

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY070822\
 Data File : VY009487.D
 Acq On : 08 Jul 2022 16:59
 Operator : KP/MD
 Sample : N3595-07
 Misc : 5.23g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 20220489A-7A

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\82Y070722S.M
 Title : SW846 8260

Signal : TIC: VY009487.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.857	3	6	16	rVB2	17518	31326	3.47%	0.460%
2	2.217	59	65	74	rBV2	13548	26494	2.93%	0.389%
3	3.235	226	232	243	rVB4	5414	12748	1.41%	0.187%
4	3.936	338	347	356	rBV	33792	90846	10.06%	1.333%
5	4.015	356	360	375	rVB2	9444	24803	2.75%	0.364%
6	4.186	375	388	403	rBV	47397	129469	14.33%	1.900%
7	4.704	462	473	485	rBV2	16072	53960	5.97%	0.792%
8	5.735	631	642	652	rBV4	6472	20443	2.26%	0.300%
9	6.978	837	846	855	rBV	12316	33175	3.67%	0.487%
10	7.710	957	966	971	rBV	95680	219332	24.28%	3.219%
11	7.783	971	978	990	rVB	272883	618253	68.45%	9.074%
12	8.137	1027	1036	1048	rBV	98077	216760	24.00%	3.181%
13	8.685	1117	1126	1141	rBV	399632	794268	87.94%	11.657%
14	10.173	1363	1370	1377	rBV	403472	703373	77.88%	10.323%
15	11.154	1525	1531	1534	rBV8	4124	9911	1.10%	0.145%
16	11.483	1578	1585	1593	rBV	531805	895797	99.18%	13.147%
17	11.691	1613	1619	1623	rBV7	10215	23147	2.56%	0.340%
18	11.837	1638	1643	1646	rBV7	6534	12914	1.43%	0.190%
19	11.983	1663	1667	1671	rBV4	7892	15631	1.73%	0.229%
20	12.227	1705	1707	1713	rVB3	20945	26889	2.98%	0.395%
21	12.307	1714	1720	1727	rBV10	16720	51192	5.67%	0.751%
22	12.483	1740	1749	1756	rBV4	451122	903170	100.00%	13.255%
23	12.569	1760	1763	1766	rVV5	14182	19287	2.14%	0.283%
24	12.733	1783	1790	1795	rBV8	30040	91700	10.15%	1.346%
25	12.837	1796	1807	1812	rVV7	42885	136086	15.07%	1.997%
26	12.995	1829	1833	1837	rBV2	20216	29069	3.22%	0.427%
27	13.062	1841	1844	1850	rVB4	58338	96972	10.74%	1.423%
28	13.172	1858	1862	1870	rVB7	34268	83688	9.27%	1.228%
29	13.282	1875	1880	1885	rVV	123061	209402	23.19%	3.073%
30	13.349	1888	1891	1894	rBV4	24191	36307	4.02%	0.533%
31	13.422	1895	1903	1908	rVV	471479	814836	90.22%	11.959%
32	13.471	1908	1911	1919	rVB	77703	158482	17.55%	2.326%
33	13.959	1988	1991	1995	rVB3	39068	55360	6.13%	0.812%
34	14.251	2035	2039	2041	rBV3	38370	55099	6.10%	0.809%
35	14.385	2054	2061	2064	rBV3	53095	113562	12.57%	1.667%

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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

Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y070722S.M
Title : SW846 8260

