

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY092721\
 Data File : VY006171.D
 Acq On : 27 Sep 2021 18:17
 Operator : SY/MD
 Sample : M3951-01
 Misc : 6.48G/5ML/MSVOA_Y/SOIL
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 WC-20210924

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\82Y091421S.M

Title : SW846 8260

Signal : TIC: VY006171.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.722	467	476	484	rBV3	4314	13184	1.68%	0.315%
2	7.722	959	968	974	rBV	91555	217704	27.69%	5.196%
3	7.795	974	980	993	rVB	156505	352073	44.79%	8.404%
4	8.149	1027	1038	1051	rVB	91098	204651	26.03%	4.885%
5	8.697	1116	1128	1138	rBV	212406	422015	53.68%	10.073%
6	10.185	1364	1372	1380	rBV	344420	587242	74.70%	14.017%
7	11.490	1578	1586	1596	rBV	300075	497630	63.30%	11.878%
8	12.489	1742	1750	1757	rBV2	435632	786139	100.00%	18.764%
9	12.642	1769	1775	1783	rVB6	5317	10386	1.32%	0.248%
10	12.806	1797	1802	1806	rBV5	5184	9990	1.27%	0.238%
11	13.288	1872	1881	1883	rBV7	4581	10595	1.35%	0.253%
12	13.337	1885	1889	1894	rVV3	10909	20314	2.58%	0.485%
13	13.428	1895	1904	1910	rVV	282239	450825	57.35%	10.761%
14	13.483	1910	1913	1919	rVV5	4536	8955	1.14%	0.214%
15	13.751	1952	1957	1960	rBV6	6017	11044	1.40%	0.264%
16	13.965	1987	1992	1997	rBV	17865	32081	4.08%	0.766%
17	14.129	2015	2019	2027	rVV8	6915	18277	2.32%	0.436%
18	14.203	2027	2031	2036	rBV6	4642	8203	1.04%	0.196%
19	14.282	2036	2044	2054	rBV4	16321	53289	6.78%	1.272%
20	14.391	2054	2062	2066	rBV	18045	41364	5.26%	0.987%
21	14.465	2070	2074	2083	rVB6	12160	32655	4.15%	0.779%
22	14.580	2090	2093	2096	rBV4	4966	8014	1.02%	0.191%
23	14.733	2115	2118	2123	rVB4	13910	21823	2.78%	0.521%
24	14.879	2132	2142	2147	rBV6	29171	78840	10.03%	1.882%
25	14.940	2148	2152	2157	rBV3	25167	41222	5.24%	0.984%
26	15.001	2157	2162	2164	rBV3	28228	49253	6.27%	1.176%
27	15.282	2204	2208	2210	rBV4	27936	47038	5.98%	1.123%
28	16.763	2447	2451	2455	rBV3	84854	154780	19.69%	3.694%

