

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD102423\
 Data File : VD077399.D
 Acq On : 24 Oct 2023 17:16
 Operator : JC/SY
 Sample : 05005-01
 Misc : 5.13G/5.0ml/MSVOA_D/SOIL
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 N-1(0-5)

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\82D101723S.M
 Title : SW846 8260

Signal : TIC: VD077399.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.693	11	18	19	rBV	4755	6939	1.13%	0.180%
2	1.734	19	25	36	rVV	325441	614291	100.00%	15.910%
3	2.581	159	169	174	rBV5	11642	32972	5.37%	0.854%
4	4.269	446	456	466	rVB2	6199	16862	2.74%	0.437%
5	4.805	535	547	555	rBV5	25927	79585	12.96%	2.061%
6	7.805	1047	1057	1063	rBV2	89442	215799	35.13%	5.589%
7	7.875	1063	1069	1081	rVB2	144507	334963	54.53%	8.675%
8	8.228	1119	1129	1141	rVB	64615	155950	25.39%	4.039%
9	8.775	1214	1222	1238	rBV	235122	492954	80.25%	12.767%
10	9.834	1397	1402	1408	rBV5	4040	6747	1.10%	0.175%
11	10.269	1468	1476	1484	rBV	236138	434909	70.80%	11.264%
12	10.663	1538	1543	1551	rBV2	6683	11612	1.89%	0.301%
13	11.581	1691	1699	1709	rBV	294897	509852	83.00%	13.205%
14	11.793	1730	1735	1738	rBV7	5293	10723	1.75%	0.278%
15	12.081	1780	1784	1786	rBV4	5840	8634	1.41%	0.224%
16	12.322	1823	1825	1830	rVB5	9703	11056	1.80%	0.286%
17	12.428	1832	1843	1847	rBV5	9716	28201	4.59%	0.730%
18	12.575	1862	1868	1875	rVB	137146	227504	37.04%	5.892%
19	12.669	1880	1884	1890	rBV8	6303	12540	2.04%	0.325%
20	12.740	1892	1896	1899	rVB6	5648	7876	1.28%	0.204%
21	12.828	1905	1911	1913	rBV6	4373	6258	1.02%	0.162%
22	12.898	1918	1923	1927	rVV6	8376	16113	2.62%	0.417%
23	13.045	1942	1948	1950	rBV6	6829	10150	1.65%	0.263%
24	13.451	2015	2017	2022	rBV5	6655	11842	1.93%	0.307%
25	13.516	2022	2028	2040	rVB	166601	295126	48.04%	7.644%
26	13.839	2078	2083	2089	rBV9	17803	36211	5.89%	0.938%
27	14.057	2116	2120	2125	rVB3	15249	26954	4.39%	0.698%
28	14.469	2188	2190	2194	rVB5	9758	12576	2.05%	0.326%
29	14.704	2226	2230	2234	rBV7	9847	18844	3.07%	0.488%
30	14.769	2236	2241	2245	rVV6	26143	52747	8.59%	1.366%
31	14.816	2247	2249	2256	rVB7	19898	36230	5.90%	0.938%
32	15.034	2283	2286	2290	rBV6	10933	15077	2.45%	0.390%
33	15.298	2328	2331	2335	rBV6	15740	26818	4.37%	0.695%
34	16.269	2492	2496	2501	rVB6	14315	26505	4.31%	0.686%
35	16.604	2546	2553	2562	rBV6	15486	49702	8.09%	1.287%

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ClientSampleId :
N-1(0-5)

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\82D101723S.M
Title : SW846 8260