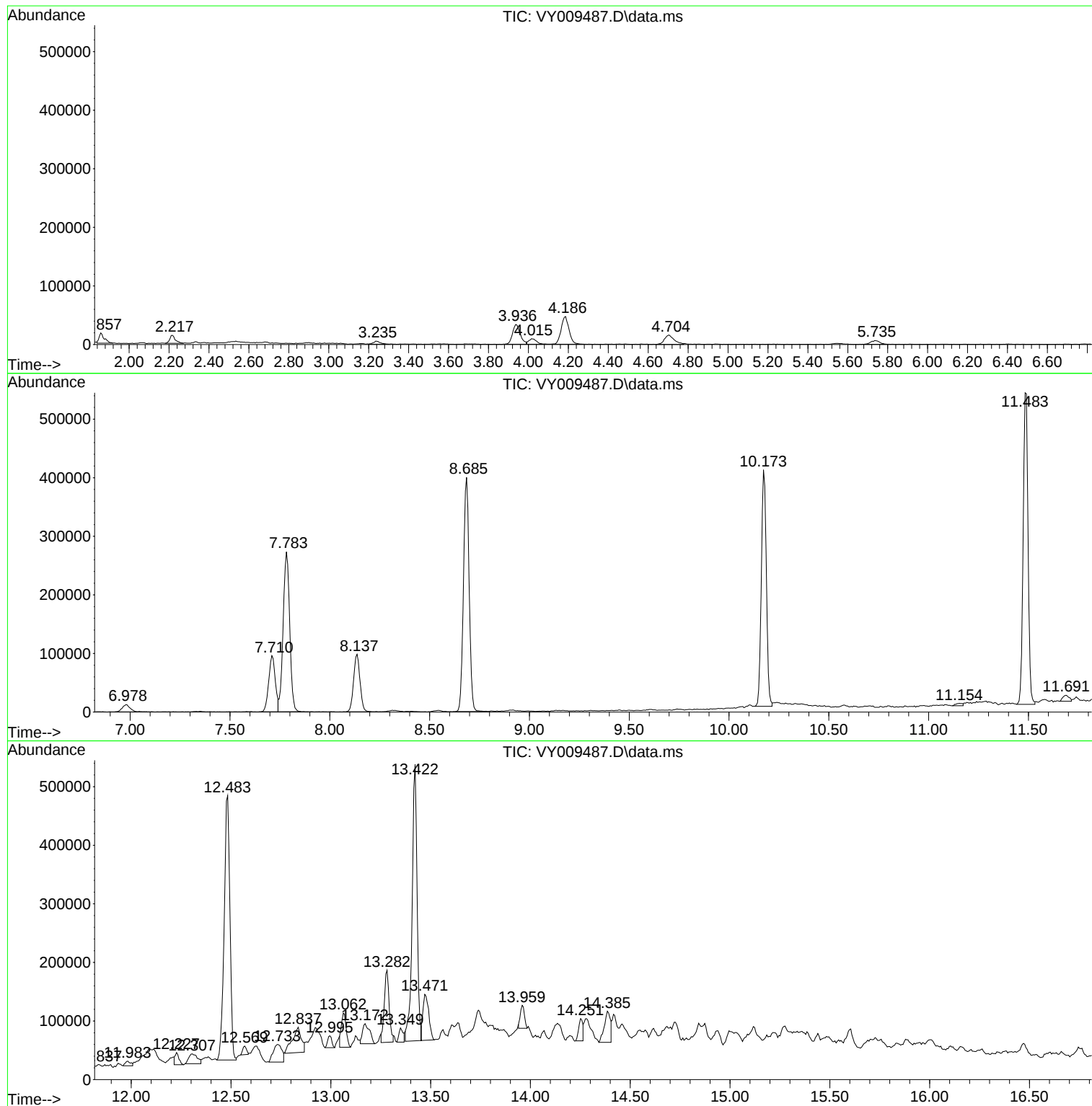
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y070722S.M
Quant Title : SW846 8260

