

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD102021\
 Data File : VD070777.D
 Acq On : 20 Oct 2021 15:52
 Operator : VA/SY
 Sample : M4284-02
 Misc : 5.03G/5.00ml/MSVOA_D/SOIL
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 20878-SOLID

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D101521S.M
 Title : SW846 8260

Signal : TIC: VD070777.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.150	370	379	390	rBV	182543	514238	18.96%	2.595%
2	4.409	413	423	431	rBV2	34723	102610	3.78%	0.518%
3	4.962	508	517	533	rVB3	43603	137773	5.08%	0.695%
4	5.985	681	691	700	rBV7	12385	36652	1.35%	0.185%
5	7.208	889	899	910	rBV3	31109	83474	3.08%	0.421%
6	7.908	1007	1018	1023	rBV	353331	835393	30.80%	4.216%
7	7.973	1023	1029	1040	rVB	585188	1349044	49.74%	6.808%
8	8.326	1077	1089	1104	rBV	333363	791791	29.19%	3.996%
9	8.861	1168	1180	1189	rBV2	952222	1922678	70.89%	9.703%
10	10.338	1421	1431	1437	rBV	1497929	2712342	100.00%	13.688%
11	10.397	1437	1441	1446	rVB	62366	113077	4.17%	0.571%
12	10.514	1456	1461	1467	rBV3	20432	35916	1.32%	0.181%
13	10.720	1488	1496	1501	rBV3	17494	33958	1.25%	0.171%
