

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY110321\
 Data File : VY006608.D
 Acq On : 03 Nov 2021 17:54
 Operator : SY/MD
 Sample : M4472-01
 Misc : 5.00G/5ML/MSVOA_Y/SOIL
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 WC-2-JS

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_Y\methods\82Y102221S.M
 Title : SW846 8260

Signal : TIC: VY006608.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.735	468	478	489	rVB3	6402	19576	6.98%	1.014%
2	5.765	635	647	655	rBV3	2485	7518	2.68%	0.390%
3	7.728	960	969	974	rBV	33694	81076	28.89%	4.201%
4	7.795	974	980	992	rVB	67784	155918	55.56%	8.080%
5	8.149	1027	1038	1047	rBV	35356	77414	27.59%	4.012%
6	8.697	1119	1128	1138	rBV	102522	204435	72.85%	10.594%
7	9.752	1296	1301	1308	rVB5	2012	4745	1.69%	0.246%
8	10.185	1365	1372	1380	rVV	161242	280638	100.00%	14.543%
9	10.587	1432	1438	1442	rBV3	2175	4991	1.78%	0.259%
10	11.489	1579	1586	1597	rBV	130913	222324	79.22%	11.521%
11	11.703	1616	1621	1630	rBV10	2781	7554	2.69%	0.391%
12	12.483	1743	1749	1757	rVB	88231	141152	50.30%	7.314%
13	12.788	1795	1799	1802	rBV3	1831	2905	1.04%	0.151%
14	12.843	1805	1808	1814	rVB5	1687	2984	1.06%	0.155%
15	13.075	1833	1846	1854	rBV5	12572	30946	11.03%	1.604%
16	13.172	1859	1862	1870	rVB7	3341	6682	2.38%	0.346%
17	13.288	1877	1881	1885	rVV6	2828	5412	1.93%	0.280%
18	13.355	1887	1892	1896	rVV	11593	20431	7.28%	1.059%
19	13.428	1898	1904	1910	rVV	93352	156413	55.73%	8.105%
20	13.483	1910	1913	1914	rVV3	2939	3705	1.32%	0.192%
21	13.513	1914	1918	1922	rVB4	4962	8884	3.17%	0.460%
22	13.611	1929	1934	1941	rBV7	8204	22096	7.87%	1.145%
23	13.678	1941	1945	1948	rBV4	6174	8565	3.05%	0.444%
24	13.788	1957	1963	1968	rBV2	31183	51505	18.35%	2.669%
25	13.855	1970	1974	1980	rVV2	15831	30283	10.79%	1.569%
26	13.904	1980	1982	1985	rVB3	5316	5490	1.96%	0.284%
27	13.965	1986	1992	1995	rBV5	5751	11184	3.99%	0.580%
28	14.044	2002	2005	2007	rBV2	3699	4559	1.62%	0.236%
29	14.080	2007	2011	2016	rVV	25789	36237	12.91%	1.878%
30	14.294	2036	2046	2048	rBV9	8610	26475	9.43%	1.372%
31	14.379	2057	2060	2064	rVB3	7968	9022	3.21%	0.468%
32	14.538	2082	2086	2089	rBV	7206	10045	3.58%	0.521%
33	14.617	2095	2099	2104	rVB4	8465	14361	5.12%	0.744%
34	14.721	2111	2116	2118	rBV4	9694	16857	6.01%	0.874%
35	14.757	2118	2122	2127	rVB	22521	35170	12.53%	1.822%
36	14.861	2133	2139	2141	rBV6	8959	18943	6.75%	0.982%

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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

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37	15.062	2169	2172	2176	rVB5	6538	8664	3.09%	0.449%
38	15.220	2195	2198	2202	rVV4	7358	9609	3.42%	0.498%
39	15.281	2206	2208	2215	rVB3	12764	19066	6.79%	0.988%
40	15.342	2215	2218	2223	rVB4	7879	11352	4.05%	0.588%
41	15.501	2239	2244	2251	rBV2	40658	83168	29.64%	4.310%
42	15.568	2253	2255	2258	rVB3	10986	13410	4.78%	0.695%
43	16.007	2324	2327	2338	rVB8	8320	22202	7.91%	1.150%
44	16.281	2369	2372	2380	rVB5	8249	15811	5.63%	0.819%

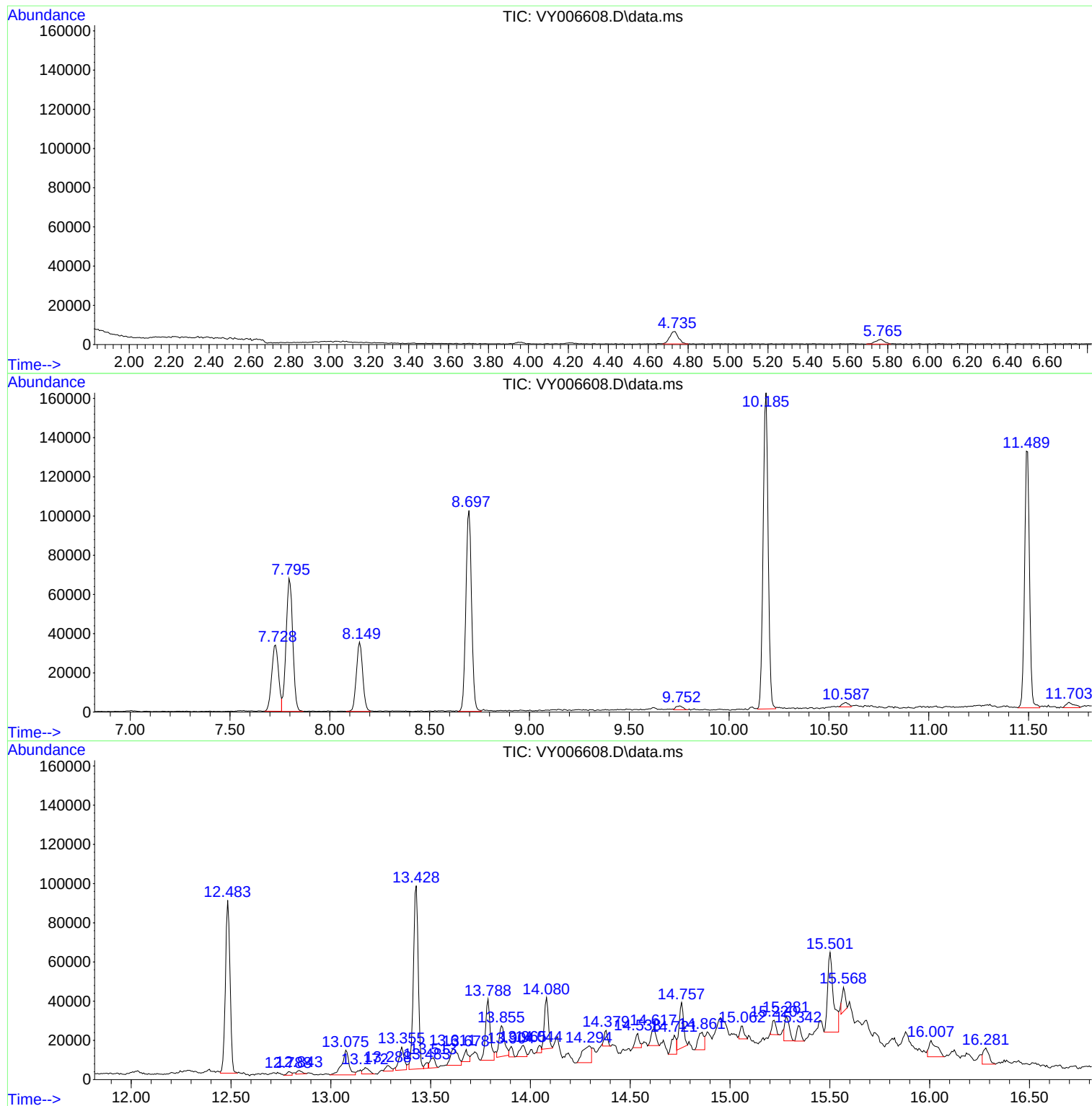
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102221S.M
Quant Title : SW846 8260

