

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY042924\
 Data File : VY018082.D
 Acq On : 29 Apr 2024 20:41
 Operator : SY/MD
 Sample : P2307-01
 Misc : 5.02g/5.0mL/MSVOA_Y/SOIL/A
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 WC-1-VOC

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\82Y041624S.M
 Title : SW846 8260

Signal : TIC: VY018082.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	13622	22789	1.38%	0.190%
2	4.704	463	473	488	rBV2	14292	43265	2.61%	0.360%
3	7.716	955	967	972	rBV	249752	593498	35.85%	4.945%
4	7.783	972	978	994	rVB	370782	852328	51.48%	7.101%
5	8.136	1027	1036	1050	rBV	188113	422094	25.49%	3.517%
6	8.685	1118	1126	1141	rBV	612217	1221558	73.78%	10.177%
7	9.746	1293	1300	1310	rVB2	11244	23504	1.42%	0.196%
8	10.179	1363	1371	1386	rVB	987371	1655630	100.00%	13.793%
9	11.489	1578	1586	1598	rBV	877764	1435972	86.73%	11.963%
10	11.691	1613	1619	1625	rBV5	7294	16724	1.01%	0.139%
11	12.123	1682	1690	1697	rVB7	7534	18914	1.14%	0.158%
12	12.483	1739	1749	1756	rBV	636061	1045476	63.15%	8.710%
13	12.642	1768	1775	1782	rVB5	29990	73376	4.43%	0.611%
14	12.745	1782	1792	1796	rBV9	11547	35077	2.12%	0.292%
15	12.837	1800	1807	1812	rBV3	29108	63952	3.86%	0.533%
16	12.946	1819	1825	1830	rBV6	16518	36402	2.20%	0.303%
17	13.007	1831	1835	1836	rVV3	15139	20428	1.23%	0.170%
18	13.038	1837	1840	1842	rVV2	40135	61016	3.69%	0.508%
19	13.068	1843	1845	1857	rVB3	50293	91052	5.50%	0.759%
20	13.172	1857	1862	1868	rBV2	29802	52636	3.18%	0.439%
21	13.282	1873	1880	1889	rBV	149098	252594	15.26%	2.104%
22	13.355	1889	1892	1896	rBV3	26041	41870	2.53%	0.349%
23	13.422	1896	1903	1908	rBV	751976	1212498	73.23%	10.102%
24	13.477	1908	1912	1923	rVB	111538	237463	14.34%	1.978%
25	13.562	1923	1926	1930	rBV3	16673	24165	1.46%	0.201%
26	13.617	1931	1935	1938	rBV5	20412	37972	2.29%	0.316%
27	13.696	1943	1948	1950	rBV4	18390	32744	1.98%	0.273%
28	13.879	1974	1978	1981	rBV4	19271	34177	2.06%	0.285%
29	14.074	2007	2010	2013	rVB3	15390	17515	1.06%	0.146%
30	14.123	2014	2018	2028	rVB5	99888	222277	13.43%	1.852%
31	14.221	2028	2034	2035	rBV6	15198	31909	1.93%	0.266%
32	14.282	2039	2044	2052	rVB	193880	339361	20.50%	2.827%
33	14.391	2055	2062	2068	rVV2	285531	556295	33.60%	4.635%
34	14.458	2069	2073	2085	rVB2	108036	219350	13.25%	1.827%
35	14.727	2114	2117	2122	rVB2	38095	55205	3.33%	0.460%
36	14.873	2136	2141	2147	rVB2	134275	234472	14.16%	1.953%

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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\82Y041624S.M
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37	14.940	2147	2152	2157	rBV	110208	177104	10.70%	1.475%
38	15.001	2157	2162	2164	rBV	79546	134915	8.15%	1.124%
39	15.214	2194	2197	2202	rVB2	27428	48332	2.92%	0.403%
40	15.275	2203	2207	2215	rBV2	73435	201267	12.16%	1.677%
41	15.586	2246	2258	2259	rBV5	23475	82467	4.98%	0.687%
42	15.885	2303	2307	2312	rVB8	11855	23346	1.41%	0.195%