14	11.085	1552	1558	1564	rBV5	15609	28548	1.05%	0.144%
15	11.638	1644	1652	1662	rBV	1327800	2275646	83.90%	11.484%
16	11.738	1664	1669	1675	rVB2	31451	50400	1.86%	0.254%
17	11.844	1680	1687	1694	rVB2	89421	171196	6.31%	0.864%
18	12.167	1734	1742	1750	rVB2	35288	64724	2.39%	0.327%
19	12.473	1787	1794	1802	rBV4	25076	45456	1.68%	0.229%
20	12.620	1812	1819	1827	rBV	938605	1586956	58.51%	8.009%
21	12.873	1856	1862	1865	rBV	47429	78209	2.88%	0.395%
22	12.944	1870	1874	1882	rVB4	61507	110986	4.09%	0.560%
23	13.108	1891	1902	1910	rBV6	19988	53220	1.96%	0.269%
24	13.255	1922	1927	1932	rBV	92115	136353	5.03%	0.688%
25	13.408	1946	1953	1957	rBV5	21675	40755	1.50%	0.206%
26	13.502	1961	1969	1973	rVV	68019	113443	4.18%	0.572%
27	13.561	1973	1979	1986	rVV	1268049	2137998	78.82%	10.789%
28	13.626	1986	1990	2002	rVB2	211132	374732	13.82%	1.891%
29	13.767	2009	2014	2016	rBV5	20624	35065	1.29%	0.177%
30	13.873	2027	2032	2037	rBV7	15112	28445	1.05%	0.144%
31	14.020	2052	2057	2065	rBV6	27651	65134	2.40%	0.329%
32	14.232	2086	2093	2097	rBV7	18285	40780	1.50%	0.206%
33	14.332	2105	2110	2117	rVB4	35042	58799	2.17%	0.297%