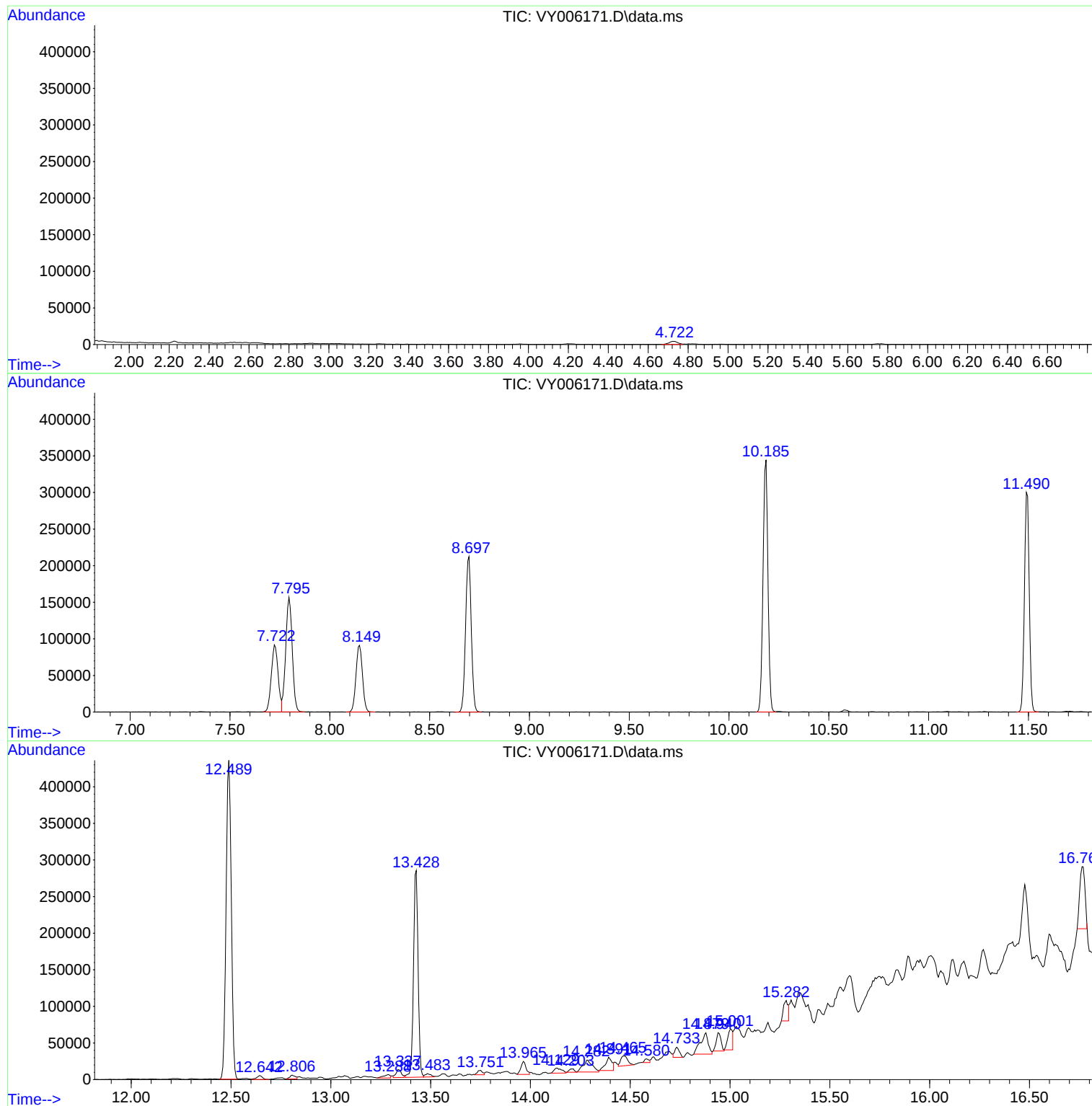
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ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
WC-20210924

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y091421S.M
Quant Title : SW846 8260