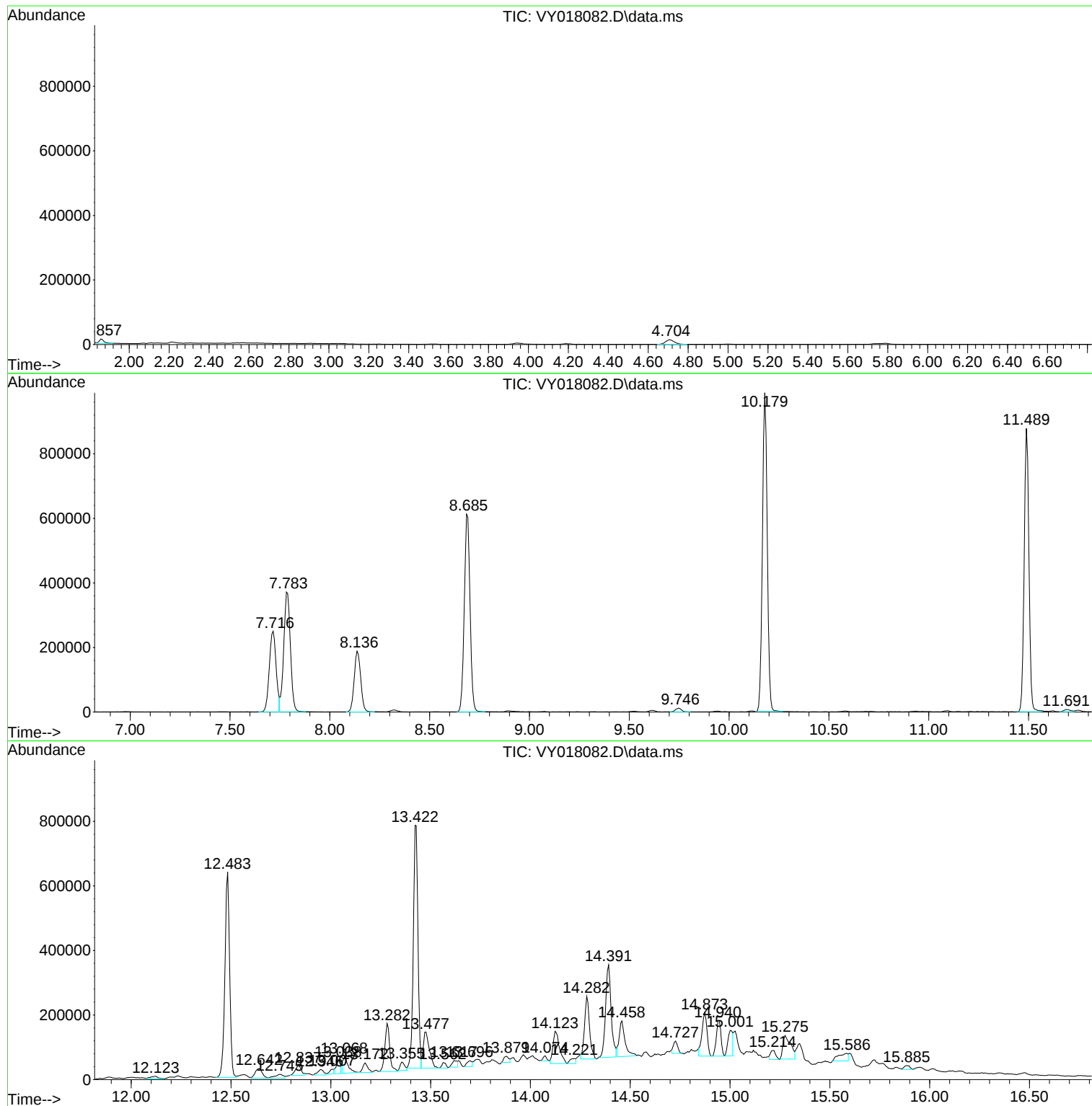
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Quant Title : SW846 8260