34	14.414	2118	2124	2130	rBV3	106925	181524	6.69%	0.916%
35	14.467	2130	2133	2137	rVV2	18626	27404	1.01%	0.138%
36	14.520	2137	2142	2144	rVV2	122389	179022	6.60%	0.903%

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37	14.549	2144	2147	2159	rVV	230871	388382	14.32%	1.960%
38	14.649	2159	2164	2168	rVV7	19587	36751	1.35%	0.185%
39	14.702	2168	2173	2177	rVV8	17894	35981	1.33%	0.182%
40	14.743	2177	2180	2185	rVB4	19253	30455	1.12%	0.154%
41	14.820	2185	2193	2199	rBV5	46493	101479	3.74%	0.512%
42	14.879	2199	2203	2210	rVB7	29507	58121	2.14%	0.293%
43	15.085	2231	2238	2248	rBV4	66221	134718	4.97%	0.680%
44	15.196	2252	2257	2259	rBV3	120301	187829	6.92%	0.948%
45	15.226	2259	2262	2267	rVV2	178996	279866	10.32%	1.412%
46	15.273	2267	2270	2276	rVB6	37984	57013	2.10%	0.288%
47	15.355	2278	2284	2287	rBV2	220592	392433	14.47%	1.980%
48	15.396	2287	2291	2298	rVB	457505	748770	27.61%	3.779%
49	15.514	2309	2311	2318	rVB7	18207	30329	1.12%	0.153%
50	15.708	2335	2344	2348	rBV7	20789	54918	2.02%	0.277%
51	16.073	2398	2406	2410	rBV5	80302	163883	6.04%	0.827%
52	16.126	2410	2415	2422	rVV4	86551	167284	6.17%	0.844%