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



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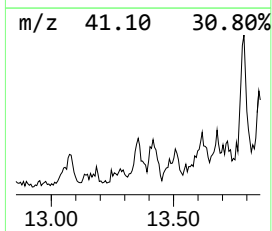
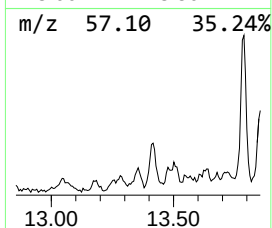
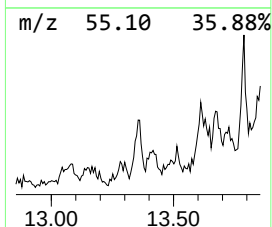
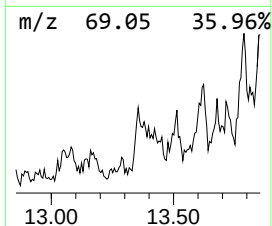
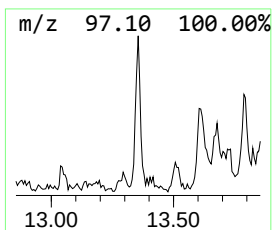
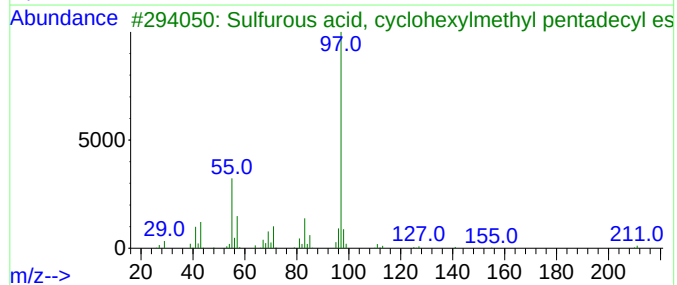
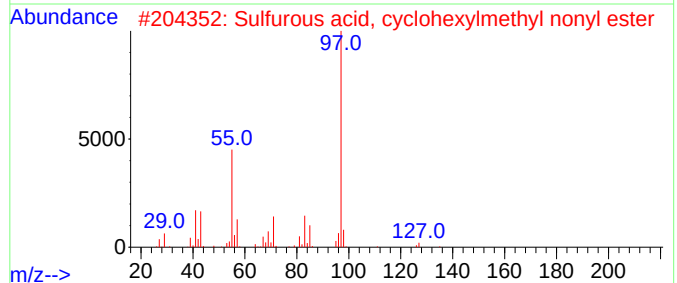
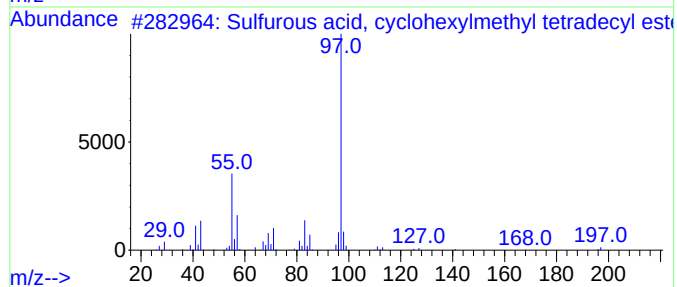
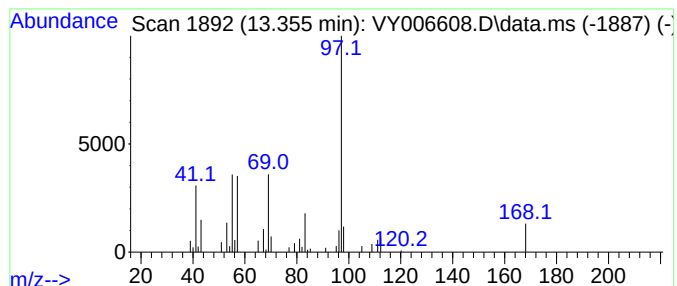
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102221S.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfurous acid, cyclohexylm... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.355	6.53 ug/l	20431	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, cyclohexylmethyl...	374	C21H42O3S	1000309-22-2	59
2			Sulfurous acid, cyclohexylmethyl...	304	C16H32O3S	1000309-21-8	59
3			Sulfurous acid, cyclohexylmethyl...	388	C22H44O3S	1000309-22-3	59
4			Sulfurous acid, cyclohexylmethyl...	346	C19H38O3S	1000309-22-0	59
5			Sulfurous acid, cyclohexylmethyl...	262	C13H26O3S	1000309-21-5	59



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Instrument :
MSVOA_Y
ClientSampleId :
WC-2-JS

