

Naphthalene, 1,2,4a,5,6,8a-hexahyd 68752 000483-75-0 98

ro-4,7-dimethyl-1-(1-methylethyl)-

.beta.-copaene 68520 1000374-18-9 94

.gamma.-Muurolene 68584 030021-74-0 93

13 10.211 1.09 C:\Database\NIST14.L

cis-Calamenene 66834 072937-55-4 90

1H-Indene, 2,3-dihydro-1,1,5,6-tet 43061 000942-43-8 87

ramethyl-

1H-Indene, 2,3-dihydro-1,1,4,5-tet 43063 016204-57-2 80

ramethyl-

14 10.595 0.84 C:\Database\NIST14.L

Bicyclo[4.1.0]heptane,-3-cycloprop 36538 1000223-00-6 72
yl,-7-hydroxymethyl, trans

Bicyclo[4.1.0]heptane,-3-cycloprop 36539 1000223-00-7 64
yl,-7-hydroxymethyl, (cis)

Preg-4-en-3-one, 17.alpha.-hydroxy 172241 1000294-64-4 59
-17.beta.-cyano-

15 10.995 33.38 C:\Database\NIST14.L

Caryophyllene oxide 83535 001139-30-6 87

Caryophyllene oxide 83533 001139-30-6 53

(Z,Z)-3,6-Nonadienal 17953 021944-83-2 49

16 11.270 1.07 C:\Database\NIST14.L

Santolina triene 16072 002153-66-4 58

Preg-4-en-3-one, 17.alpha.-hydroxy 172241 1000294-64-4 47
-17.beta.-cyano-

2,6-Octadiyne 5177 000764-73-8 25

17 11.607 1.72 C:\Database\NIST14.L

Bicyclo[4.4.0]dec-1-ene, 2-isoprop 68697 150320-52-8 92
yl-5-methyl-9-methylene-

(1R,2S,6S,7S,8S)-8-Isopropyl-1-met 68812 018252-44-3 89
hyl-3-methylenetricyclo[4.4.0.02,7
]decane-rel-

(+)-epi-Bicyclosquiphellandrene 68646 054274-73-6 86

18	11.804	0.67	C:\Database\NIST14.L	
			1-Octen-3-yne	5496 017679-92-4 66
			Preg-4-en-3-one, 17.alpha.-hydroxy	172241 1000294-64-4 64
			-17.beta.-cyano-	
			1-Octen-3-yne	5495 017679-92-4 44
19	11.954	1.01	C:\Database\NIST14.L	
			1,5-Decadiyne	15153 053963-03-4 52
			Santolina triene	16072 002153-66-4 46
			Dicyclopentadiene diepoxide	34612 000081-21-0 38
20	11.996	0.86	C:\Database\NIST14.L	
			Naphthalene, 1,6-dimethyl-4-(1-met	63658 000483-78-3 97
			hylethyl)-	
			Azulene, 1,4-dimethyl-7-(1-methyle	63653 000489-84-9 95
			thyl)-	
			Azulene, 1,4-dimethyl-7-(1-methyle	63655 000489-84-9 93
			thyl)-	
21	14.367	0.71	C:\Database\NIST14.L	
			2-Carene	16041 000554-61-0 46
			3-Carene	16028 013466-78-9 46
			Cyclohexene, 1-methyl-4-(1-methyle	16230 000586-62-9 46
			thylidene)-	

Area Percent Report

Data Path : C:\msdchem\1\methods\scan.M\

Data File : S1.D

Acq On : 19 Nov 2024 14:34

Operator :

Sample : S1

Misc :

ALS Vial : 1 Sample Multiplier: 1

Integration Parameters: autoint1.e

Integrator: ChemStation

Method : C:\msdchem\1\methods\PAHs.M

Title :