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



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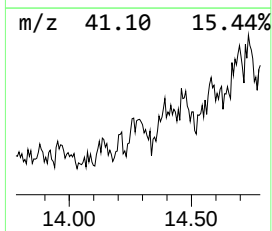
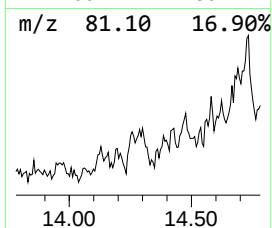
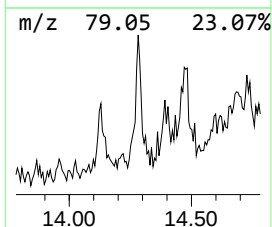
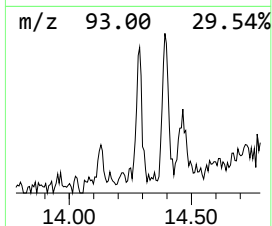
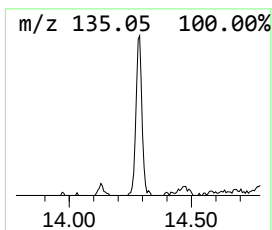
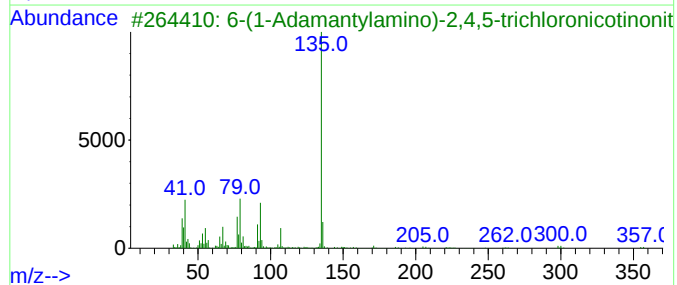
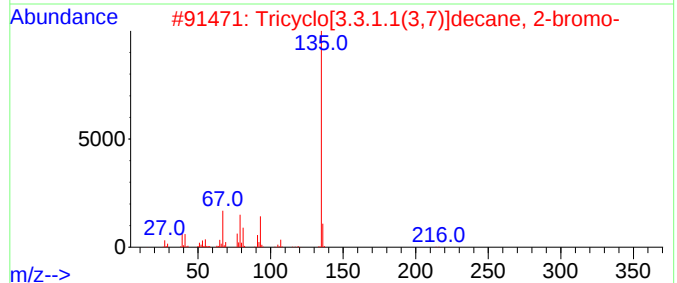
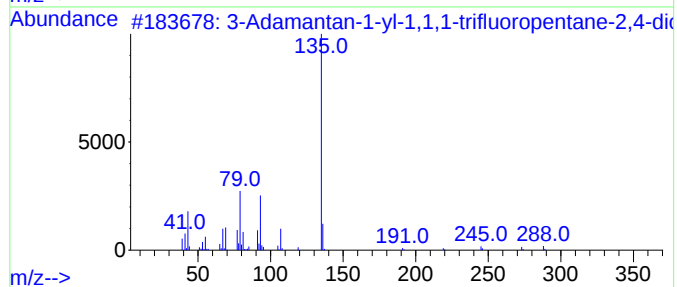
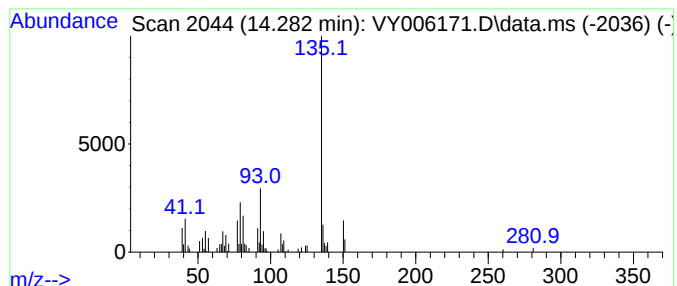
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y091421S.M
Quant Title : SW846 8260

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

Peak Number 1 3-Adamantan-1-yl-1,1,1-trif... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.282	5.91 ug/l	53289	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Adamantan-1-yl-1,1,1-trifluoro...	288	C15H19F3O2	1000311-44-8	72		
2	Tricyclo[3.3.1.1(3,7)]decane, 2-...	214	C10H15Br	007314-85-4	64		
3	6-(1-Adamantylamino)-2,4,5-trich...	355	C16H16Cl3N3	339165-88-7	64		
4	Tricyclo[3.3.1.1(3,7)]decane, 1-...	181	C10H15NO2	007575-82-8	64		
5	N-Methylenedeadamantan-1-amine	163	C11H17N	033103-90-1	59		