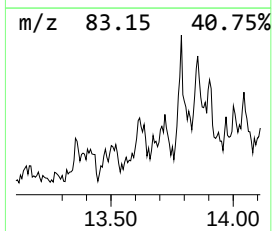
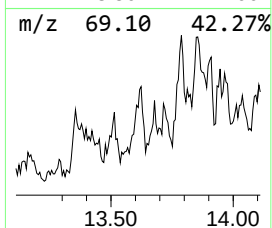
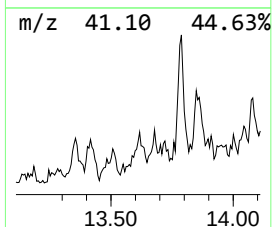
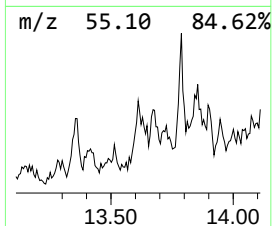
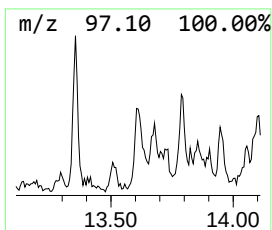
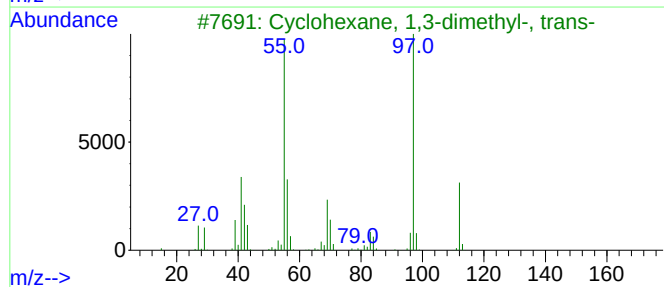
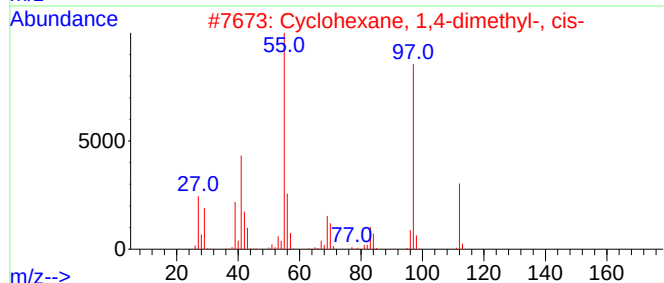
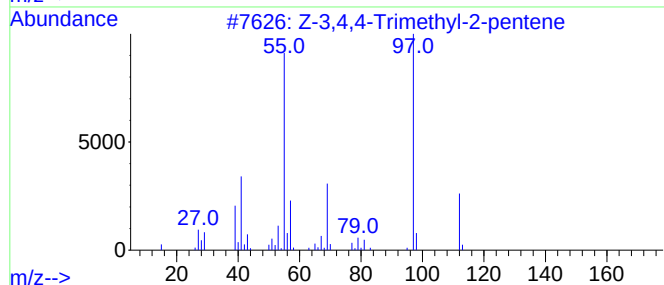
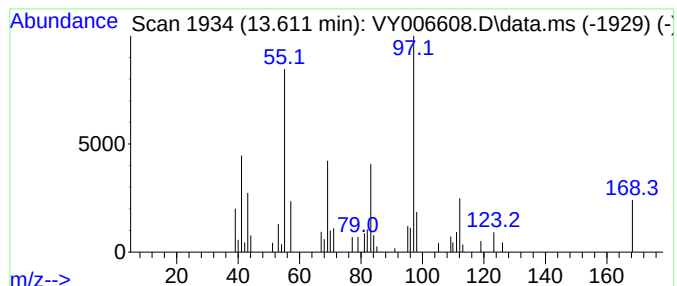
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102221S.M
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TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Z-3,4,4-Trimethyl-2-pentene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.611	7.06 ug/l	22096	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Z-3,4,4-Trimethyl-2-pentene	112	C8H16	039761-64-3	55
2			Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	49
3			Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	49
4			Cyclohexane, 1,4-dimethyl-	112	C8H16	000589-90-2	49
5			2-Pentene, 2,4,4-trimethyl-	112	C8H16	000107-40-4	46



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Instrument :
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ClientSampleId :
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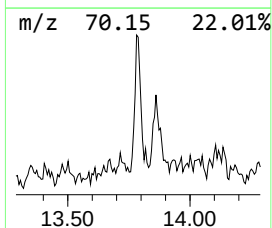
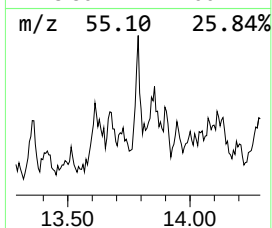
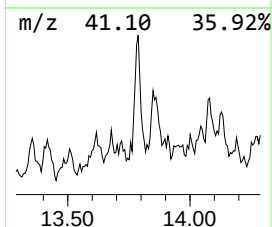
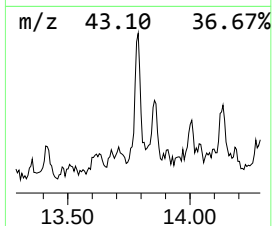
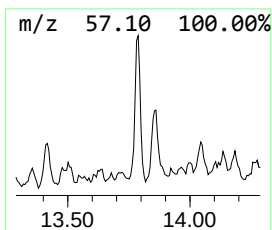
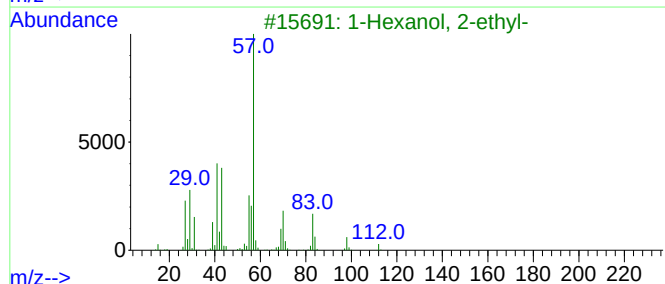
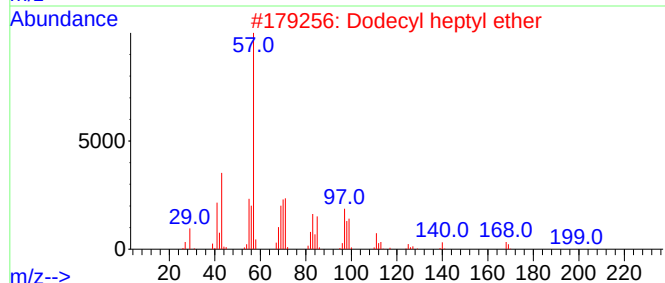
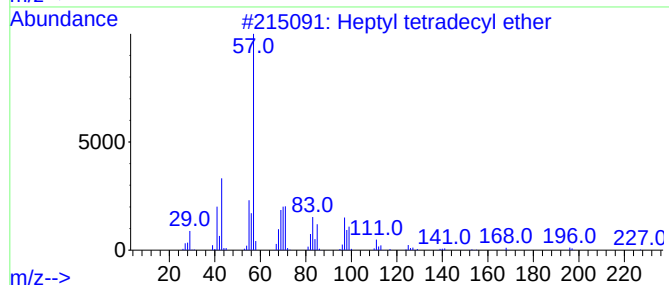
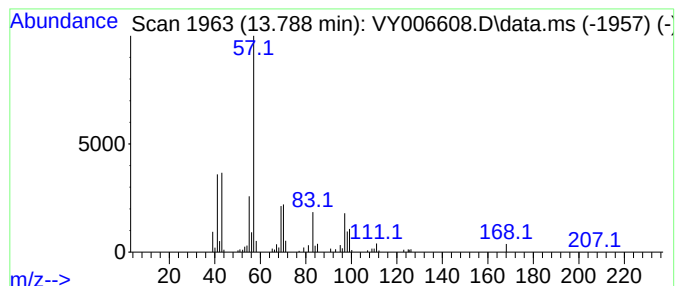
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102221S.M
Quant Title : SW846 8260