53	16.290	2436	2443	2446	rBV3	72994	145909	5.38%	0.736%
54	16.337	2446	2451	2461	rVB2	127899	247803	9.14%	1.251%

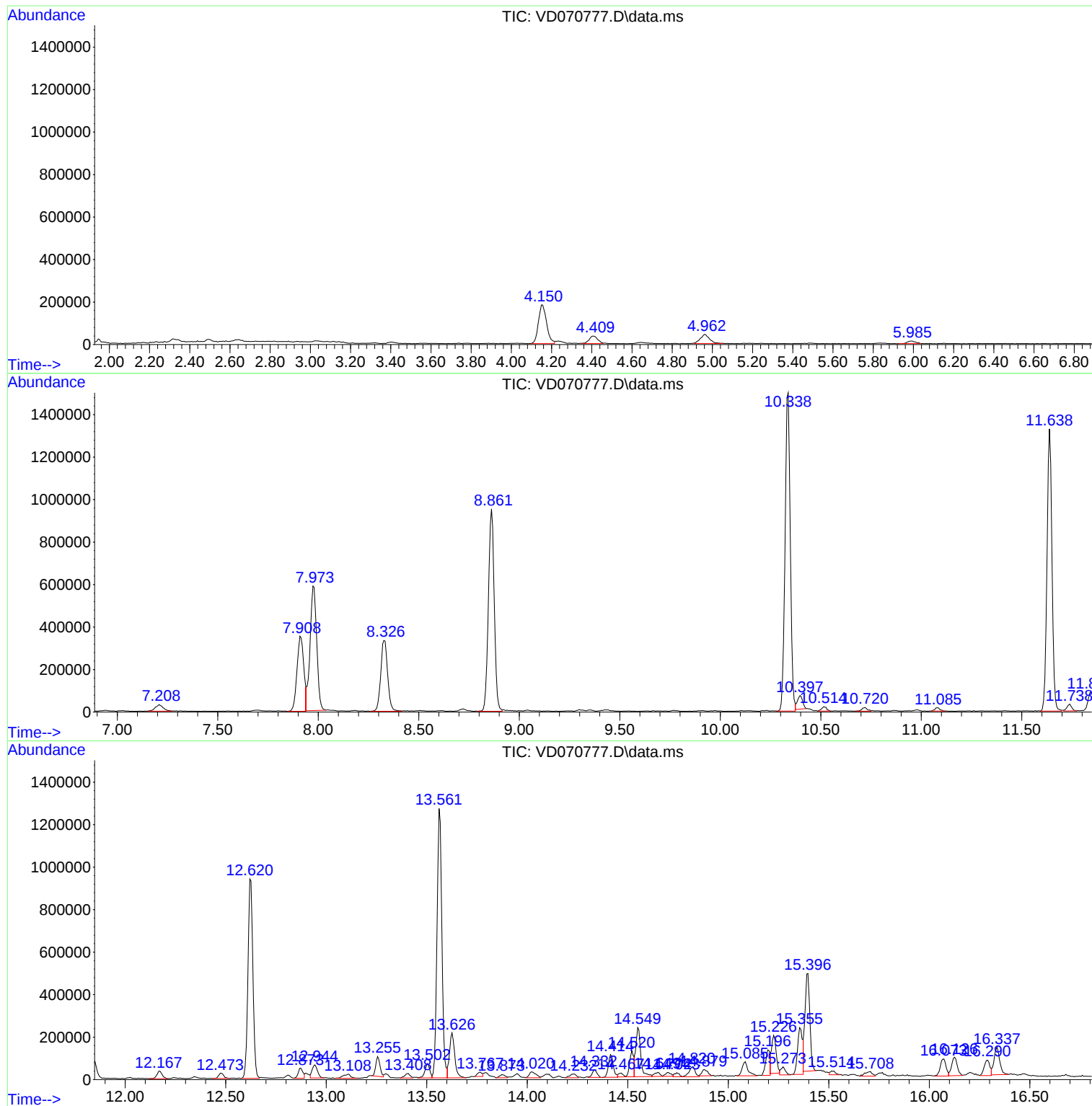
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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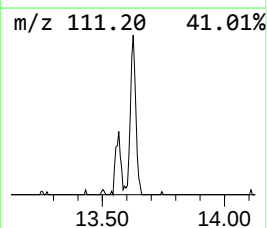
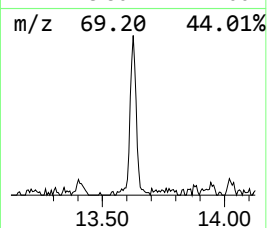
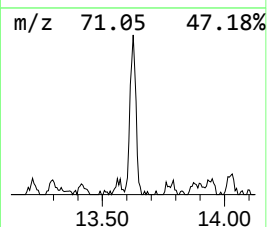
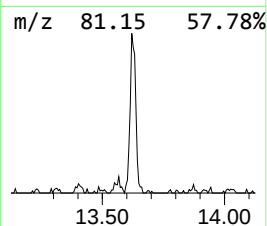
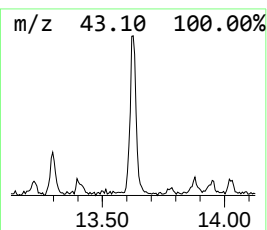
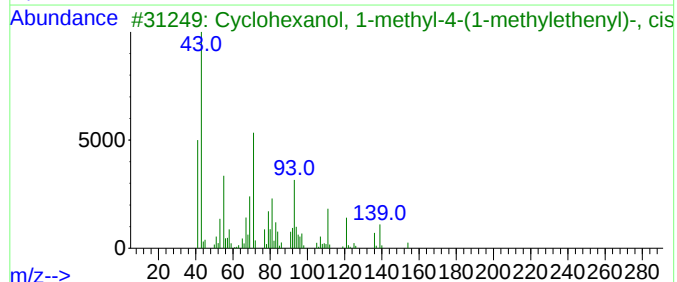
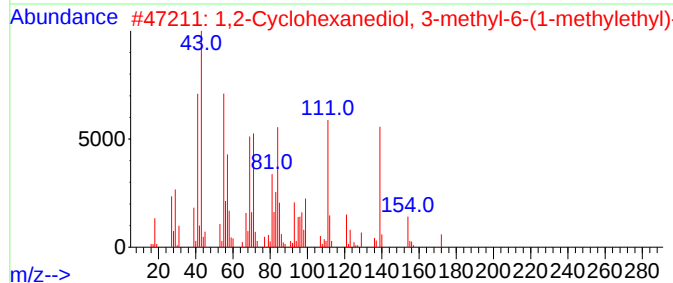
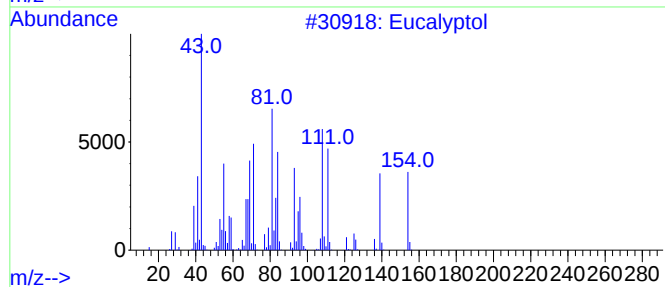
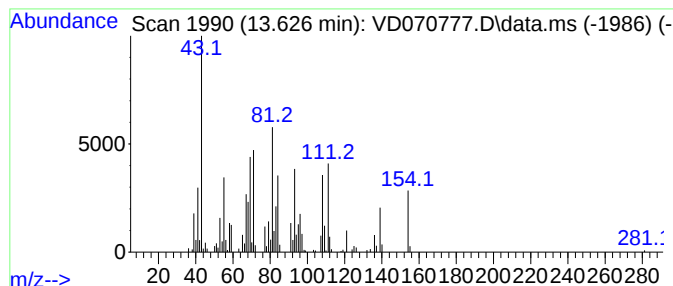
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D101521S.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Eucalyptol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.626	8.76 ug/l	374732	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eucalyptol	154	C10H18O	000470-82-6	95
2			1,2-Cyclohexanediol, 3-methyl-6-...	172	C10H20O2	042962-93-6	43
3			Cyclohexanol, 1-methyl-4-(1-meth...	154	C10H18O	007299-41-4	43
4			2-Heptanone, 3-propylidene-	154	C10H18O	032064-70-3	42
