

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY020422\
 Data File : VY007392.D
 Acq On : 04 Feb 2022 14:15
 Operator : SY/MD
 Sample : N1381-07
 Misc : 6.09g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 DB-07(13.5-15)-02-02-22

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\82Y020222S.M
 Title : SW846 8260

Signal : TIC: VY007392.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.948	340	349	359	rBV	6208	17370	1.02%	0.187%
2	7.716	958	967	973	rBV	93049	226432	13.24%	2.433%
3	7.789	973	979	988	rVB	154357	344681	20.15%	3.703%
4	8.142	1028	1037	1048	rBV	87822	196330	11.48%	2.109%
5	8.691	1118	1127	1136	rBV	244698	487257	28.49%	5.235%
6	9.929	1324	1330	1339	rBV8	6816	18823	1.10%	0.202%
7	10.179	1362	1371	1379	rBV	387278	682465	39.90%	7.333%
8	10.349	1393	1399	1404	rBV7	7417	21715	1.27%	0.233%
9	10.605	1433	1441	1449	rBV7	12349	35283	2.06%	0.379%
10	10.752	1461	1465	1469	rBV3	13284	22821	1.33%	0.245%
11	11.087	1516	1520	1525	rVB	31476	52201	3.05%	0.561%
12	11.300	1550	1555	1564	rVB8	16594	43851	2.56%	0.471%
13	11.489	1580	1586	1595	rVB	364569	589953	34.49%	6.339%
14	11.685	1613	1618	1621	rVV4	15984	30318	1.77%	0.326%
15	11.752	1622	1629	1638	rVB7	29498	93120	5.44%	1.001%
16	11.837	1638	1643	1647	rBV6	13626	24495	1.43%	0.263%
17	11.892	1647	1652	1657	rBV5	17711	28130	1.64%	0.302%
18	11.989	1663	1668	1669	rBV2	16457	25002	1.46%	0.269%
19	12.056	1676	1679	1682	rBV3	16923	27710	1.62%	0.298%
20	12.117	1687	1689	1695	rVB3	22569	35412	2.07%	0.380%
21	12.300	1714	1719	1723	rBV5	35265	72740	4.25%	0.782%
22	12.489	1743	1750	1757	rBV2	949672	1710572	100.00%	18.379%
23	12.642	1770	1775	1781	rVB2	68704	110995	6.49%	1.193%
24	12.812	1797	1803	1811	rBV8	55295	159728	9.34%	1.716%
25	12.940	1821	1824	1830	rVB3	53769	93600	5.47%	1.006%
26	13.062	1837	1844	1849	rVB8	39302	99502	5.82%	1.069%
27	13.129	1851	1855	1858	rBV5	24366	45952	2.69%	0.494%
28	13.166	1858	1861	1862	rBV3	17182	18422	1.08%	0.198%
29	13.422	1895	1903	1912	rVB	260006	530468	31.01%	5.700%
30	13.562	1923	1926	1930	rVB4	52653	78127	4.57%	0.839%
31	13.611	1930	1934	1937	rBV2	39630	63564	3.72%	0.683%
32	13.745	1951	1956	1968	rBV10	99618	264696	15.47%	2.844%
33	13.959	1987	1991	2003	rVB3	118672	252546	14.76%	2.713%
34	14.123	2014	2018	2027	rVB4	107503	244803	14.31%	2.630%
35	14.257	2035	2040	2041	rBV2	110029	158003	9.24%	1.698%
36	14.282	2041	2044	2054	rVB	160302	317088	18.54%	3.407%

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Start Thrs: 0.2

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Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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37	14.391	2058	2062	2065	rBV	105170	179408	10.49%	1.928%
38	14.465	2070	2074	2080	rVB4	86396	187410	10.96%	2.014%
39	14.727	2114	2117	2123	rVB4	100693	163243	9.54%	1.754%
40	14.873	2138	2141	2147	rVB2	151048	232525	13.59%	2.498%
41	14.940	2148	2152	2157	rVB	133057	211660	12.37%	2.274%
42	15.001	2157	2162	2164	rBV	114894	197358	11.54%	2.120%
43	15.275	2201	2207	2215	rBV4	157914	459647	26.87%	4.939%
44	15.446	2231	2235	2238	rBV4	37540	75958	4.44%	0.816%
45	16.470	2400	2403	2417	rVB5	92940	245802	14.37%	2.641%
46	16.598	2420	2424	2426	rBV4	24098	42223	2.47%	0.454%
47	16.757	2447	2450	2455	rVB4	47847	87759	5.13%	0.943%