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

Peak Number 3 Heptyl tetradecyl ether Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.788	16.46 ug/l	51505	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptyl tetradecyl ether	312	C21H44O	1000406-39-3	59
2			Dodecyl heptyl ether	284	C19H40O	1010406-39-2	56
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	47
4			Heptane, 3-ethyl-	128	C9H20	015869-80-4	43
5			2,4-Dimethylpentan-3-yl isobutyl...	216	C12H24O3	1000372-75-3	43



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ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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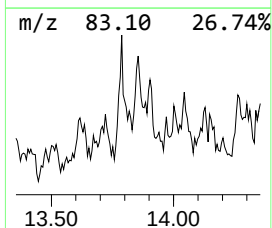
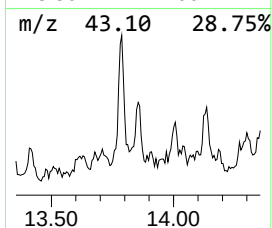
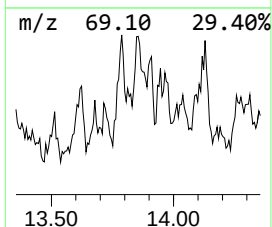
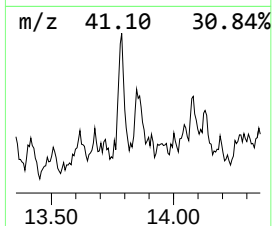
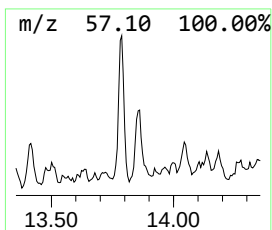
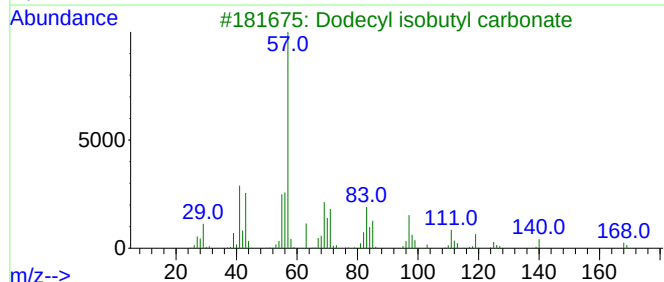
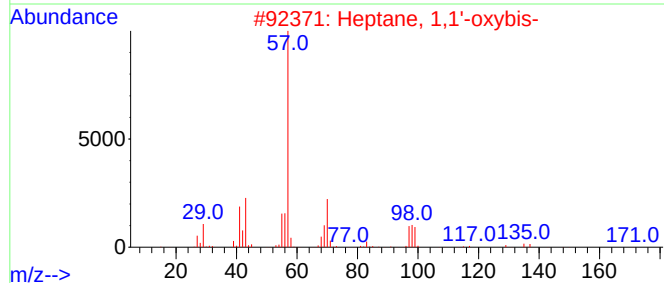
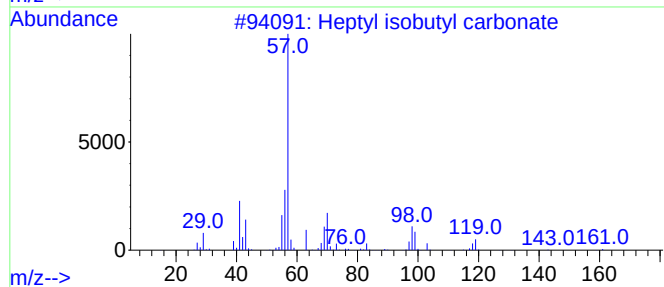
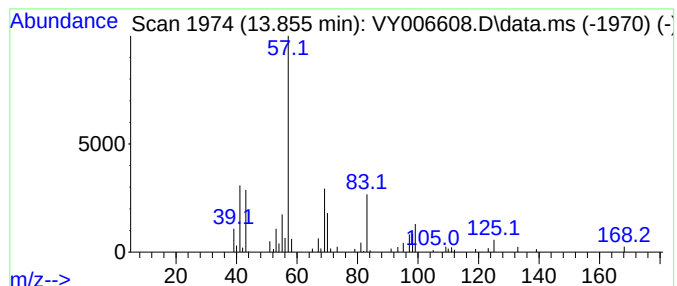
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102221S.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown13.855 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.855	9.68 ug/l	30283	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	37
2			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	37
3			Dodecyl isobutyl carbonate	286	C17H34O3	959067-22-2	36
4			Heptyl tetradecyl ether	312	C21H44O	1000406-39-3	28
5			Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	25