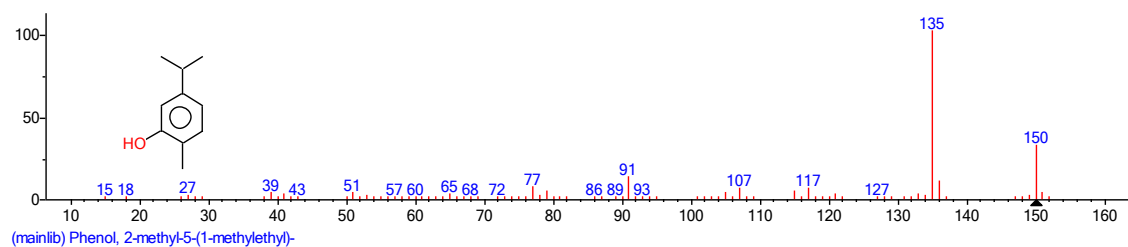
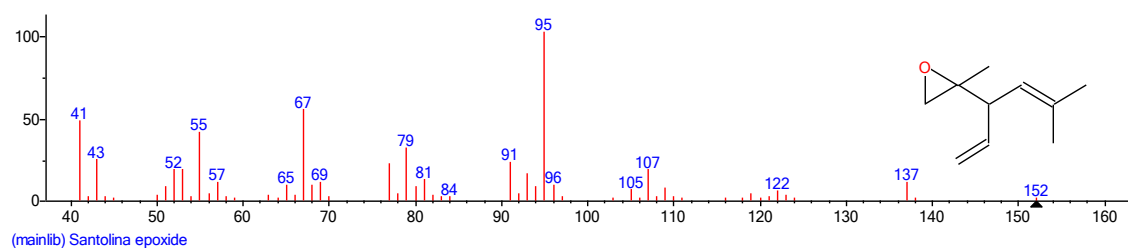
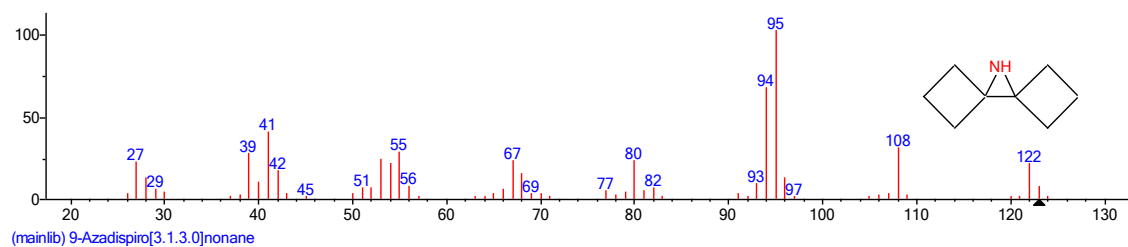
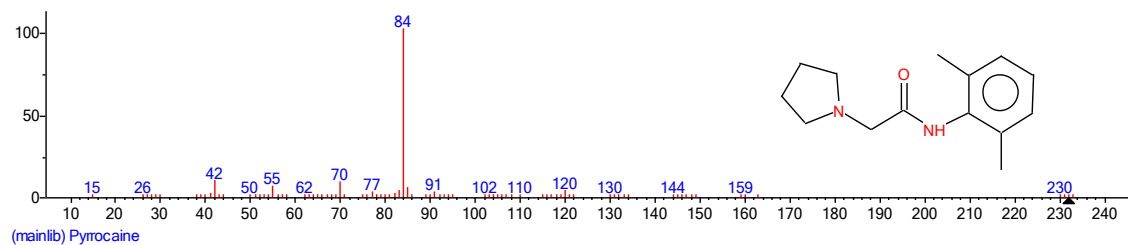
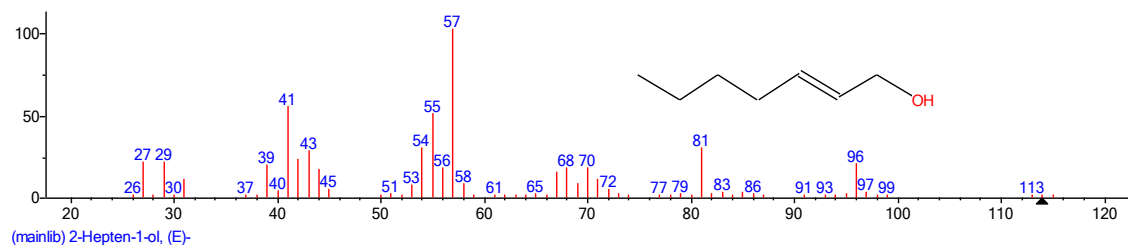
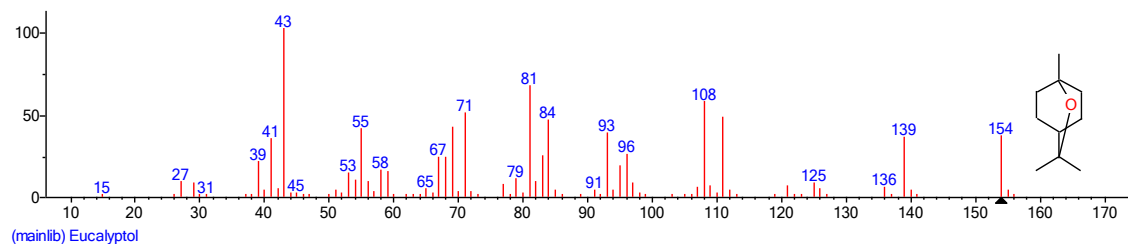
Signal : TIC: S1.D\data.ms