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



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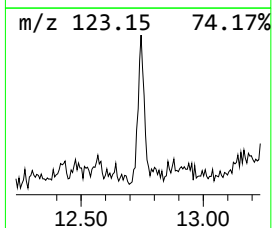
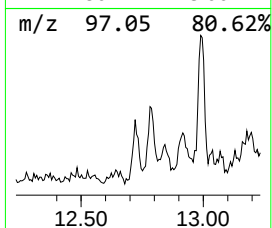
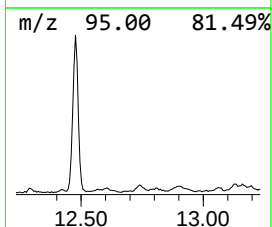
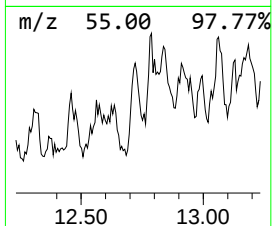
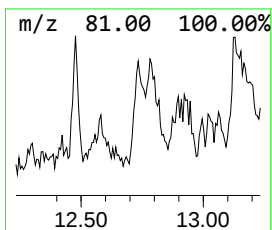
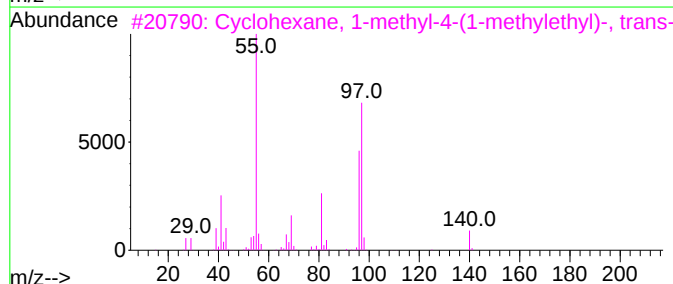
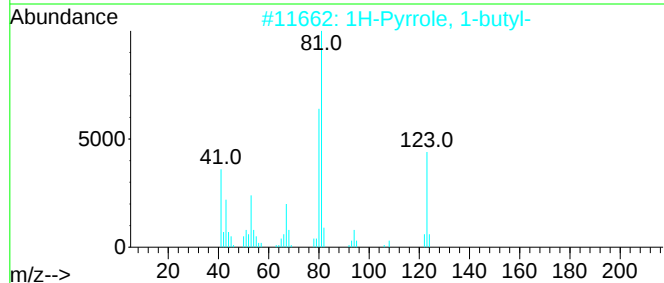
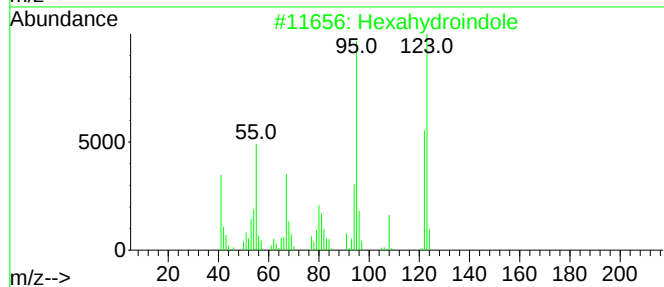
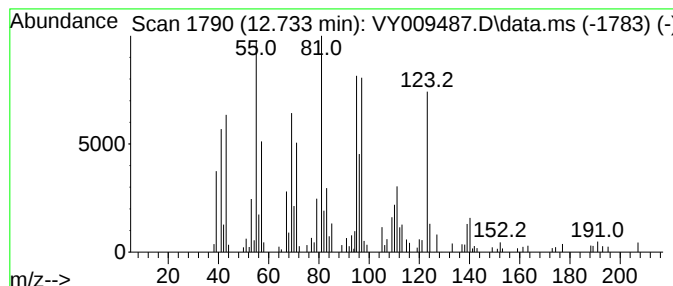
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y070722S.M
Quant Title : SW846 8260

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

Peak Number 1 unknown12.733 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.733	5.63 ug/l	91700	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexahydroindole	123	C8H13N	018159-32-5	27
2			1H-Pyrrole, 1-butyl-	123	C8H13N	000589-33-3	22
3			Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	001678-82-6	18
4			Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	006069-98-3	18
5			1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	11



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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
20220489A-7A