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



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Instrument :
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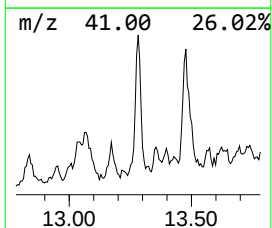
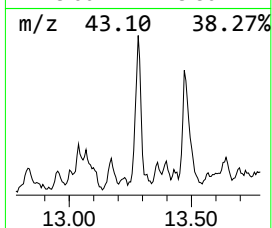
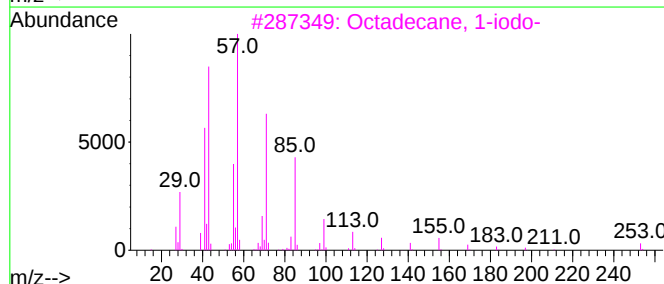
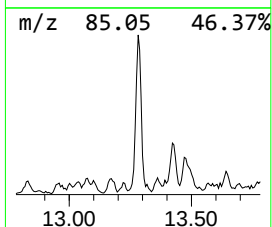
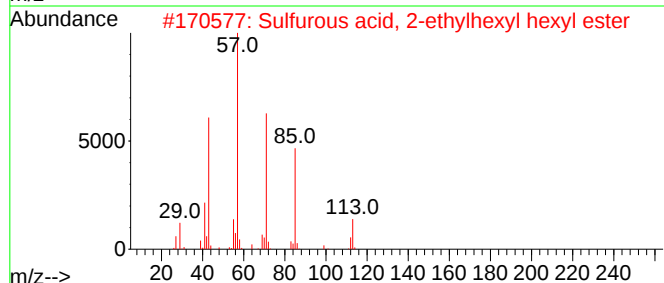
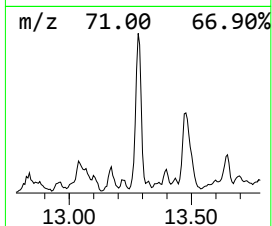
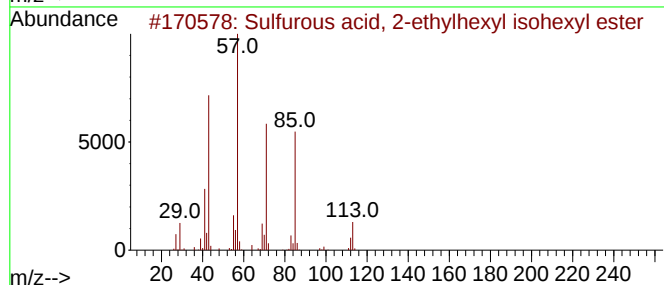
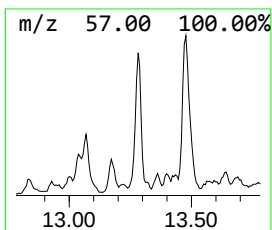
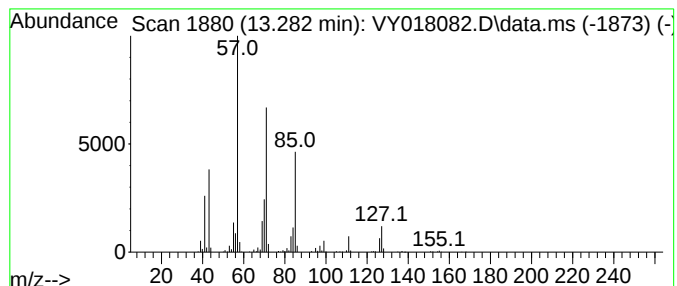
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y041624S.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfurous acid, 2-ethylhexy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.282	10.42 ug/l	252594	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	53
2			Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	53
3			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	50
4			Nonane, 5-methyl-5-propyl-	184	C13H28	017312-75-3	50
5			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	50



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Instrument :
MSVOA_Y
ClientSampleId :
WC-1-VOC