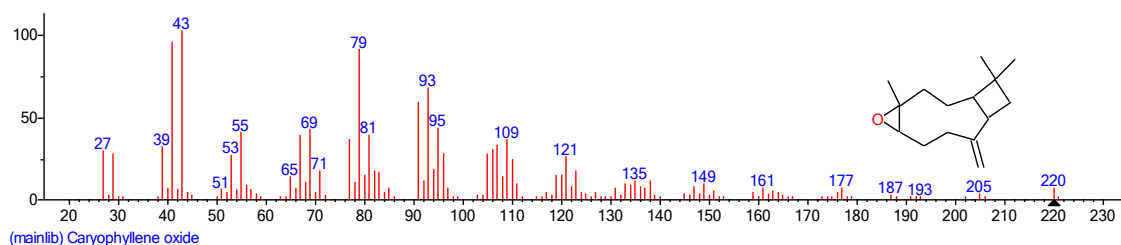
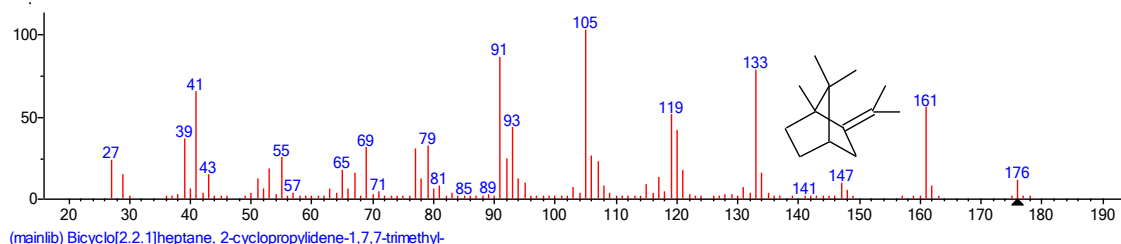
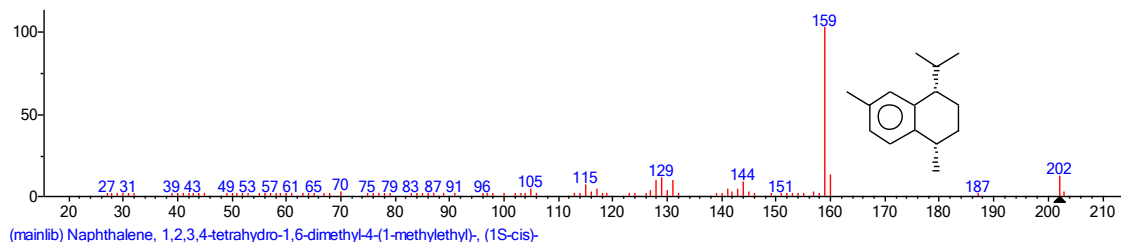
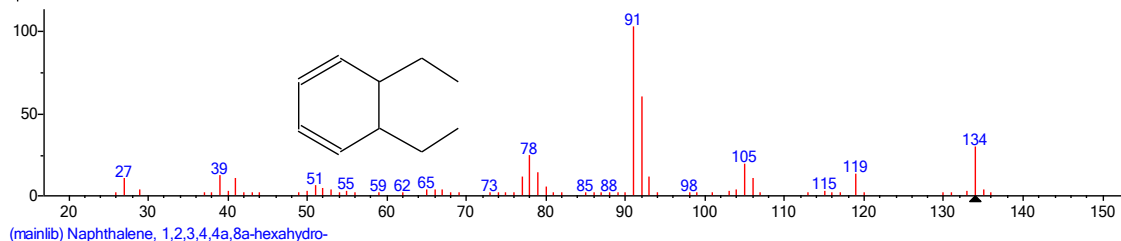
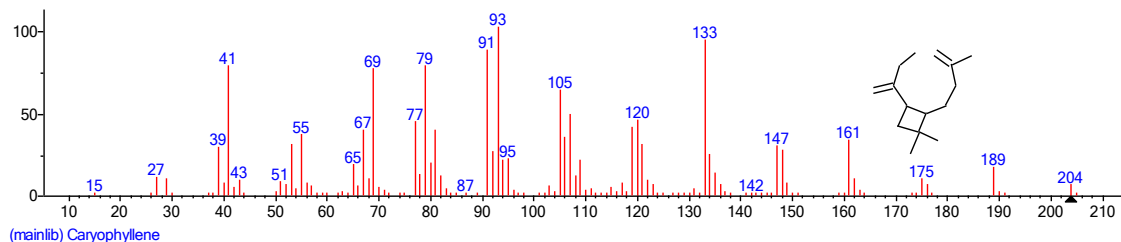
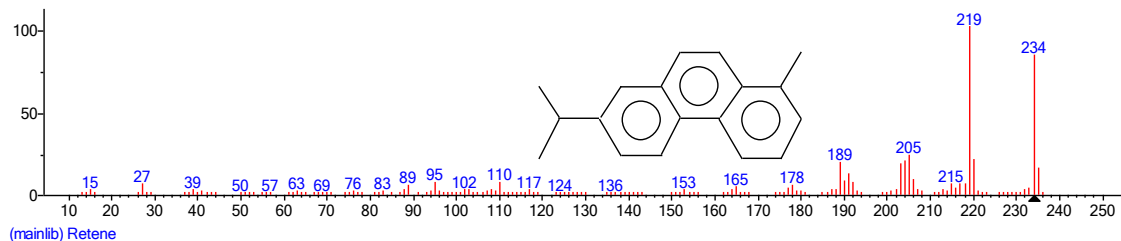
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
---	-----	-----	-----	-----	-----	-----	-----	-----	-----
1	3.606	89	100	113	PV 2	656505	16937453	7.42%	2.582%
2	3.726	113	123	176	VB 10	347660	29252462	12.82%	4.459%
3	4.521	270	276	284	PV 4	185363	3443219	1.51%	0.525%
4	5.438	424	453	459	BV 2	193942	995936	0.44%	0.152%
5	5.519	459	469	475	VV 3	379229	10130924	4.44%	1.544%