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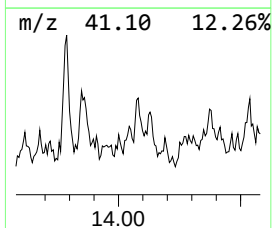
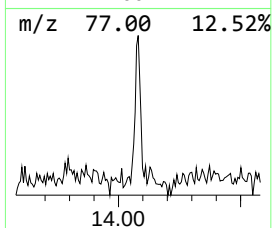
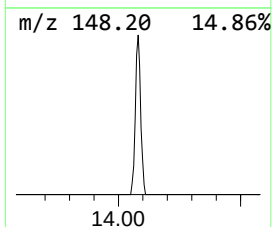
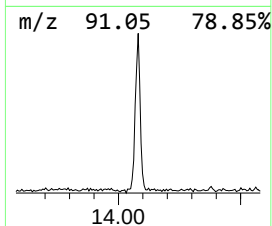
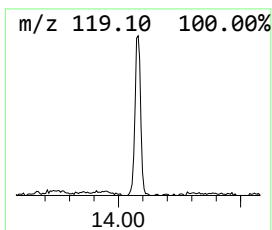
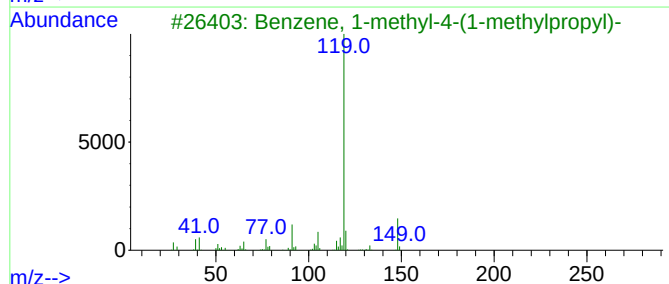
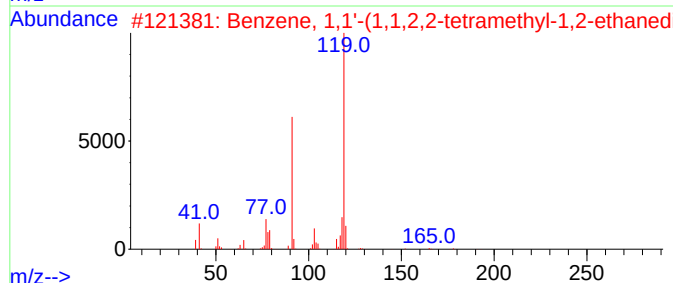
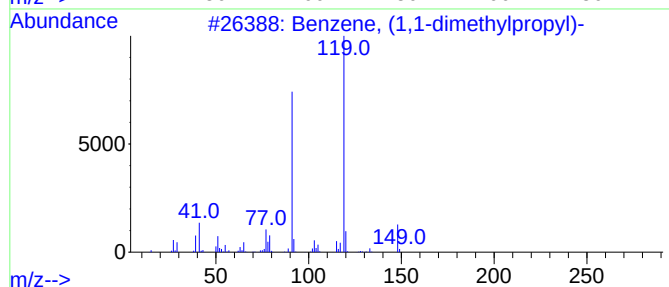
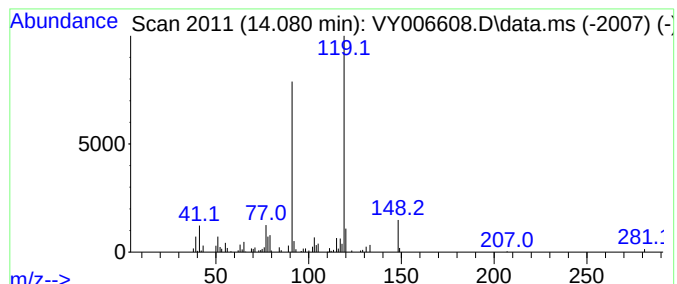
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102221S.M
Quant Title : SW846 8260

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

Peak Number 5 Benzene, (1,1-dimethylpropyl)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.080	11.58 ug/l	36237	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1,1-dimethylpropyl)-	148	C11H16	002049-95-8	95
2			Benzene, 1,1'-(1,1,2,2-tetrameth...	238	C18H22	001889-67-4	80
3			Benzene, 1-methyl-4-(1-methylpro...	148	C11H16	001595-16-0	74
4			5-Methyl-5-phenyl-3-hexanone	190	C13H18O	1000430-96-7	64
5			Benzene, tert-butyl-	134	C10H14	000098-06-6	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY110321\
Data File : VY006608.D
Acq On : 03 Nov 2021 17:54
Operator : SY/MD
Sample : M4472-01
Misc : 5.00G/5ML/MSVOA_Y/SOIL
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
WC-2-JS

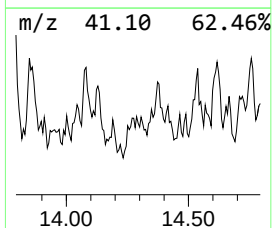
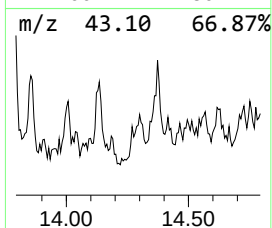
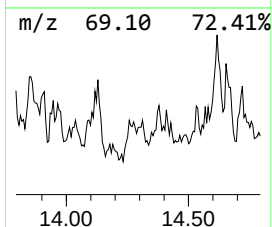
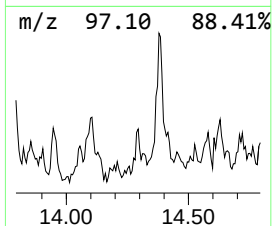
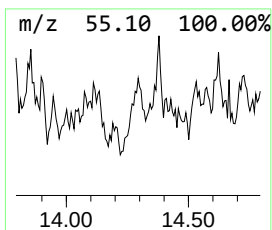
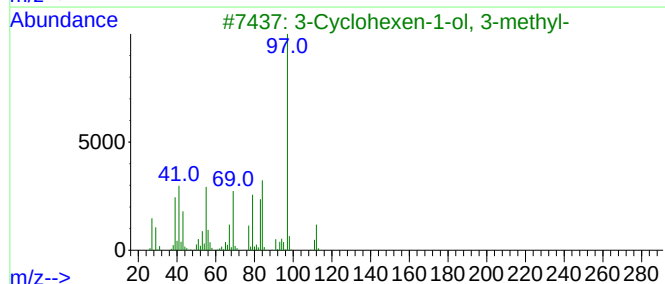
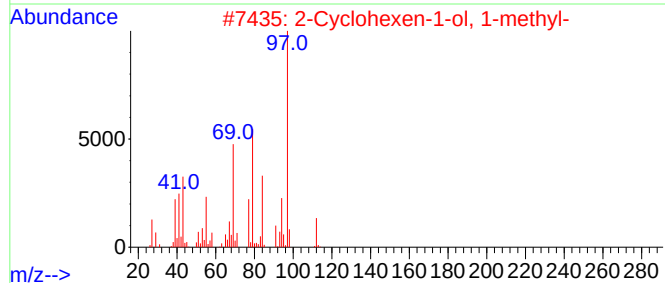
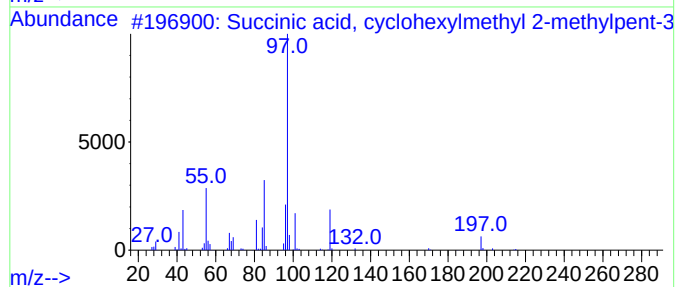
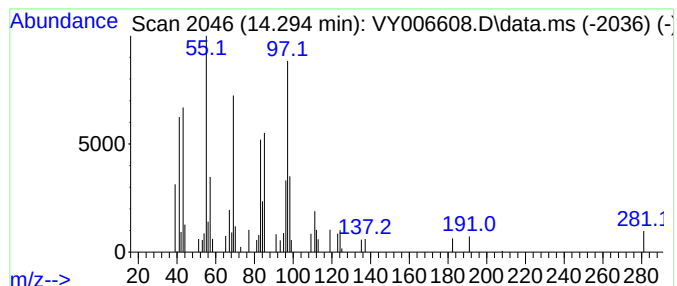
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Quant Title : SW846 8260