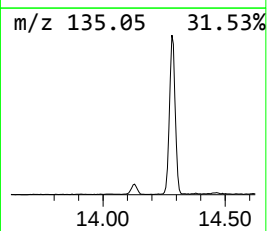
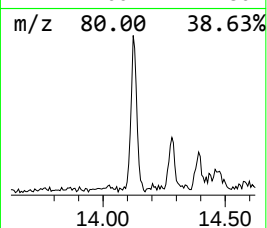
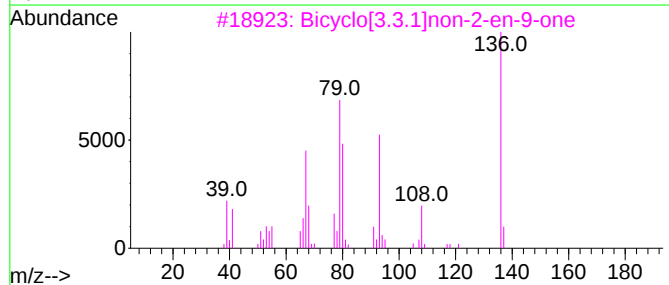
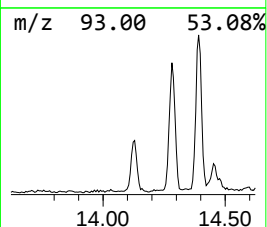
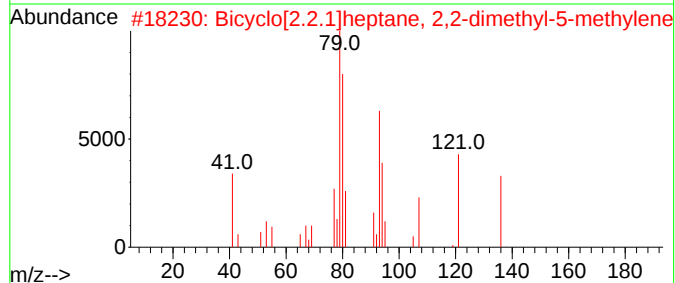
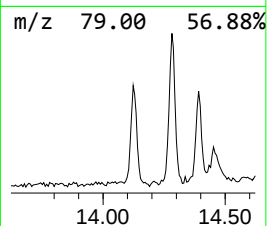
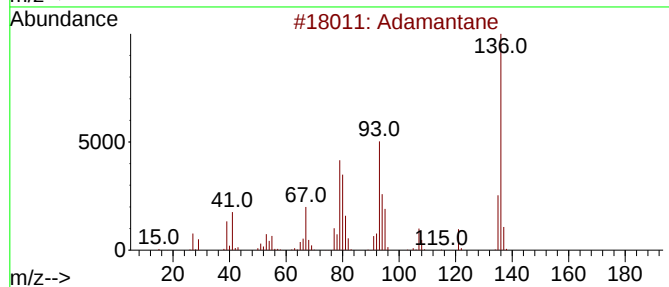
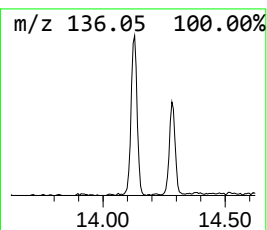
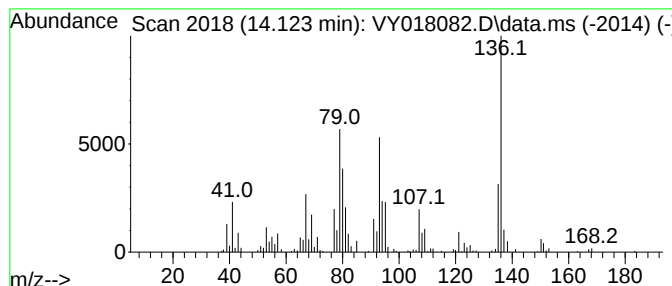
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y041624S.M
Quant Title : SW846 8260

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

Peak Number 2 Adamantane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.123	9.17 ug/l	222277	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Adamantane	136	C10H16	000281-23-2	97
2			Bicyclo[2.2.1]heptane, 2,2-dimet...	136	C10H16	000497-32-5	74
3			Bicyclo[3.3.1]non-2-en-9-one	136	C9H12O	004844-11-5	64
4			Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	000586-62-9	47
5			1,3-Cyclohexadiene, 5-butyl-	136	C10H16	030168-57-1	47