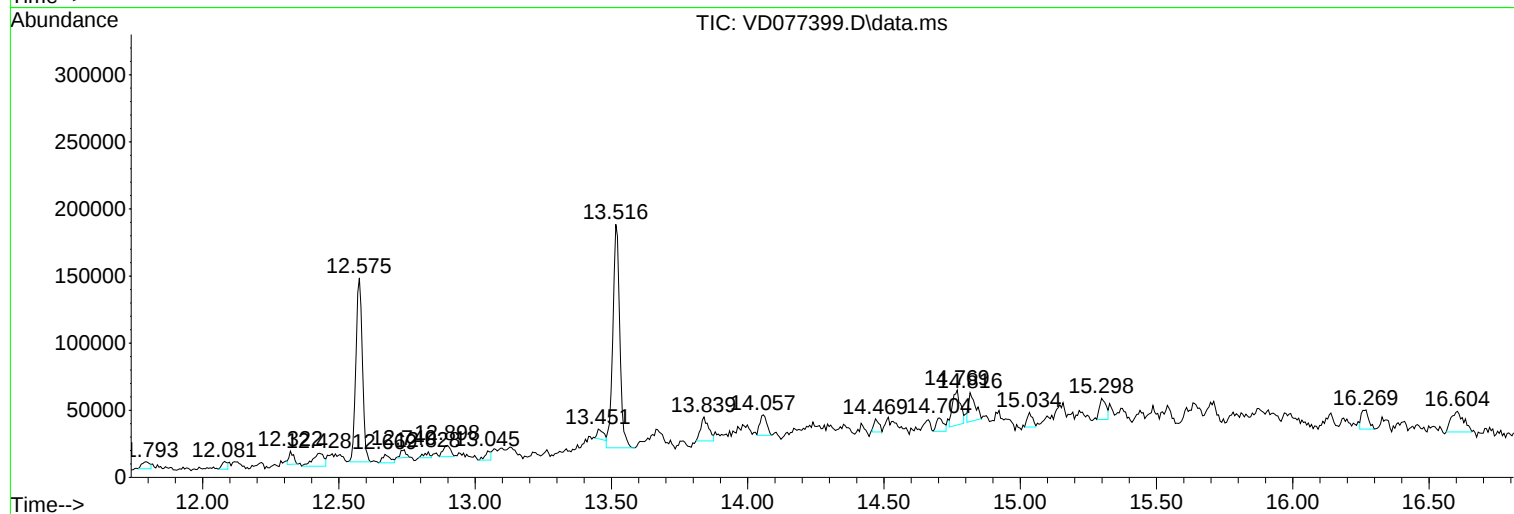
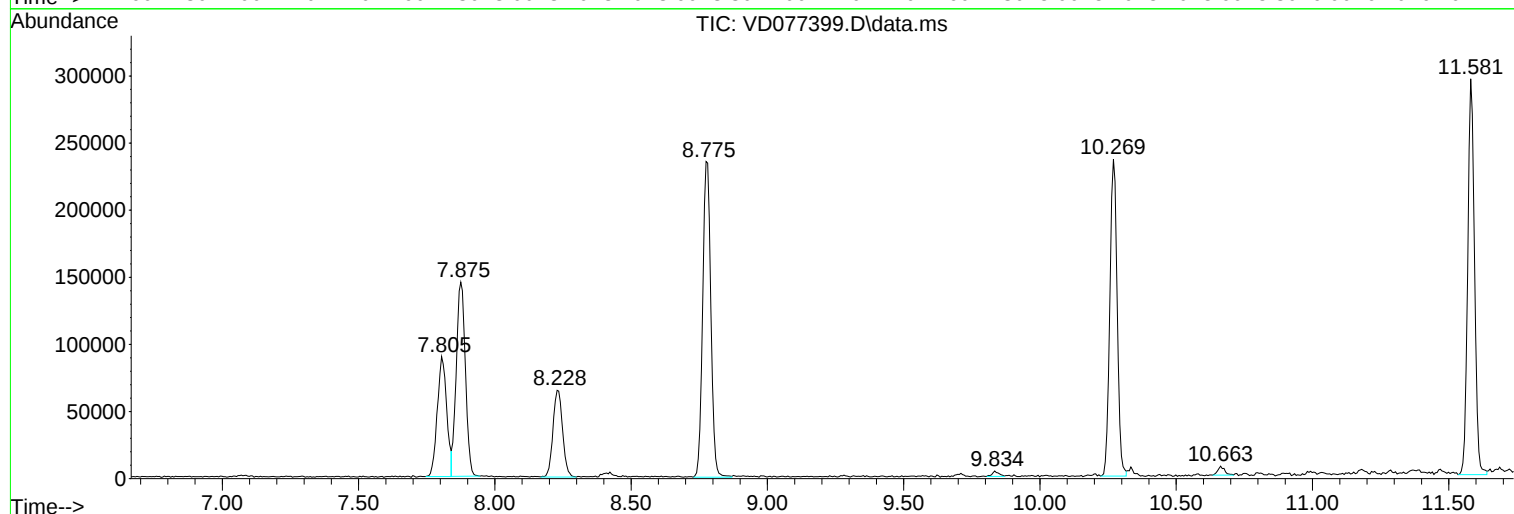
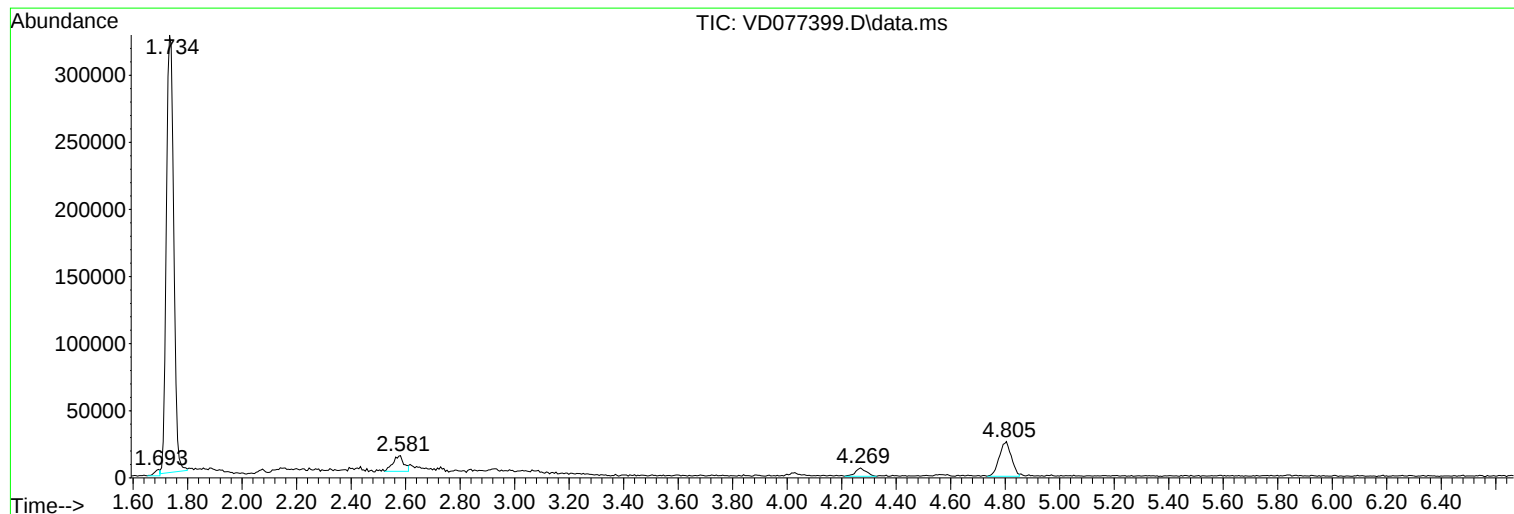
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D101723S.M
Quant Title : SW846 8260