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

Peak Number 6 unknown14.294 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.294	8.46 ug/l	26475	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Succinic acid, cyclohexylmethyl ...	298	C17H30O4	1000389-60-0	38
2			2-Cyclohexen-1-ol, 1-methyl-	112	C7H12O	023758-27-2	38
3			3-Cyclohexen-1-ol, 3-methyl-	112	C7H12O	053783-91-8	38
4			2-Heptafluorobutyropentadecane	424	C19H31F7O2	1010245-50-0	35
5			3a,7a-Epoxy-1H-inden-4(5H)-one, ...	152	C9H12O2	039746-31-1	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY110321\
Data File : VY006608.D
Acq On : 03 Nov 2021 17:54
Operator : SY/MD
Sample : M4472-01
Misc : 5.00G/5ML/MSVOA_Y/SOIL
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
WC-2-JS

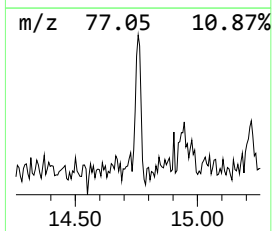
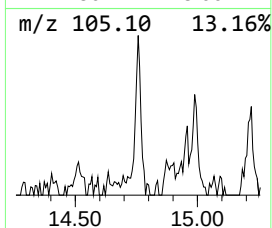
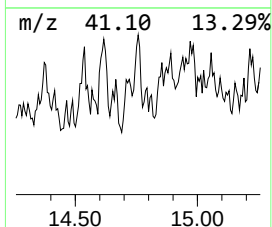
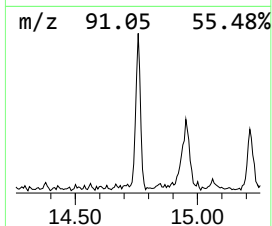
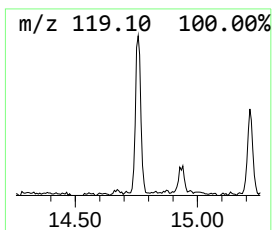
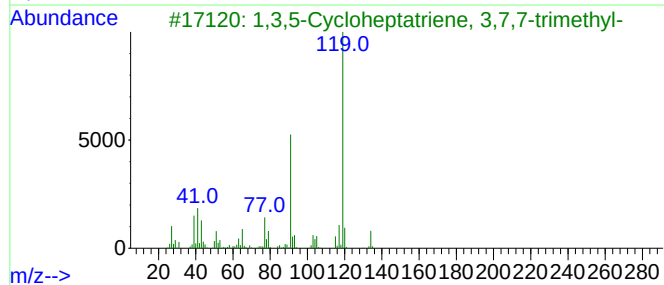
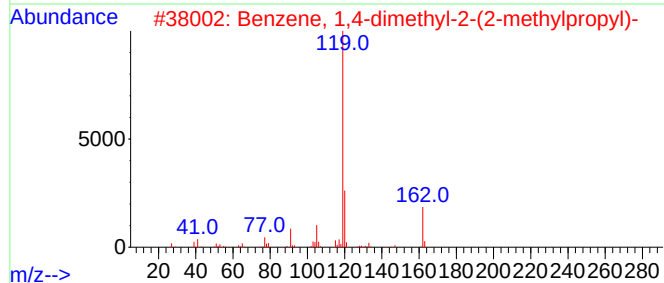
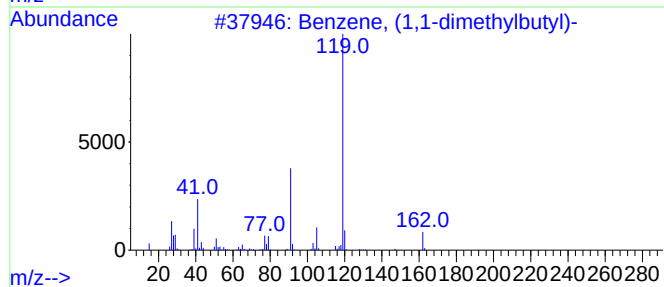
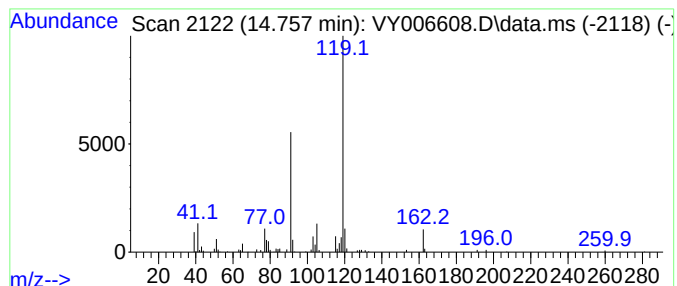
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, (1,1-dimethylbutyl)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.757	11.24 ug/l	35170	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1,1-dimethylbutyl)-	162	C12H18	001985-57-5	86
2			Benzene, 1,4-dimethyl-2-(2-methy...	162	C12H18	055669-88-0	72
3			1,3,5-Cycloheptatriene, 3,7,7-tr...	134	C10H14	003479-89-8	64
4			.alpha.,.alpha.-DIMETHYLBENZYL I...	206	C13H18O2	1000429-51-9	64
5			Benzene, (1,1-dimethylpropyl)-	148	C11H16	002049-95-8	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY110321\
Data File : VY006608.D
Acq On : 03 Nov 2021 17:54
Operator : SY/MD
Sample : M4472-01
Misc : 5.00G/5ML/MSVOA_Y/SOIL
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
WC-2-JS