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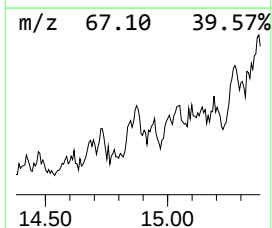
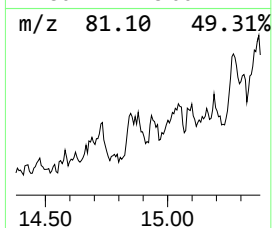
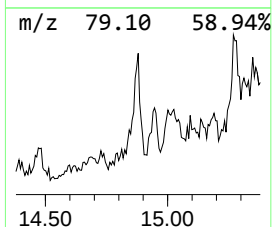
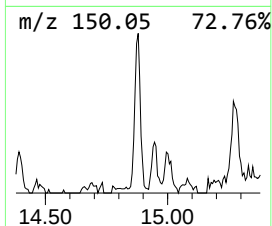
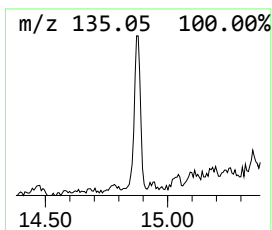
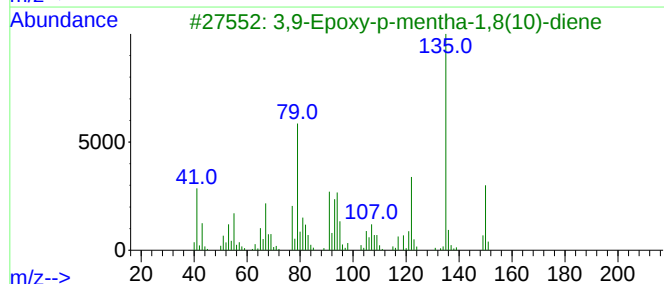
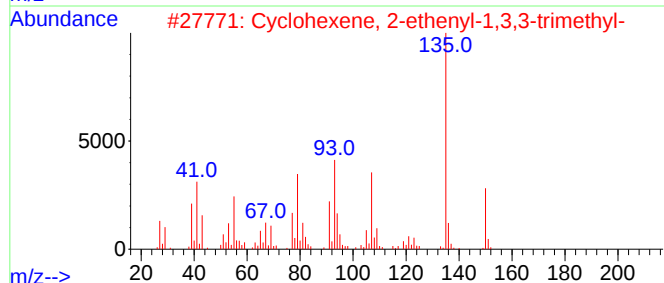
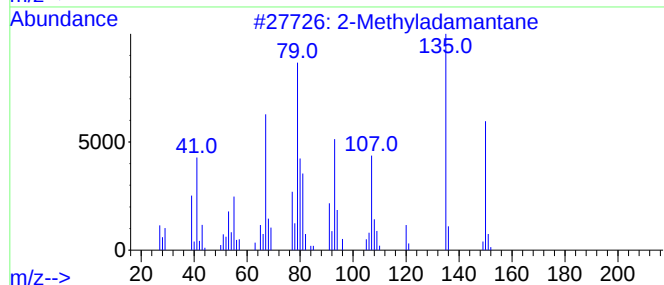
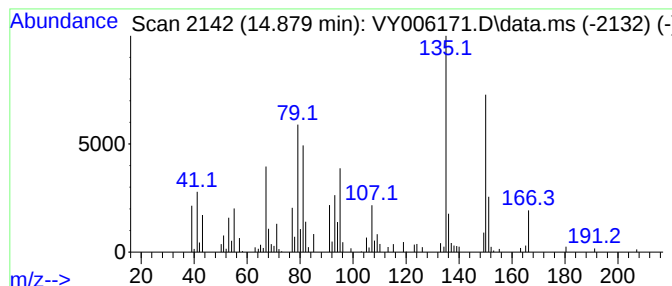
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y091421S.M
Quant Title : SW846 8260

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

Peak Number 2 2-Methyladamantane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.879	8.74 ug/l	78840	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methyladamantane	150	C11H18	000700-56-1	76
2			Cyclohexene, 2-ethenyl-1,3,3-tri...	150	C11H18	005293-90-3	64
3			3,9-Epoxy-p-mentha-1,8(10)-diene	150	C10H14O	1000111-14-8	62
4			Cyclohexanone, 2-(2-butynyl)-	150	C10H14O	054166-48-2	53
5			Cyclooctene, 3-(1-methylethenyl)-	150	C11H18	061233-78-1	46