5			3-Ethylidene- heptan-2,6-dione	154	C9H14O2	1000223-47-9	14



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Instrument :
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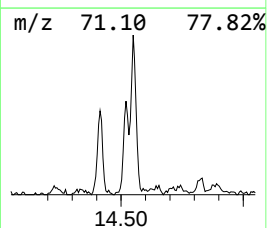
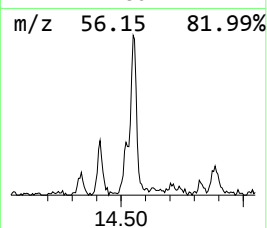
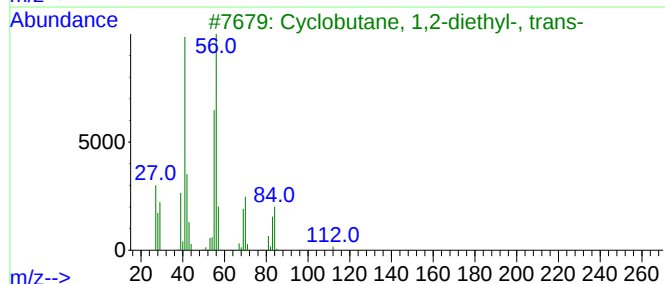
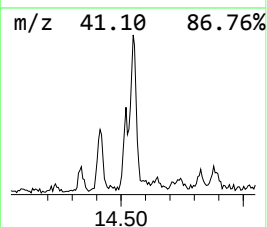
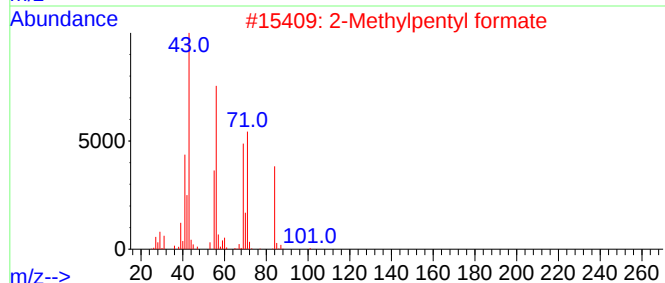
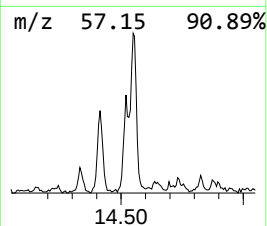
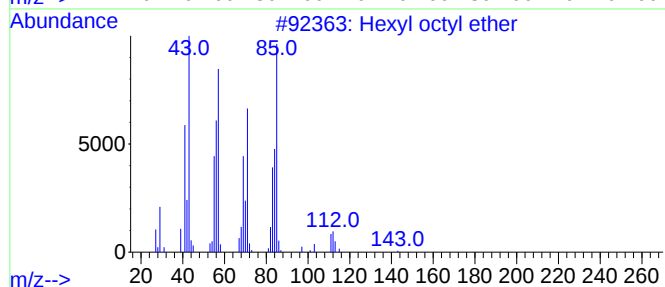
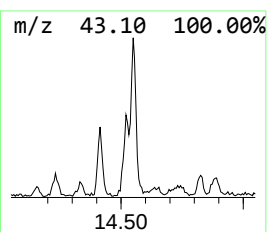
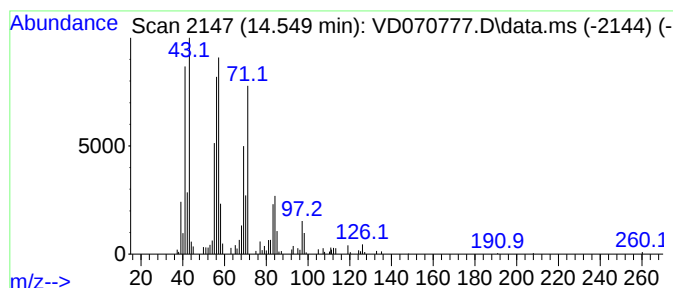
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D101521S.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Hexyl octyl ether Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.549	9.08 ug/l	388382	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexyl octyl ether	214	C14H30O	017071-54-4	64
2			2-Methylpentyl formate	130	C7H14O2	381670-34-4	52
3			Cyclobutane, 1,2-diethyl-, trans-	112	C8H16	019341-98-1	50
4			Cyclobutane, 1,2-diethyl-	112	C8H16	061141-83-1	50
5			1-Nonene	126	C9H18	000124-11-8	43



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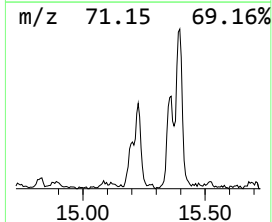