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ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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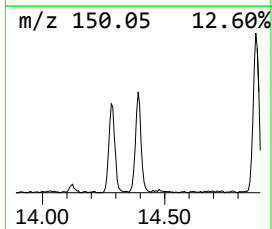
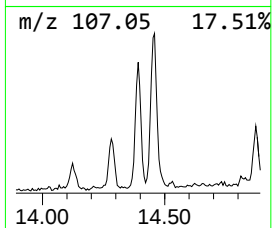
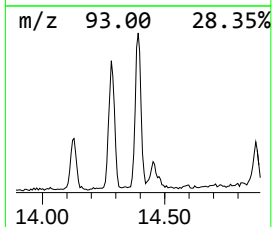
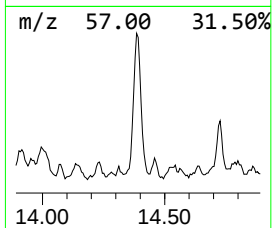
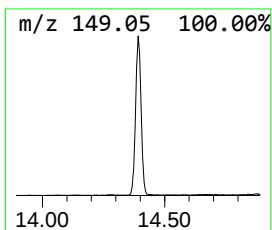
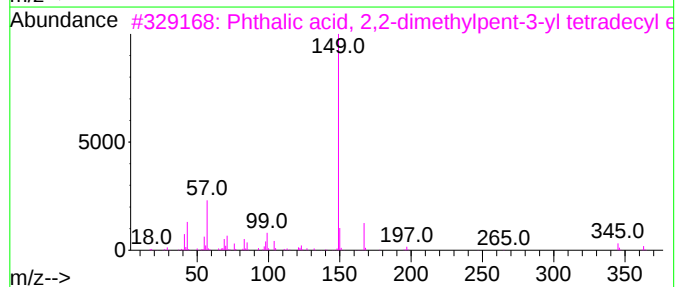
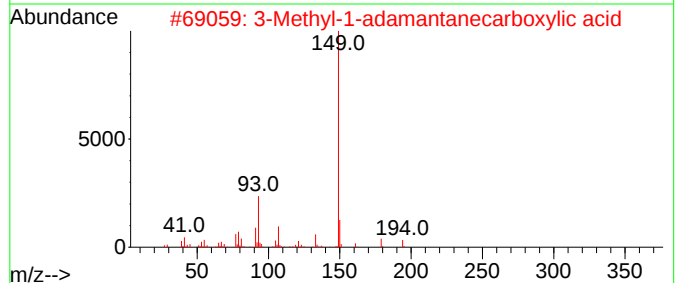
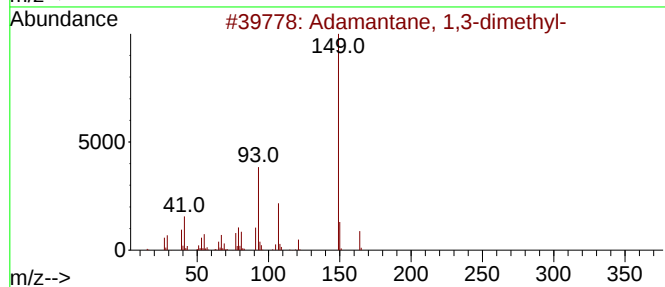
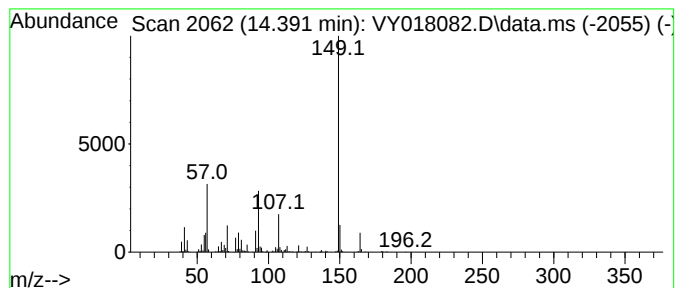
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y041624S.M
Quant Title : SW846 8260

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

Peak Number 4 Adamantane, 1,3-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.391	22.94 ug/l	556295	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	91
2			3-Methyl-1-adamantanecarboxylic ...	194	C12H18O2	1000504-38-9	53
3			Phthalic acid, 2,2-dimethylpent-...	460	C29H48O4	1000415-53-7	50
4			1-Methyl-3-ethyladamantane	178	C13H22	001687-34-9	50
5			1,4-Dimethyladamantane (isomer 1)	164	C12H20	1000460-67-0	50