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Misc : 6.48G/5ML/MSVOA_Y/SOIL
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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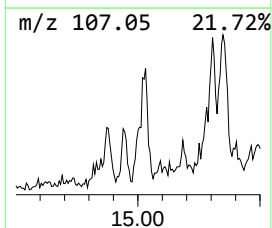
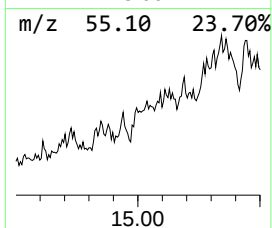
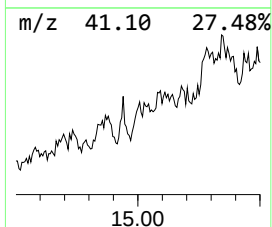
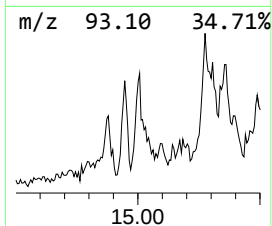
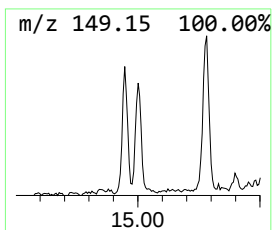
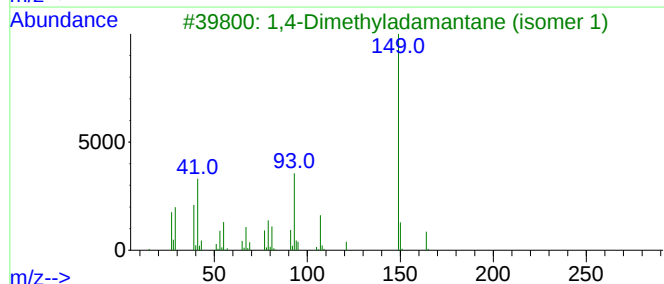
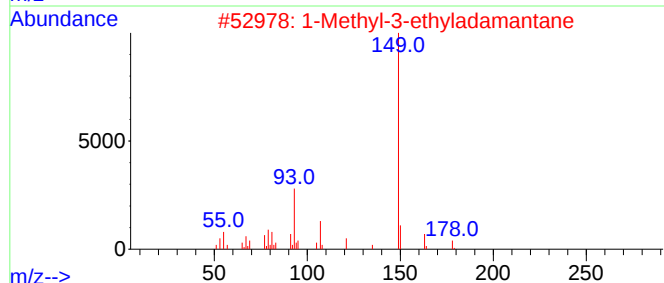
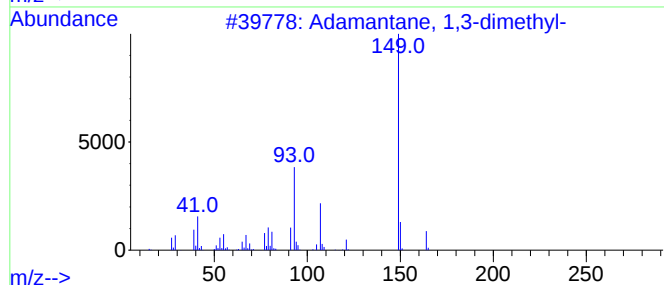
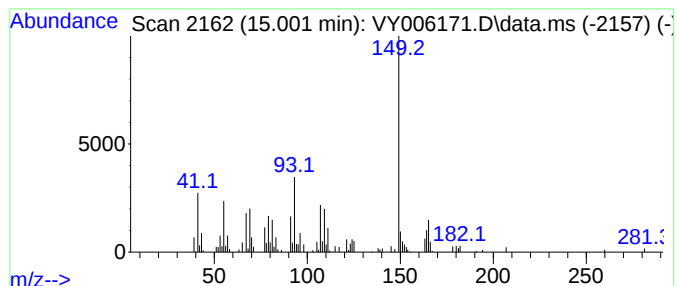
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y091421S.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.001	5.46 ug/l	49253	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	76
2			1-Methyl-3-ethyladamantane	178	C13H22	001687-34-9	70
3			1,4-Dimethyladamantane (isomer 1)	164	C12H20	1000460-67-0	70
4			Added stereo to name	164	C12H20	024145-89-9	70
5			Pyridinium, 1-(acetylamino)-2,6-...	164	C9H12N2O	031020-35-6	50