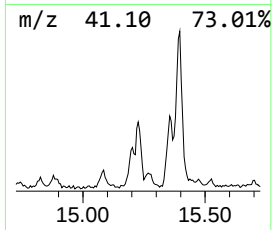
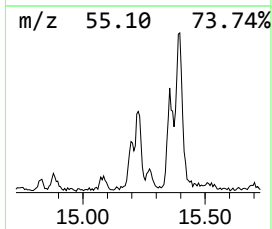
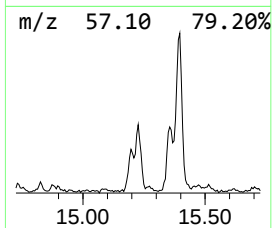
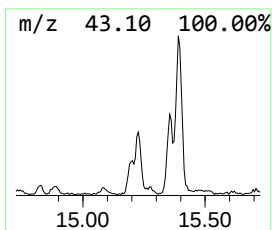
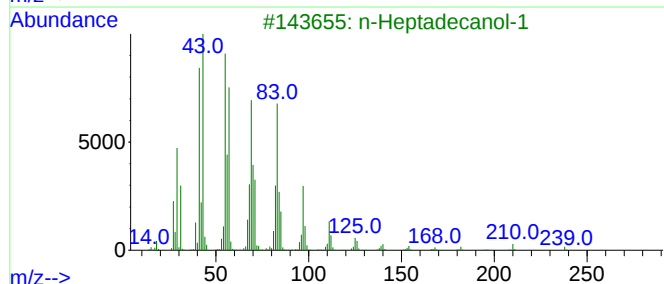
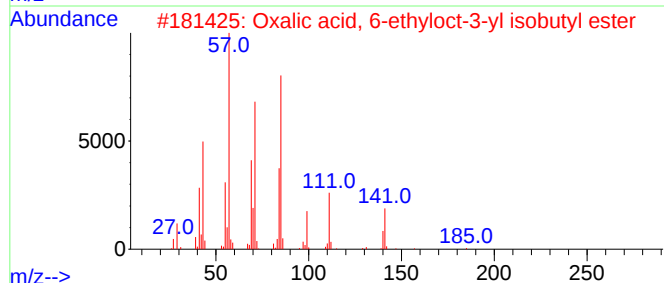
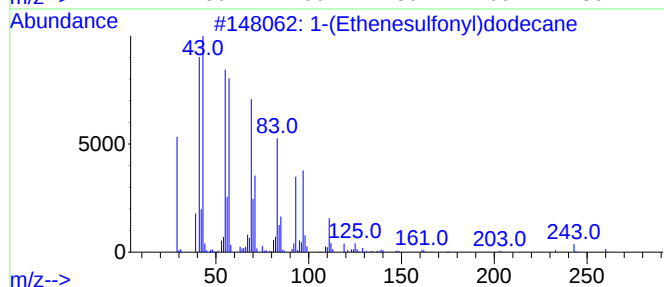
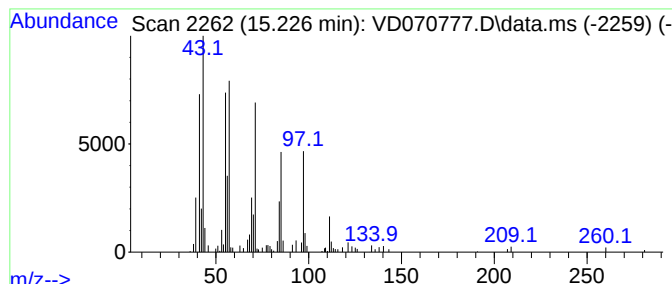
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D101521S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-(Ethenesulfonyl)dodecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.226	6.55 ug/l	279866	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-(Ethenesulfonyl)dodecane	260	C14H28O2S	030719-66-5	64
2			Oxalic acid, 6-ethyloct-3-yl iso...	286	C16H30O4	1010309-34-1	47
3			n-Heptadecanol-1	256	C17H36O	001454-85-9	47
4			Cycloheptane, methyl-	112	C8H16	004126-78-7	46
5			(2,2-Dimethylcyclobutyl)methylamine	113	C7H15N	1000195-04-0	45



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ClientSampleId :
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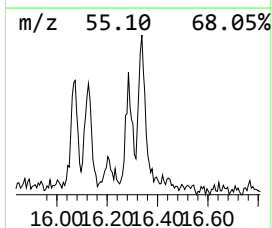
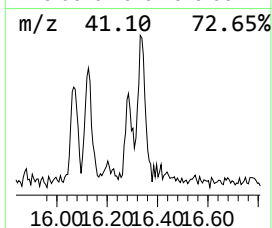