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



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N-1(0-5)

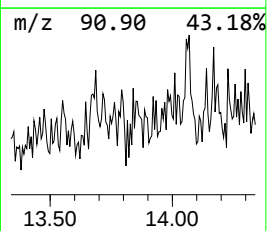
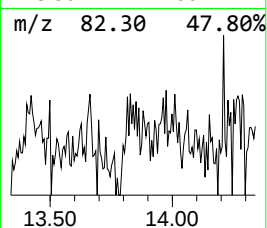
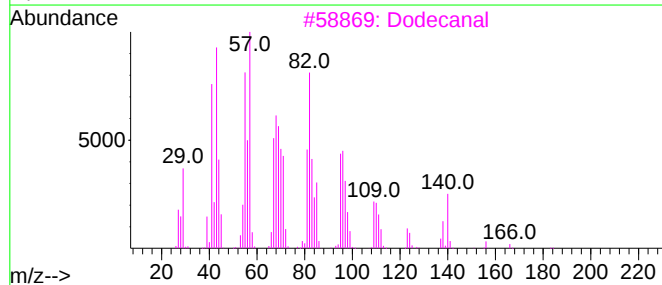
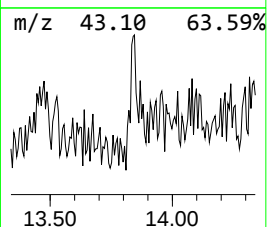
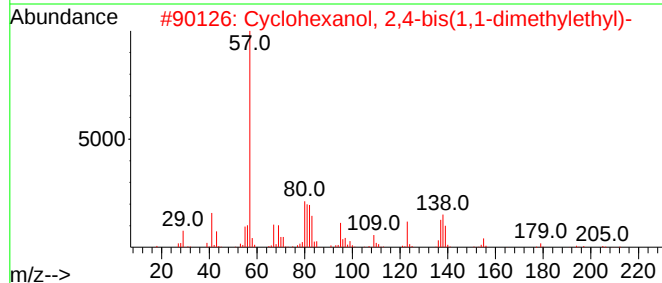
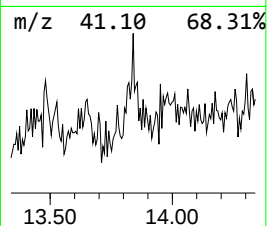
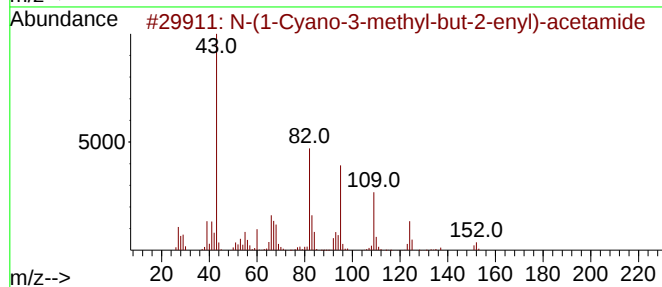
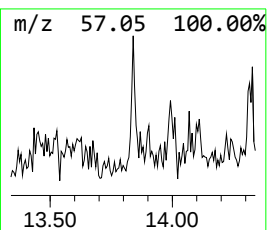
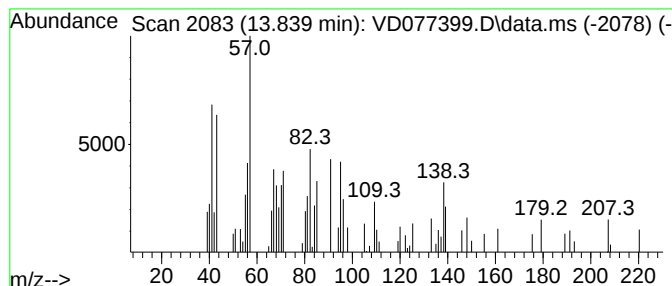
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D101723S.M
Quant Title : SW846 8260

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

Peak Number 2 unknown13.839 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.839	6.13 ug/l	36211	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N-(1-Cyano-3-methyl-but-2-enyl)-...	152	C8H12N2O	1000192-62-7	47
2			Cyclohexanol, 2,4-bis(1,1-dimeth...	212	C14H28O	055030-25-6	35
3			Dodecanal	184	C12H24O	000112-54-9	27
4			Citronellyl isobutyrate	226	C14H26O2	000097-89-2	25
5			13-Methyltetradecanal	226	C15H30O	075853-51-9	22



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Sample : 05005-01
Misc : 5.13G/5.0ml/MSVOA_D/SOIL
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
N-1(0-5)