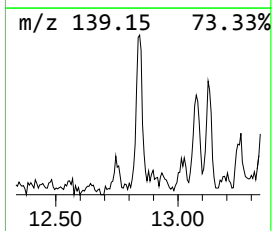
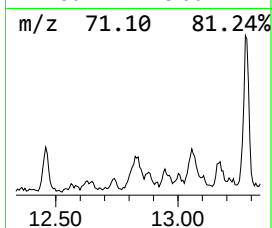
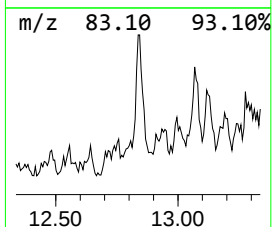
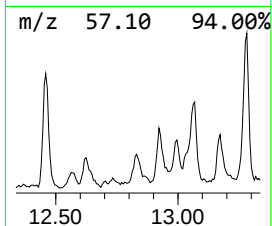
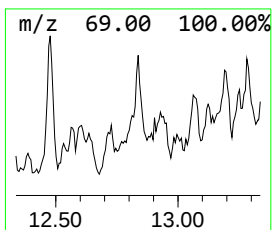
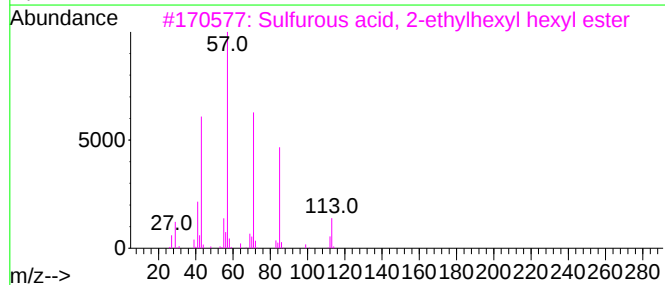
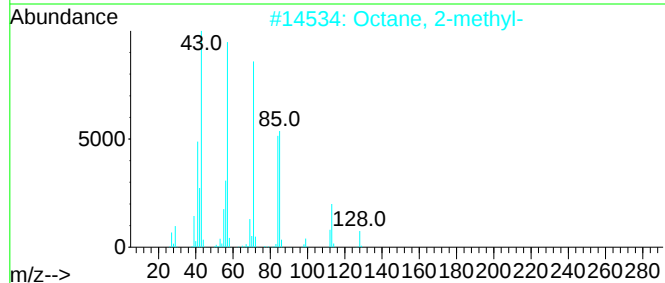
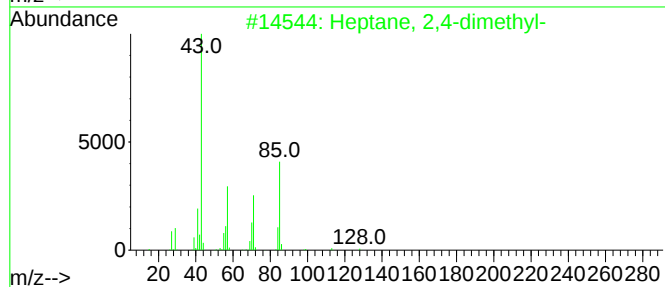
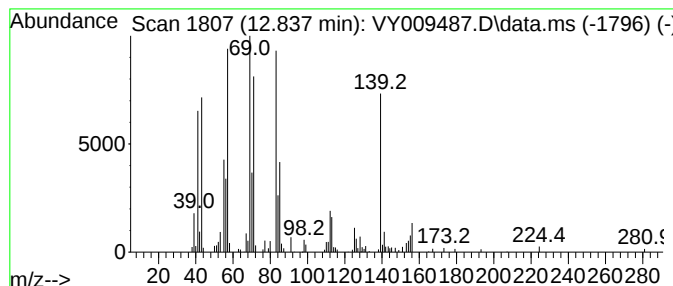
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y070722S.M
Quant Title : SW846 8260

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

Peak Number 2 unknown12.837 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.837	8.35 ug/l	136086	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	18
2			Octane, 2-methyl-	128	C9H20	003221-61-2	18
3			Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	14
4			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	14
5			3-Ethyl-3-methylheptane	142	C10H22	017302-01-1	14