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Misc : 6.48G/5ML/MSVOA_Y/SOIL
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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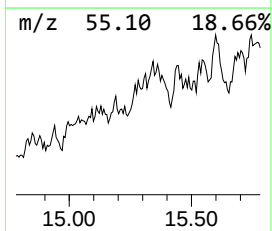
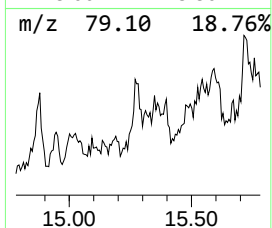
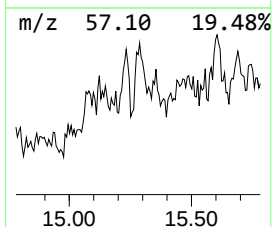
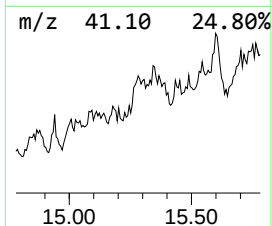
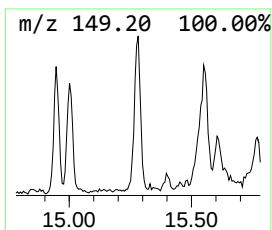
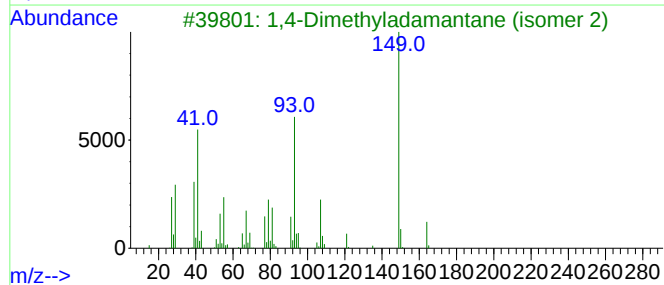
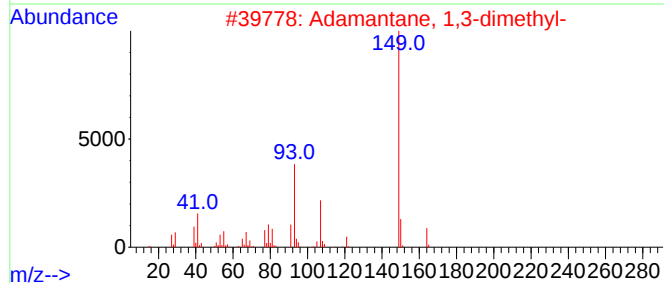
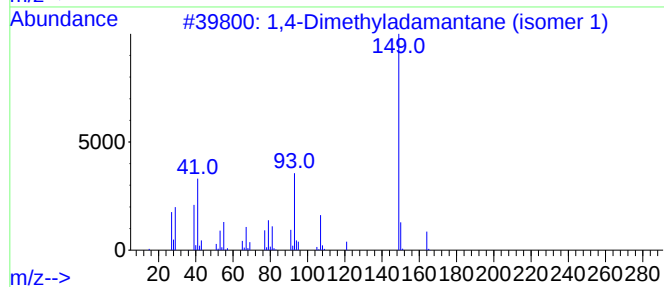
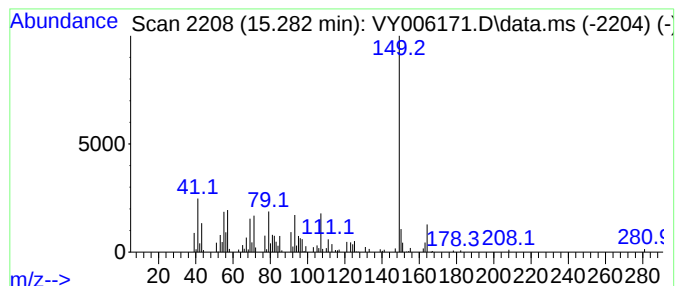
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 1,4-Dimethyladamantane (iso... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.282	5.22 ug/l	47038	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Dimethyladamantane (isomer 1)	164	C12H20	1000460-67-0	74
2			Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	72
3			1,4-Dimethyladamantane (isomer 2)	164	C12H20	1000460-67-1	72
4			2-(3-Methylbuta-1,3-dienyl)cyclo...	164	C11H16O	1000191-75-5	59
5			2'-Hydroxy-4',5'-dimethylacetoph...	164	C10H12O2	036436-65-4	59