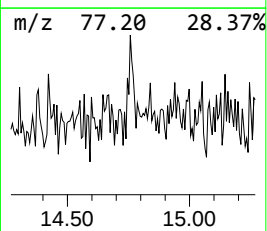
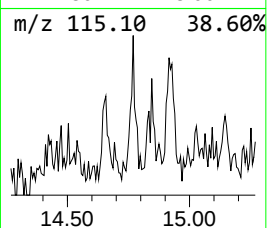
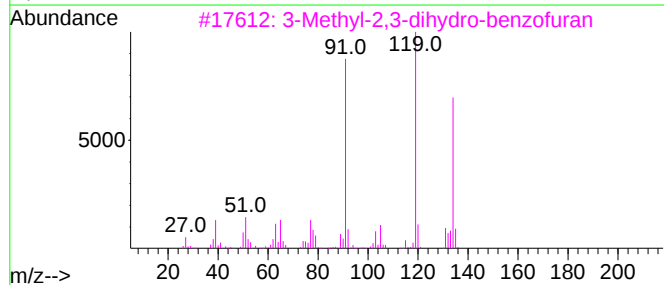
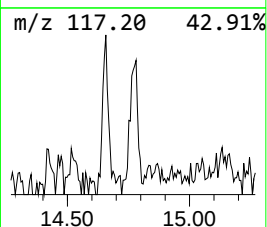
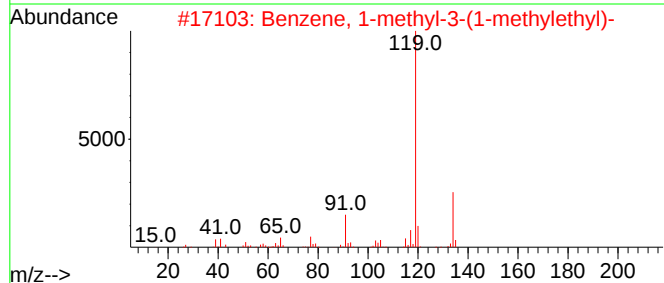
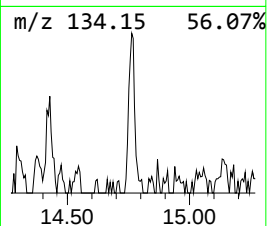
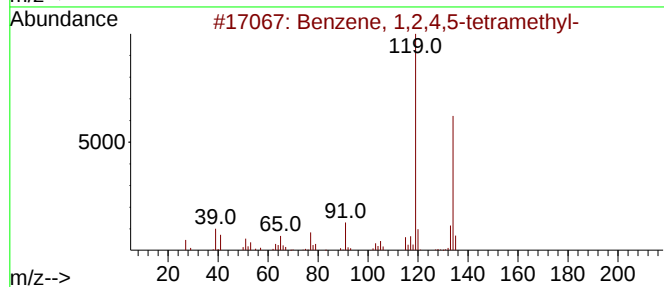
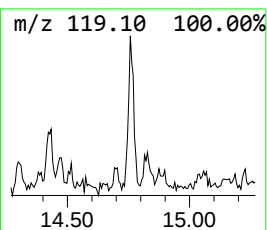
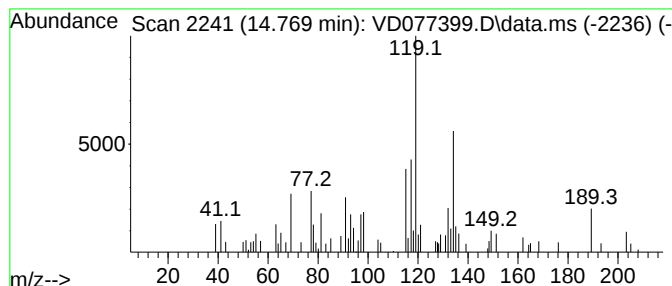
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D101723S.M
Quant Title : SW846 8260

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

Peak Number 3 unknown14.769 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.769	8.94 ug/l	52747	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	46
2			Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	000535-77-3	43
3			3-Methyl-2,3-dihydro-benzofuran	134	C9H10O	013524-73-7	43
4			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	43
5			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	43



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Sample : 05005-01
Misc : 5.13G/5.0ml/MSVOA_D/SOIL
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
N-1(0-5)