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Instrument :
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ClientSampleId :
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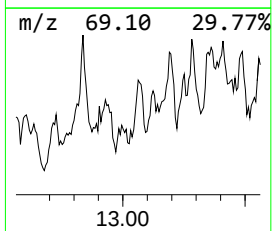
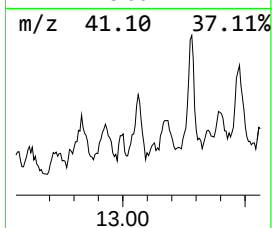
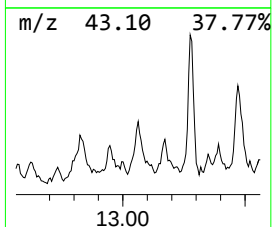
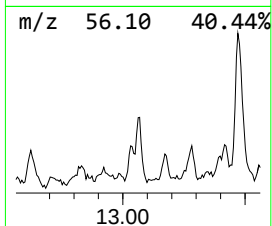
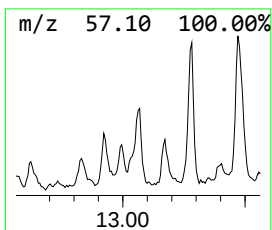
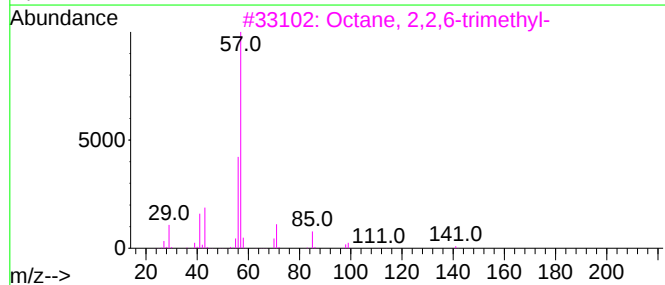
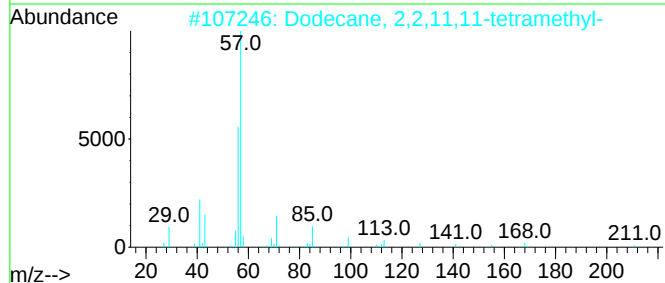
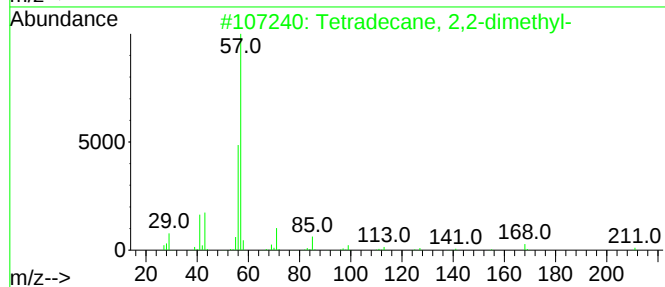
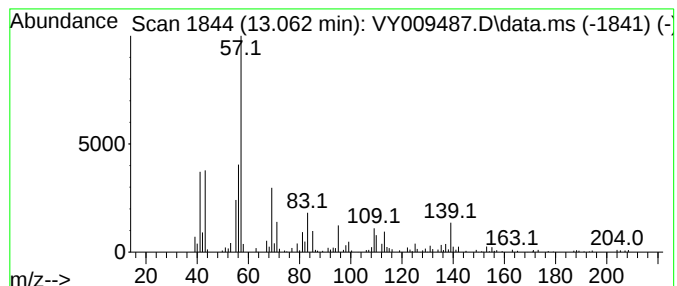
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y070722S.M
Quant Title : SW846 8260

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

Peak Number 3 unknown13.063 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.063	5.95 ug/l	96972	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane, 2,2-dimethyl-	226	C16H34	059222-86-5	47
2			Dodecane, 2,2,11,11-tetramethyl-	226	C16H34	127204-12-0	47
3			Octane, 2,2,6-trimethyl-	156	C11H24	062016-28-8	43
4			2,2,7,7-Tetramethyloctane	170	C12H26	001071-31-4	43
5			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	43



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ALS Vial : 13 Sample Multiplier: 1