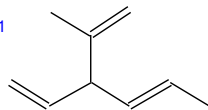
6	5.596	475	483	515 VV 7	299640	15126042	6.63%	2.306%
7	7.216	751	796	815 BV	5442845	228216414	100.00%	34.790%
8	7.337	815	819	848 VV 3	424031	16396243	7.18%	2.499%
9	8.146	965	975	989 PV 3	197701	5398683	2.37%	0.823%
10	8.940	1105	1128	1143 BV 2	1420019	32505527	14.24%	4.955%
11	9.638	1253	1263	1277 BV 2	474551	11275264	4.94%	1.719%
12	10.108	1345	1353	1366 VV	723939	15091649	6.61%	2.301%
13	10.210	1366	1373	1391 VB 3	305865	7154887	3.14%	1.091%
14	10.592	1429	1447	1457 BV 3	280808	5492130	2.41%	0.837%
15	10.993	1488	1524	1549 BV	10828613	218982772	95.95%	33.382%
16	11.271	1570	1577	1593 VV 2	320167	6996384	3.07%	1.067%
17	11.604	1619	1642	1649 PV 2	503250	11254279	4.93%	1.716%
18	11.804	1675	1680	1686 VV 4	243049	4385013	1.92%	0.668%
19	11.955	1694	1709	1713 VV 4	348918	6621364	2.90%	1.009%
20	11.995	1713	1717	1723 VV	360847	5666504	2.48%	0.864%
21	14.369	2156	2174	2183 BV	319101	4668597	2.05%	0.712%

Sum of corrected areas: 655991746

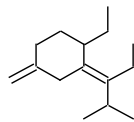
scan.M Tue Nov 19 15:11:34 2024







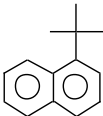
(mainlib) Santolina triene



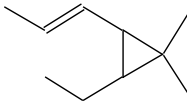
(mainlib) Bicyclo[4.4.0]dec-1-ene, 2-isopropyl-5-methyl-9-methylene-



(mainlib) 1-Octen-3-yne



(mainlib) Naphthalene, 1-(1,1-dimethylethyl)-



(mainlib) (+)-2-Carene