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ClientSampleId :
WC-1-VOC

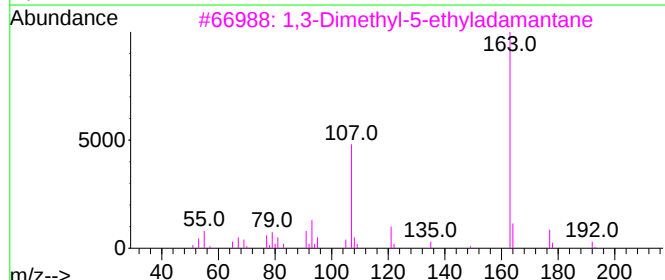
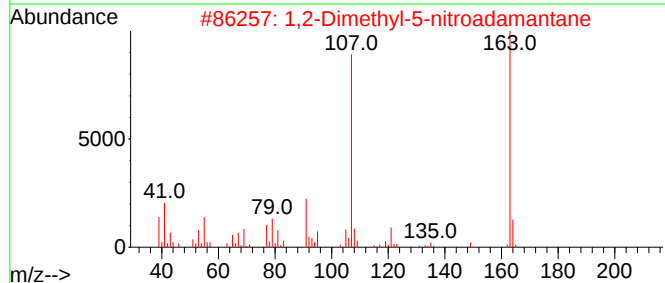
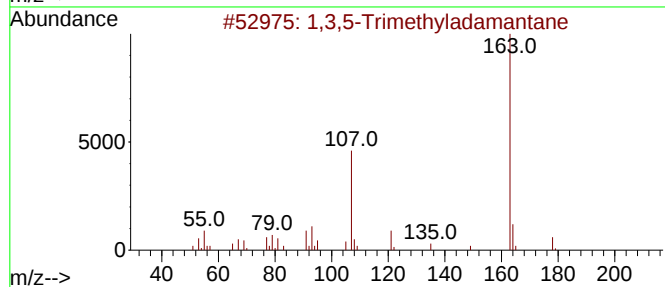
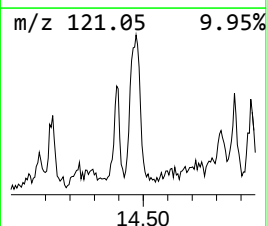
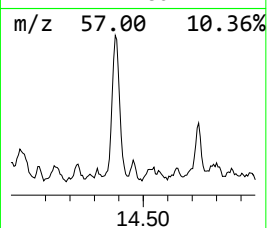
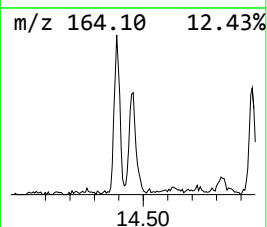
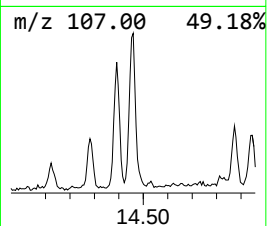
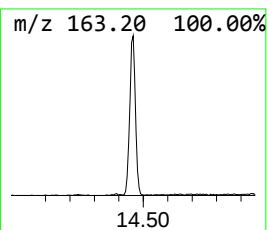
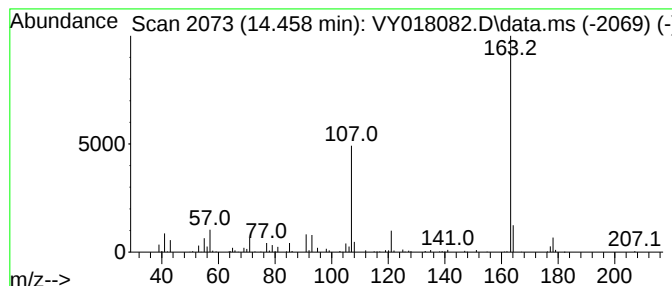
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y041624S.M
Quant Title : SW846 8260

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

Peak Number 5 1,3,5-Trimethyladamantane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.458	9.05 ug/l	219350	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3,5-Trimethyladamantane	178	C13H22	000707-35-7	80
2			1,2-Dimethyl-5-nitroadamantane	209	C12H19NO2	006588-68-7	56
3			1,3-Dimethyl-5-ethyladamantane	192	C14H24	001687-35-0	56
4			1,3-Dimethyl-5-n-propyl-adamantane	206	C15H26	019385-87-6	56
5			3,5-Dimethyl-1-adamantanecarboxy...	208	C13H20O2	014670-94-1	56



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Instrument :
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ClientSampleId :
WC-1-VOC