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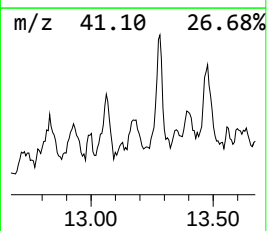
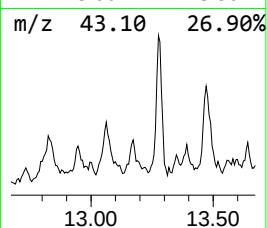
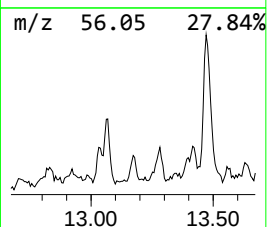
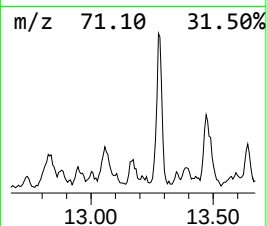
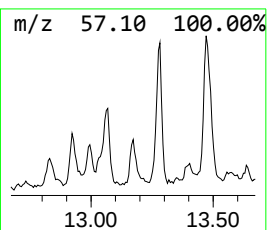
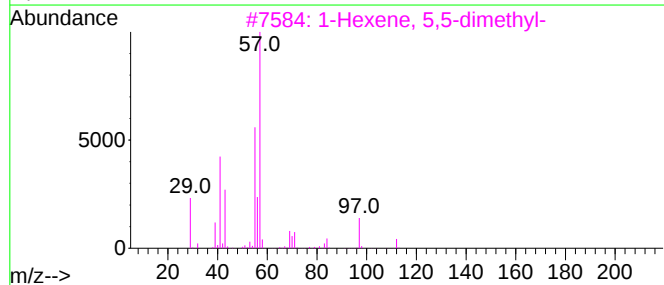
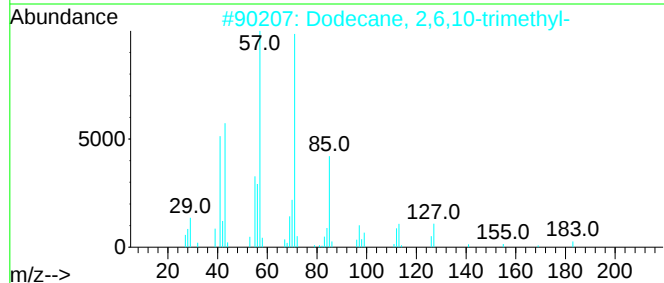
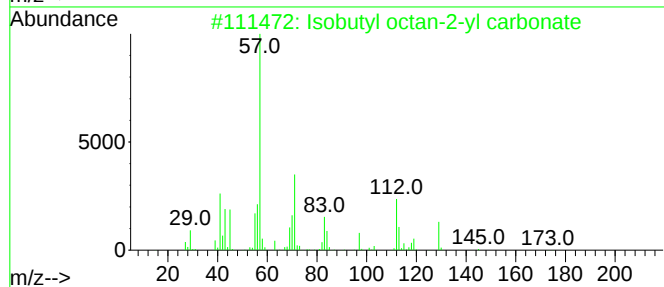
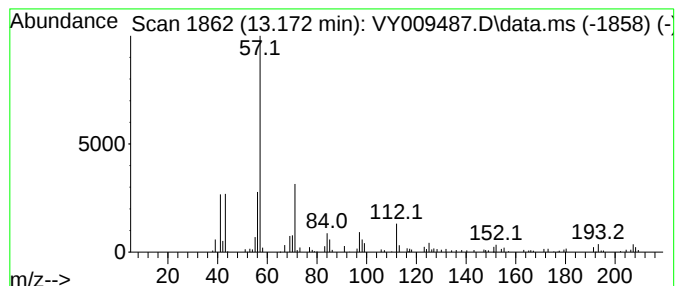
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Isobutyl octan-2-yl carbonate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.172	5.14 ug/l	83688	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isobutyl octan-2-yl carbonate	230	C13H26O3	1000372-74-7	50
2			Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	47
3			1-Hexene, 5,5-dimethyl-	112	C8H16	007116-86-1	47
4			Dodecane, 1-fluoro-	188	C12H25F	000334-68-9	42
5			Decyl isobutyl carbonate	258	C15H30O3	959226-07-4	40