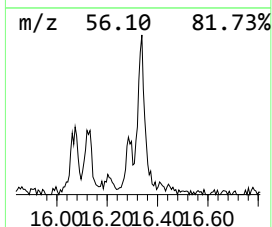
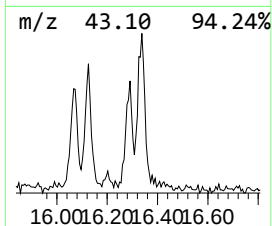
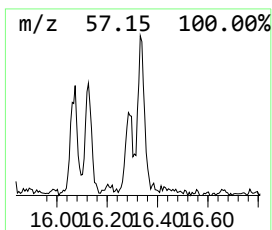
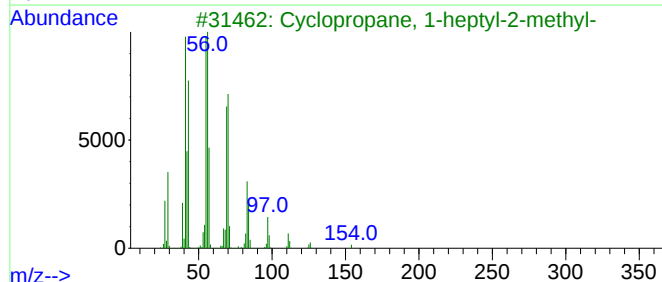
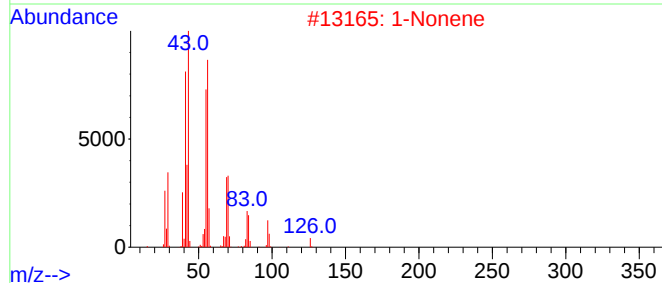
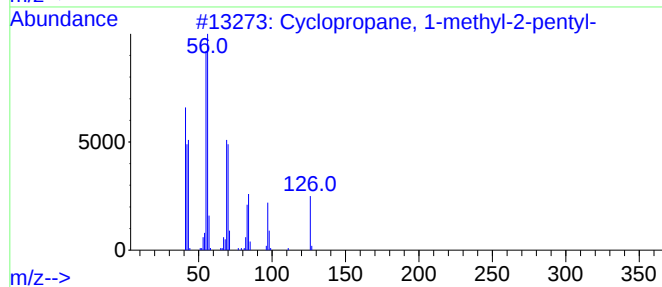
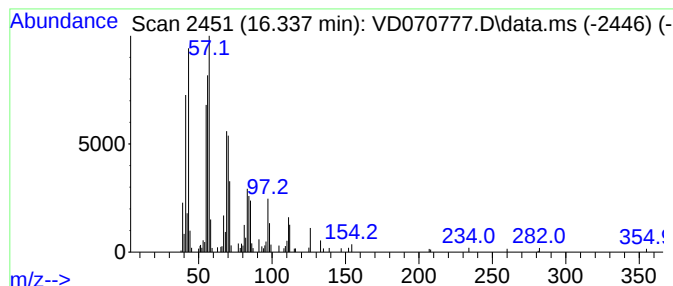
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D101521S.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Cyclopropane, 1-methyl-2-pe... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.337	5.80 ug/l	247803	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, 1-methyl-2-pentyl-	126	C9H18	041977-37-1	93
2			1-Nonene	126	C9H18	000124-11-8	87
3			Cyclopropane, 1-heptyl-2-methyl-	154	C11H22	074663-91-5	81
4			Cyclopropane, 1-methyl-2-octyl-	168	C12H24	037617-26-8	80
5			1-Undecene	154	C11H22	000821-95-4	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Eucalyptol	13.626	8.8	ug/l	374732	4	13.561	2138000	50.0
Hexyl octyl ether	14.549	9.1	ug/l	388382	4	13.561	2138000	50.0
1-(Ethenesulfon...	15.226	6.5	ug/l	279866	4	13.561	2138000	50.0
Cyclopropane, 1...	16.337	5.8	ug/l	247803	4	13.561	2138000	50.0