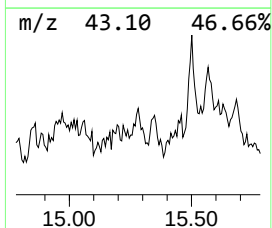
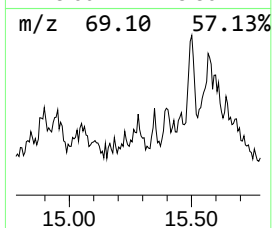
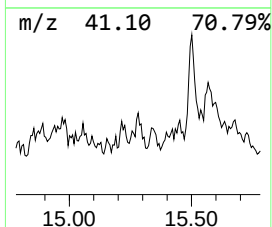
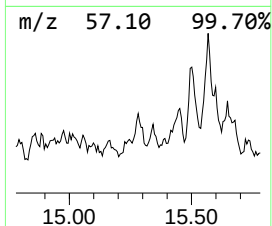
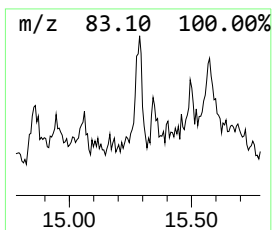
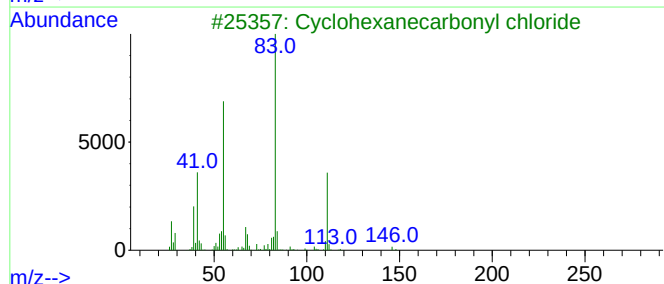
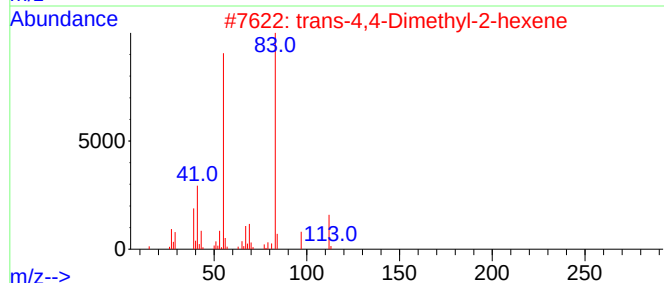
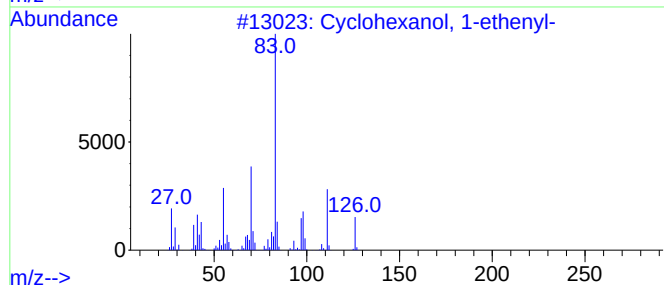
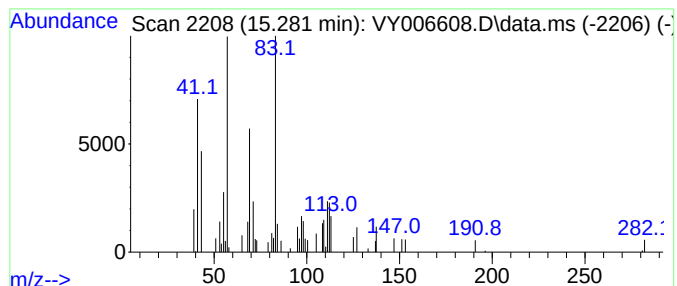
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102221S.M
Quant Title : SW846 8260

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

Peak Number 8 unknown15.281 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.281	6.09 ug/l	19066	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanol, 1-ethenyl-	126	C8H14O	001940-19-8	47
2			trans-4,4-Dimethyl-2-hexene	112	C8H16	019550-83-5	43
3			Cyclohexanecarbonyl chloride	146	C7H11ClO	002719-27-9	43
4			6-Methyl-1,7-diazabicyclo[4.1.0]...	112	C6H12N2	108602-71-7	38
5			Tetradecanoic acid, 2-hydroxy-, ...	258	C15H30O3	056009-40-6	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY110321\
Data File : VY006608.D
Acq On : 03 Nov 2021 17:54
Operator : SY/MD
Sample : M4472-01
Misc : 5.00G/5ML/MSVOA_Y/SOIL
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
WC-2-JS

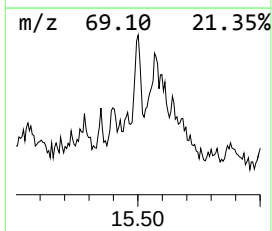
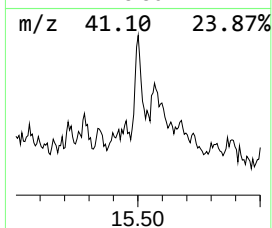
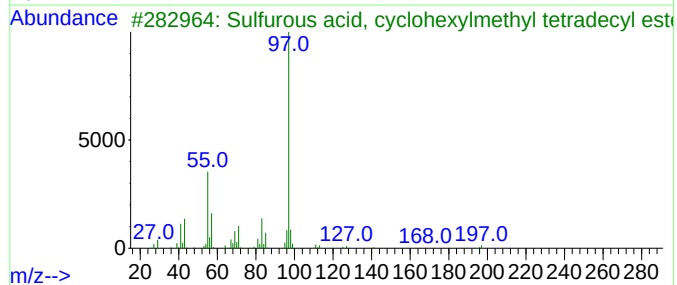
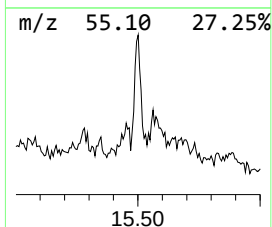
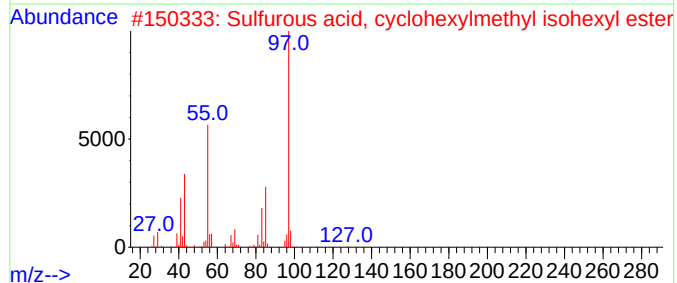
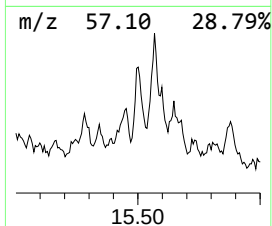
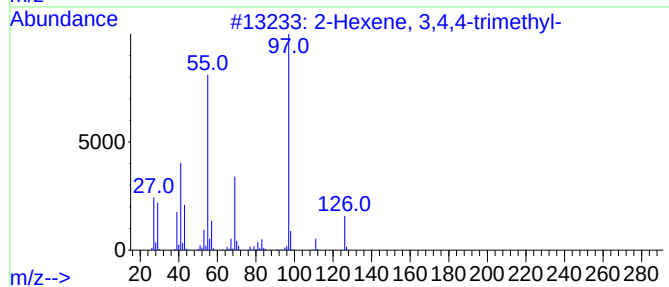
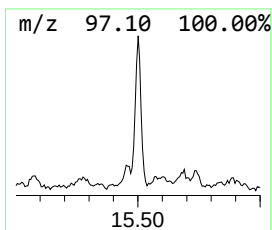
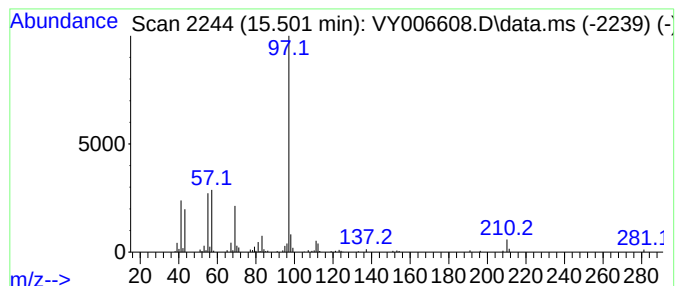
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102221S.M
Quant Title : SW846 8260