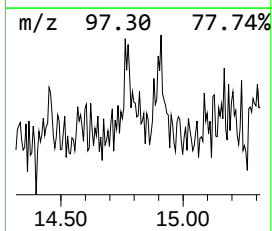
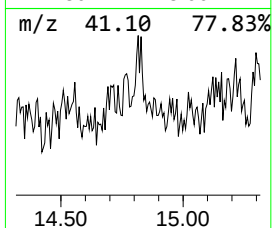
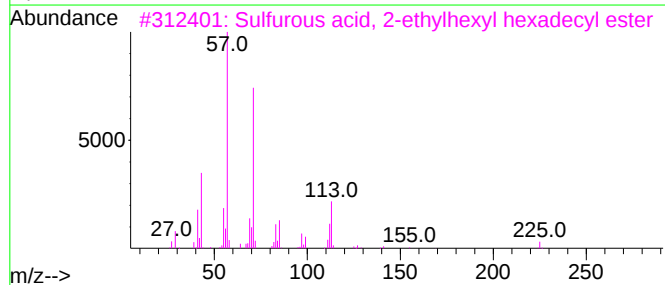
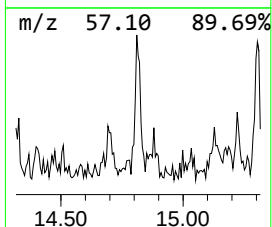
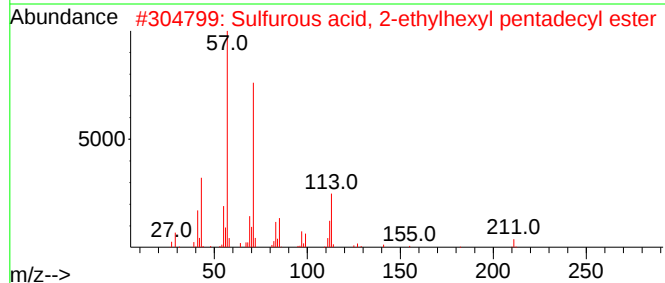
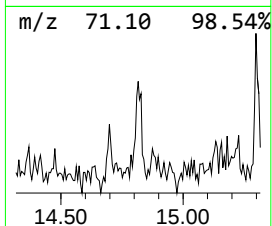
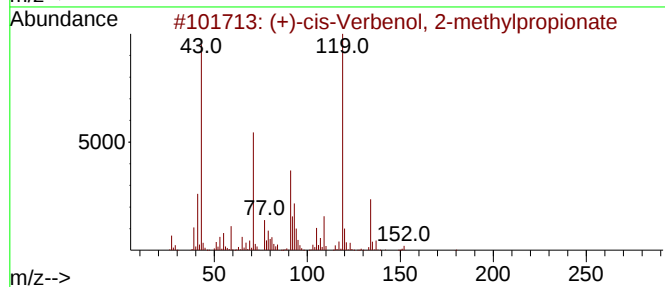
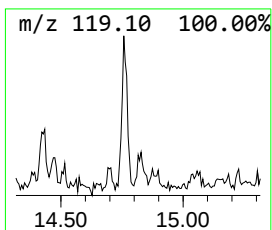
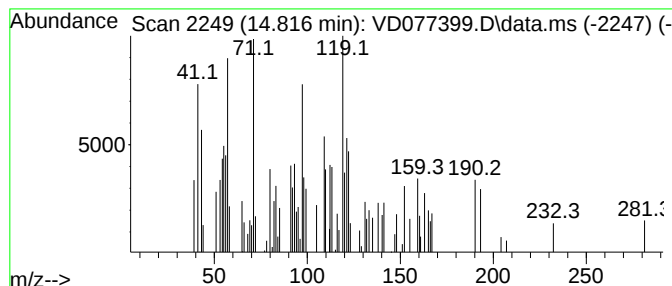
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D101723S.M
Quant Title : SW846 8260

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

Peak Number 4 unknown14.816 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.816	6.14 ug/l	36230	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+)-cis-Verbenol, 2-methylpropio...	222	C14H22O2	1000462-96-7	22		
2	Sulfurous acid, 2-ethylhexyl pen...	404	C23H48O3S	1000309-19-8	14		
3	Sulfurous acid, 2-ethylhexyl hex...	418	C24H50O3S	1000309-19-9	14		
4	Sulfurous acid, 2-ethylhexyl tet...	390	C22H46O3S	1000309-19-7	14		
5	Sorbic Acid	112	C6H8O2	000110-44-1	11		



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Misc : 5.13G/5.0ml/MSVOA_D/SOIL
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
N-1(0-5)