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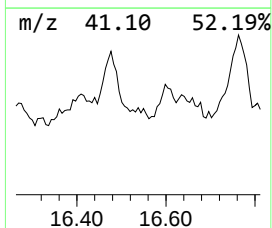
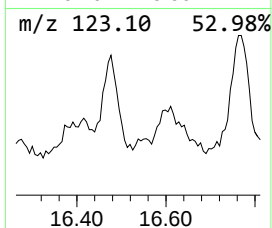
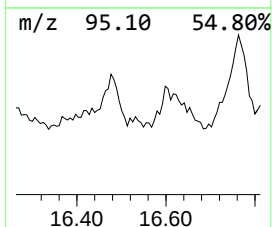
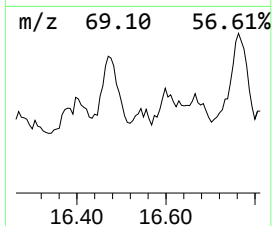
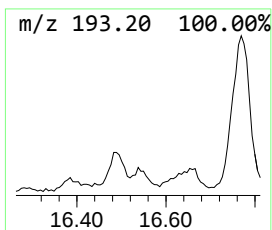
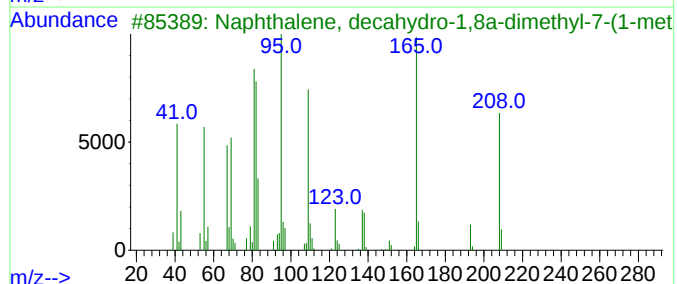
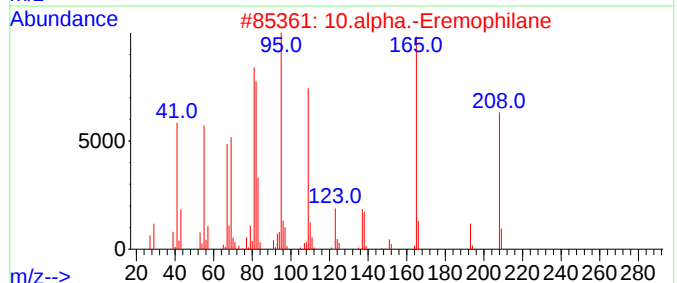
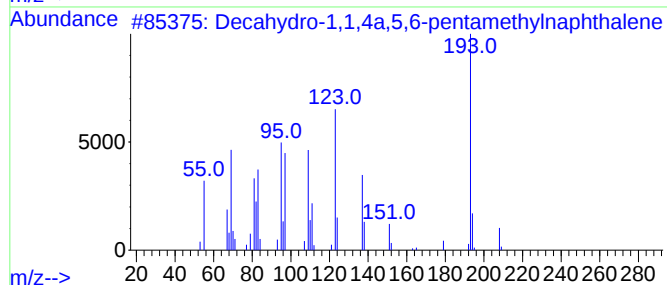
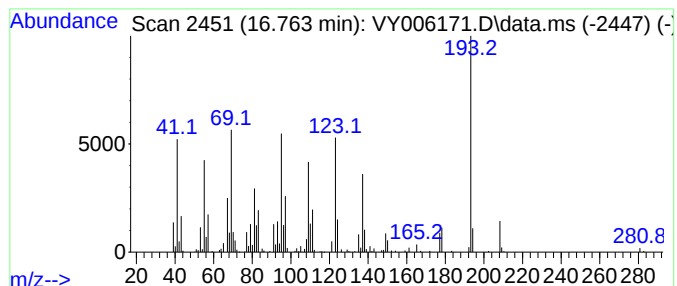
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y091421S.M
Quant Title : SW846 8260

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

Peak Number 5 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.763	17.17 ug/l	154780	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	87
2			10.alpha.-Eremophilane	208	C15H28	003242-05-5	38
3			Naphthalene, decahydro-1,8a-dime...	208	C15H28	015404-63-4	38
4			Benzhydrazide, N2-(bicyclo[2.2.1...	258	C15H15FN2O	1000274-01-8	35
5			Pyrazolo[5,1-c]-as-triazine-3-ca...	193	C6H7N7O	016111-78-7	35



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Adamantan-1-y...	14.282	5.9	ug/l	53289	4	13.428	450825	50.0
2-Methyladamantane	14.879	8.7	ug/l	78840	4	13.428	450825	50.0
Adamantane, 1,3...	15.001	5.5	ug/l	49253	4	13.428	450825	50.0
1,4-Dimethylada...	15.282	5.2	ug/l	47038	4	13.428	450825	50.0
Decahydro-1,1,4...	16.763	17.2	ug/l	154780	4	13.428	450825	50.0