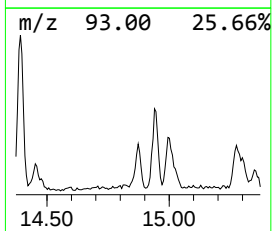
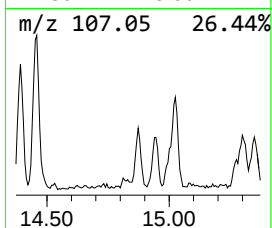
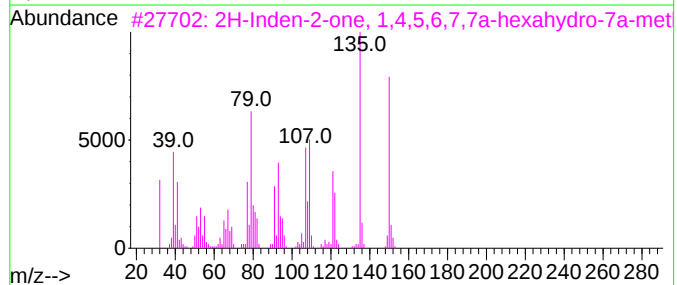
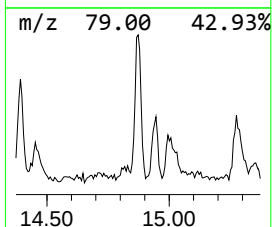
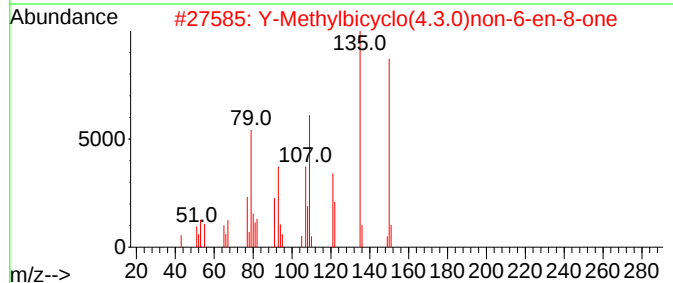
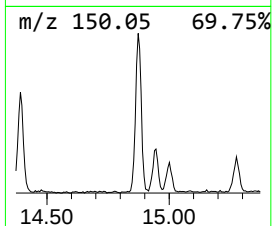
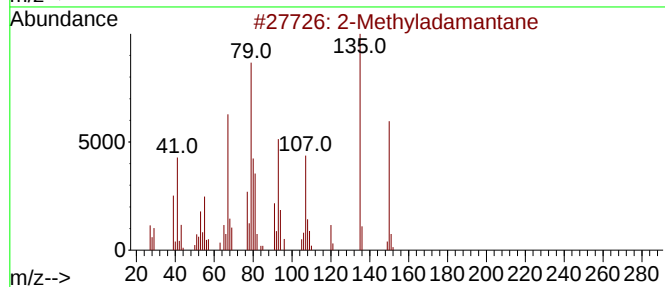
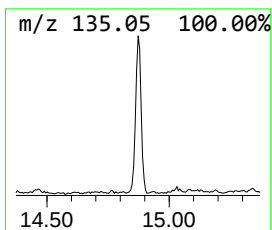
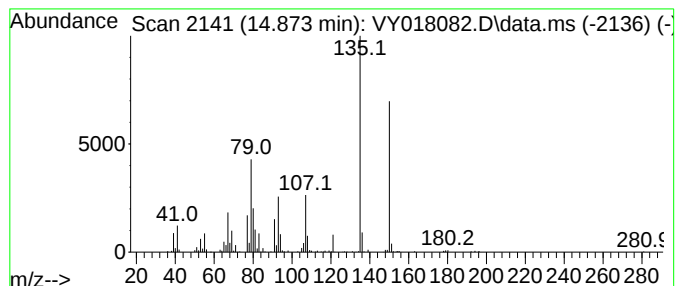
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Quant Title : SW846 8260

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

Peak Number 6 2-Methyladamantane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.873	9.67 ug/l	234472	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methyladamantane	150	C11H18	000700-56-1	91
2			Y-Methylbicyclo(4.3.0)non-6-en-8-one	150	C10H14O	1000424-65-9	87
3			2H-Inden-2-one, 1,4,5,6,7,7a-hexahydro-	150	C10H14O	054725-16-5	64
4			3,9-Epoxy-p-mentha-1,8(10)-diene	150	C10H14O	1000111-14-8	64
5			3-Methyl-2-(2-methyl-2-butenyl)-	150	C10H14O	015186-51-3	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY042924\
Data File : VY018082.D
Acq On : 29 Apr 2024 20:41
Operator : SY/MD
Sample : P2307-01
Misc : 5.02g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
WC-1-VOC