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

Peak Number 9 2-Hexene, 3,4,4-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.501	26.59 ug/l	83168	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexene, 3,4,4-trimethyl-	126	C9H18	053941-19-8	64		
2	Sulfurous acid, cyclohexylmethyl...	262	C13H26O3S	1000309-21-5	59		
3	Sulfurous acid, cyclohexylmethyl...	374	C21H42O3S	1000309-22-2	59		
4	Sulfurous acid, cyclohexylmethyl...	276	C14H28O3S	1000309-21-7	53		
5	2-Pentene, 2,4,4-trimethyl-	112	C8H16	000107-40-4	53		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY110321\
Data File : VY006608.D
Acq On : 03 Nov 2021 17:54
Operator : SY/MD
Sample : M4472-01
Misc : 5.00G/5ML/MSVOA_Y/SOIL
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
WC-2-JS

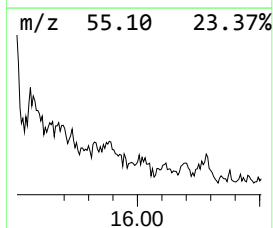
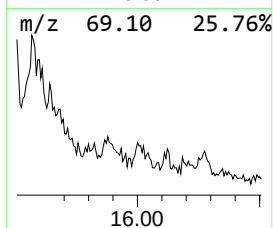
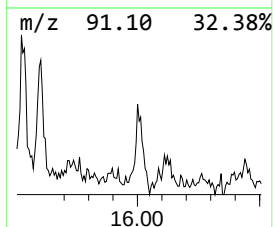
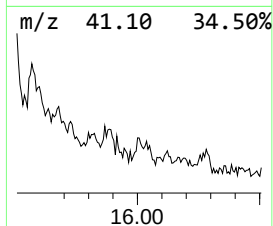
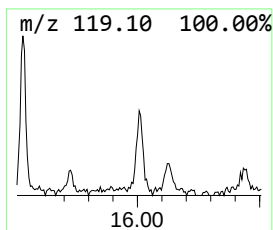
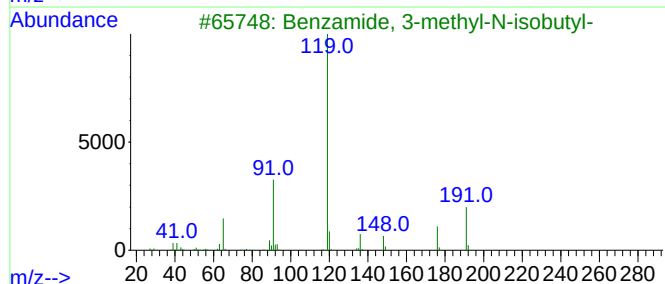
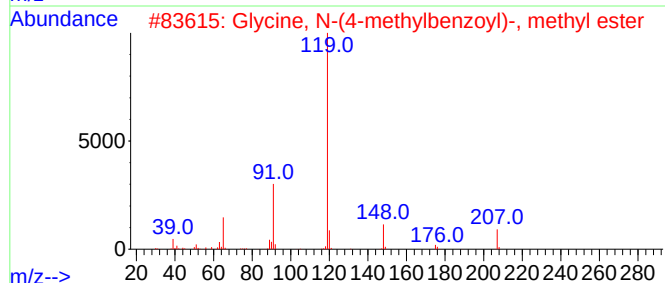
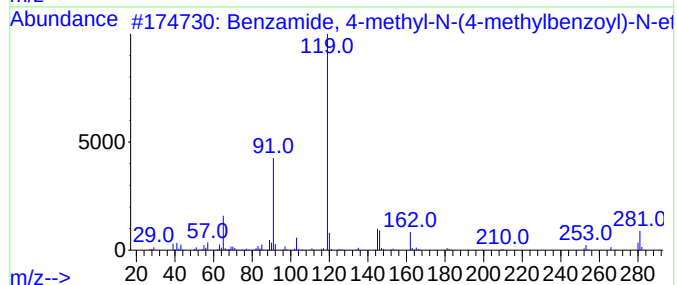
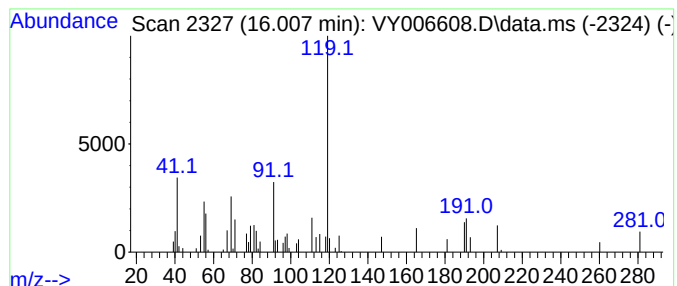
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 unknown16.007 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.007	7.10 ug/l	22202	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzamide, 4-methyl-N-(4-methylb...	281	C18H19NO2	1000407-48-1	49
2			Glycine, N-(4-methylbenzoyl)-, m...	207	C11H13NO3	001208-23-7	43
3			Benzamide, 3-methyl-N-isobutyl-	191	C12H17NO	1000407-41-0	43
4			Diethyltoluamide	191	C12H17NO	000134-62-3	40
5			Benzene, 1,1'-(1,1,2,2-tetrameth...	238	C18H22	001889-67-4	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY110321\
Data File : VY006608.D
Acq On : 03 Nov 2021 17:54
Operator : SY/MD
Sample : M4472-01
Misc : 5.00G/5ML/MSVOA_Y/SOIL
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
WC-2-JS

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102221S.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfurous acid,...	13.355	6.5	ug/l	20431	4	13.428	156413	50.0
Z-3,4,4-Trimeth...	13.611	7.1	ug/l	22096	4	13.428	156413	50.0
Heptyl tetradec...	13.788	16.5	ug/l	51505	4	13.428	156413	50.0
unknown13.855	13.855	9.7	ug/l	30283	4	13.428	156413	50.0
Benzene, (1,1-d...	14.080	11.6	ug/l	36237	4	13.428	156413	50.0
unknown14.294	14.294	8.5	ug/l	26475	4	13.428	156413	50.0
Benzene, (1,1-d...	14.757	11.2	ug/l	35170	4	13.428	156413	50.0
unknown15.281	15.281	6.1	ug/l	19066	4	13.428	156413	50.0
2-Hexene, 3,4,4...	15.501	26.6	ug/l	83168	4	13.428	156413	50.0
unknown16.007	16.007	7.1	ug/l	22202	4	13.428	156413	50.0