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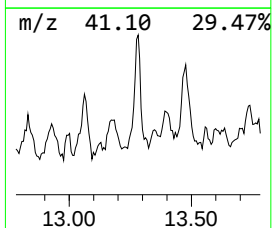
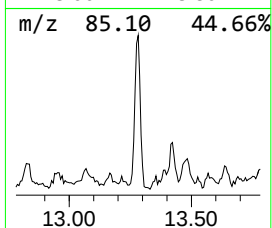
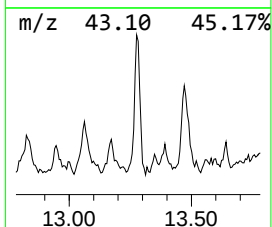
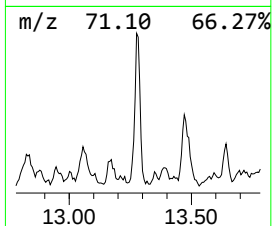
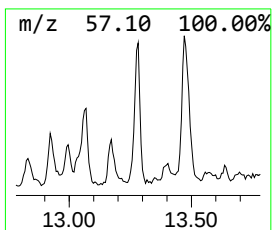
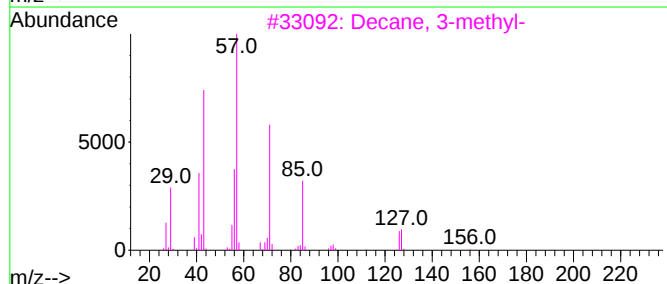
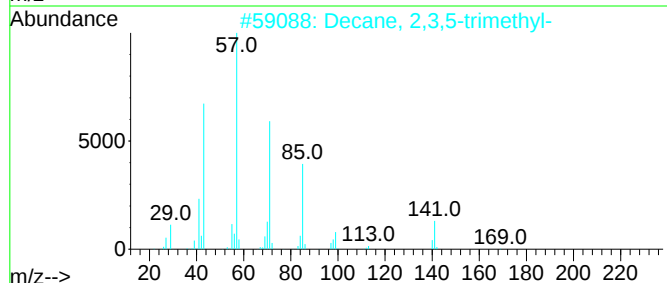
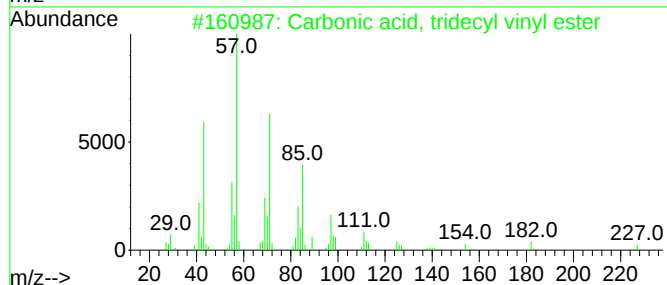
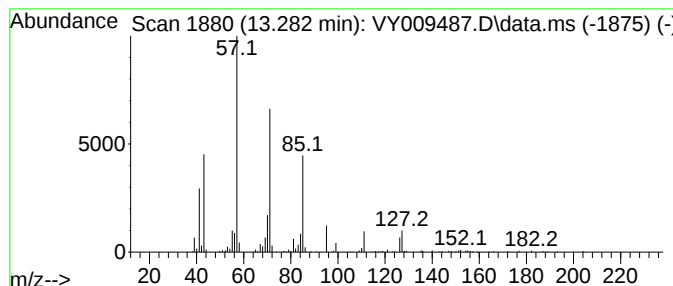
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y070722S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Carbonic acid, tridecyl vin... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.282	12.85 ug/l	209402	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, tridecyl vinyl ester	270	C16H30O3	1000382-54-7	64
2			Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	59
3			Decane, 3-methyl-	156	C11H24	013151-34-3	59
4			Tridecane	184	C13H28	000629-50-5	59
5			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY070822\
Data File : VY009487.D
Acq On : 08 Jul 2022 16:59
Operator : KP/MD
Sample : N3595-07
Misc : 5.23g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
20220489A-7A