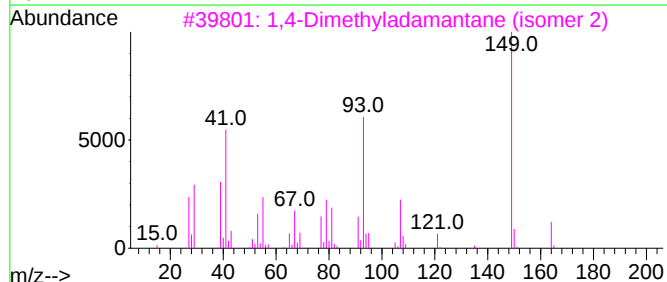
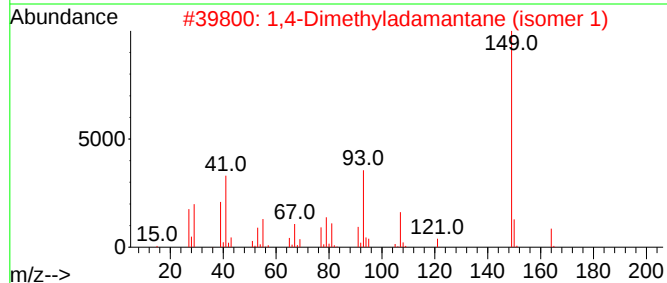
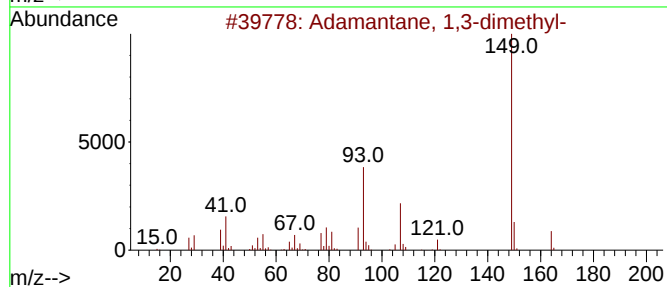
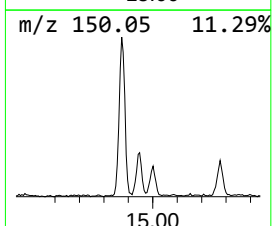
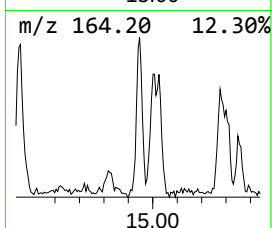
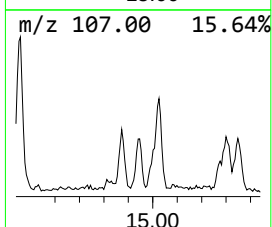
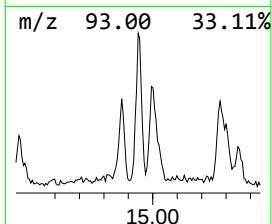
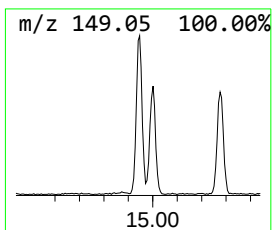
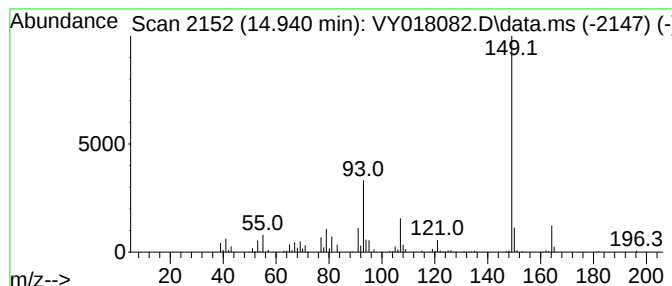
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Quant Title : SW846 8260

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

Peak Number 7 1-Methyl-3-ethyladamantane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.940	7.30 ug/l	177104	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	95
2			1,4-Dimethyladamantane (isomer 1)	164	C12H20	1000460-67-0	91
3			1,4-Dimethyladamantane (isomer 2)	164	C12H20	1000460-67-1	91
4			1-Methyl-3-ethyladamantane	178	C13H22	001687-34-9	86
5			Added stereo to name	164	C12H20	024145-88-8	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY042924\
Data File : VY018082.D
Acq On : 29 Apr 2024 20:41
Operator : SY/MD
Sample : P2307-01
Misc : 5.02g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
WC-1-VOC

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y041624S.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,...	13.282	10.4	ug/l	252594	4	13.428	1212500	50.0
Adamantane	14.123	9.2	ug/l	222277	4	13.428	1212500	50.0
Adamantane, 1,3...	14.391	22.9	ug/l	556295	4	13.428	1212500	50.0
1,3,5-Trimethyl...	14.458	9.1	ug/l	219350	4	13.428	1212500	50.0
2-Methyladamantane	14.873	9.7	ug/l	234472	4	13.428	1212500	50.0
1-Methyl-3-ethy...	14.940	7.3	ug/l	177104	4	13.428	1212500	50.0