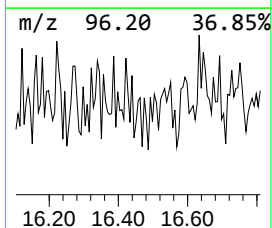
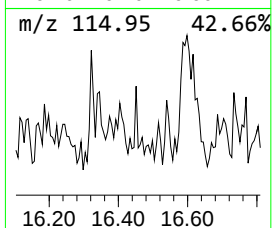
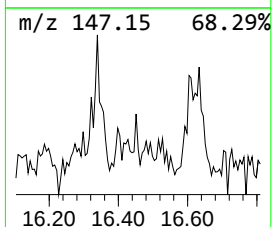
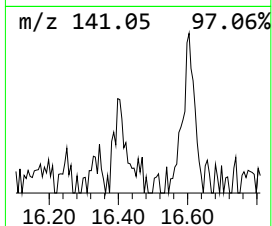
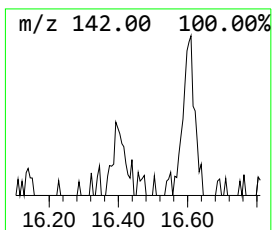
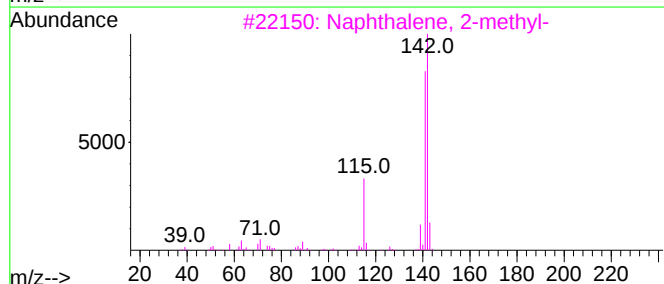
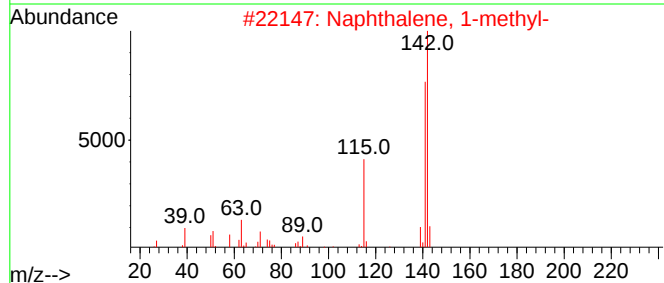
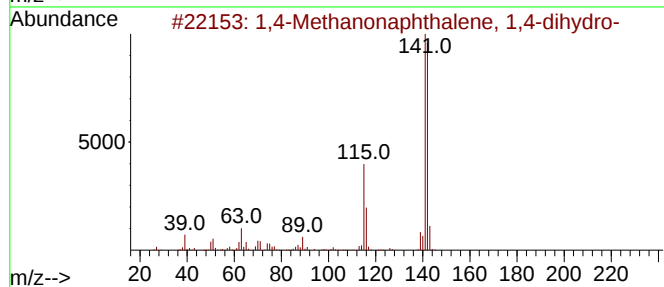
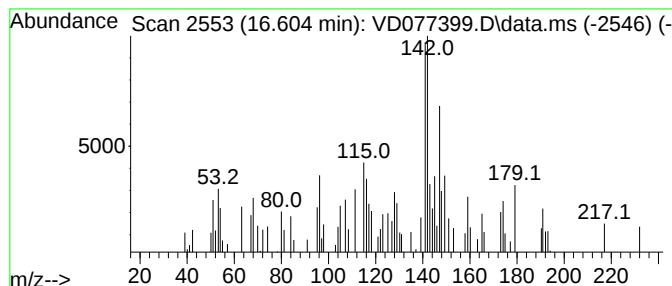
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown16.604 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.604	8.42 ug/l	49702	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	43
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	43
3			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	43
4			dimethyl selenone	142	C2H6O2Se	004371-90-8	38
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	32



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D101723S.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown14.769	14.769	8.9	ug/l	52747	4	13.516	295126	50.0
unknown14.816	14.816	6.1	ug/l	36230	4	13.516	295126	50.0
unknown16.604	16.604	8.4	ug/l	49702	4	13.516	295126	50.0