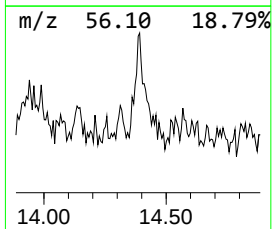
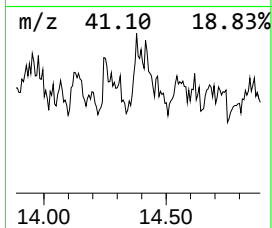
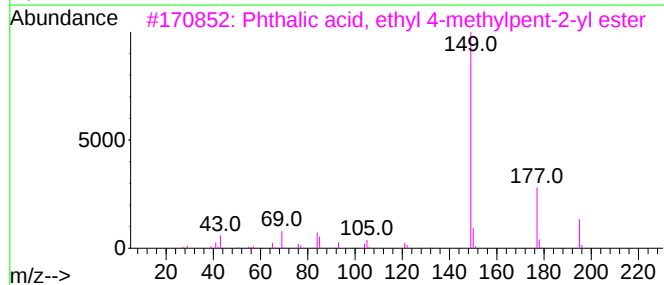
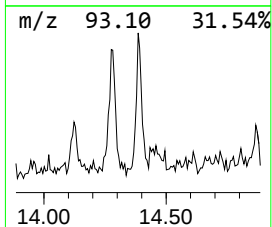
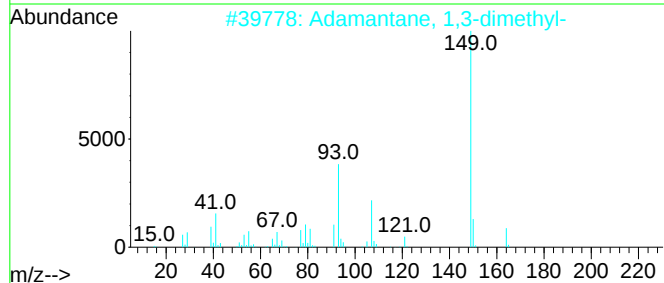
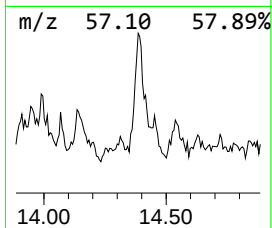
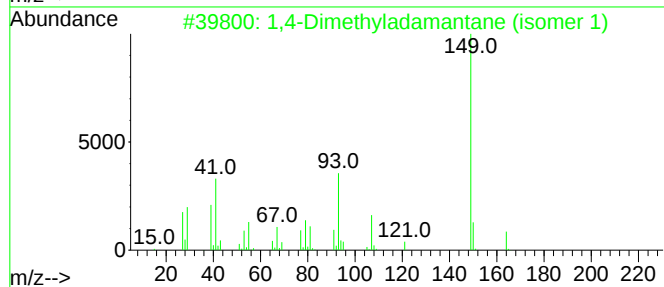
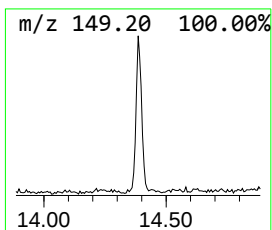
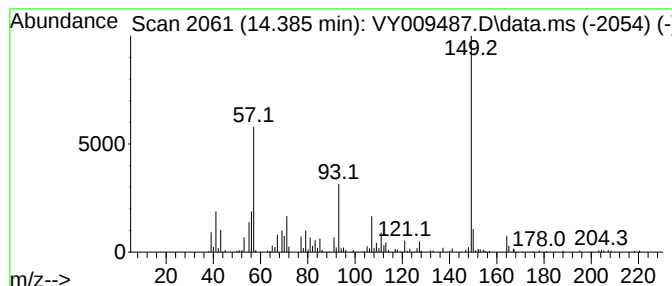
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y070722S.M
Quant Title : SW846 8260

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

Peak Number 6 1,4-Dimethyladamantane (iso... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.385	6.97 ug/l	113562	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Dimethyladamantane (isomer 1)	164	C12H20	1000460-67-0	83
2			Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	80
3			Phthalic acid, ethyl 4-methylpen...	278	C16H22O4	1000356-87-0	50
4			1-Methyl-3-ethyladamantane	178	C13H22	001687-34-9	50
5			Phthalic acid, 2-methylbutyl pro...	278	C16H22O4	1000322-81-1	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY070822\
Data File : VY009487.D
Acq On : 08 Jul 2022 16:59
Operator : KP/MD
Sample : N3595-07
Misc : 5.23g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
20220489A-7A

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y070722S.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
unknown12.733	12.733	5.6	ug/l	91700	4	13.422	814836	50.0
unknown12.837	12.837	8.3	ug/l	136086	4	13.422	814836	50.0
unknown13.063	13.063	6.0	ug/l	96972	4	13.422	814836	50.0
Isobutyl octan-...	13.172	5.1	ug/l	83688	4	13.422	814836	50.0
Carbonic acid, ...	13.282	12.9	ug/l	209402	4	13.422	814836	50.0
1,4-Dimethylada...	14.385	7.0	ug/l	113562	4	13.422	814836	50.0