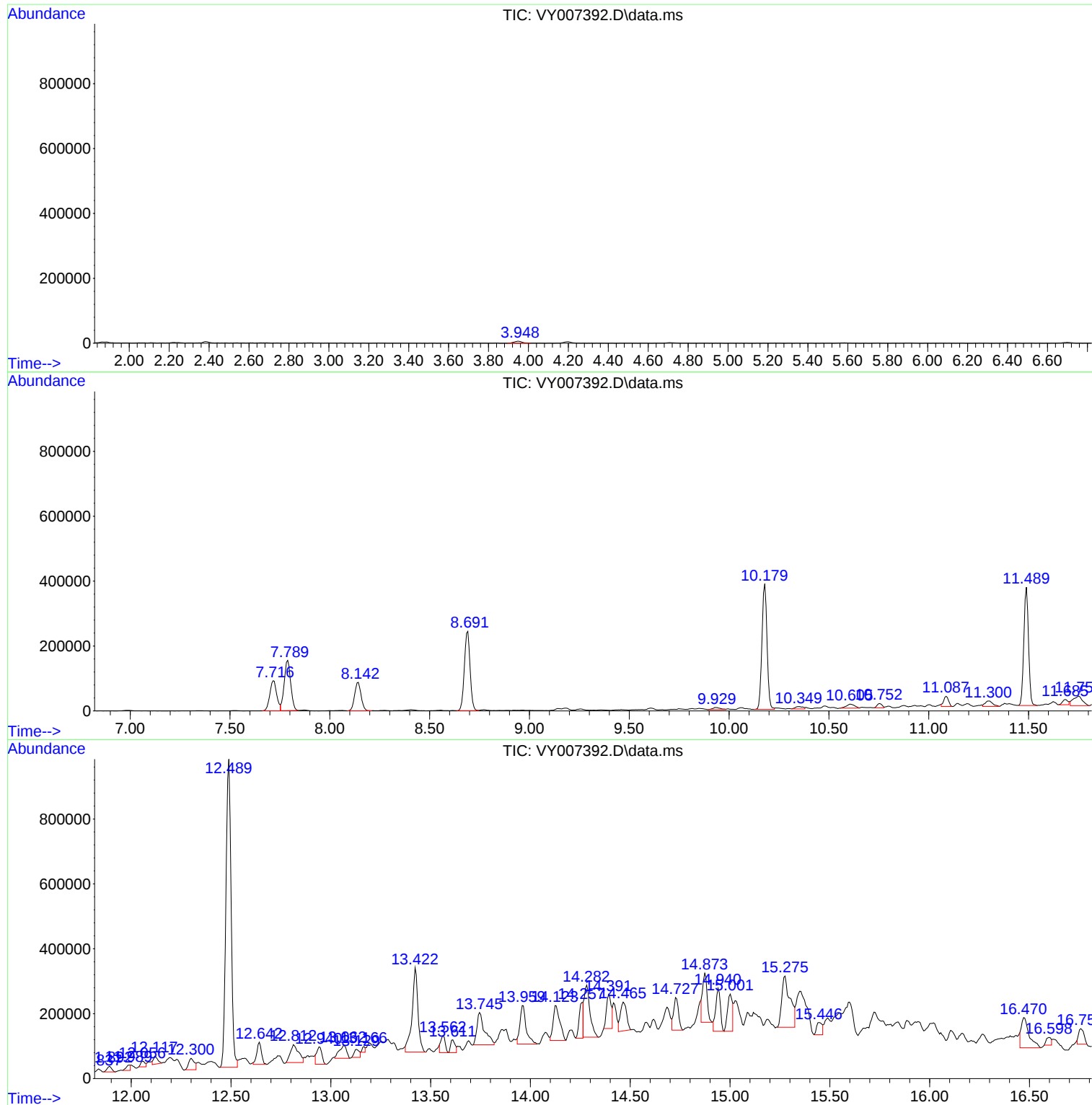
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Quant Title : SW846 8260

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



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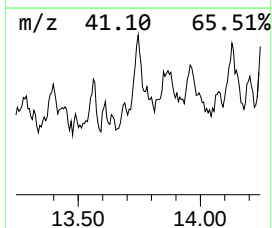
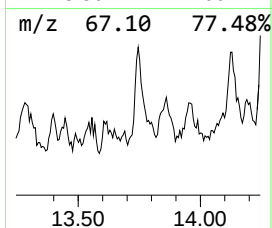
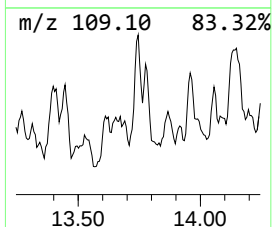
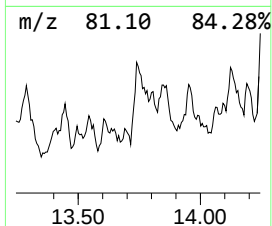
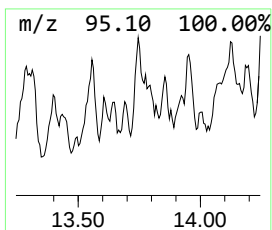
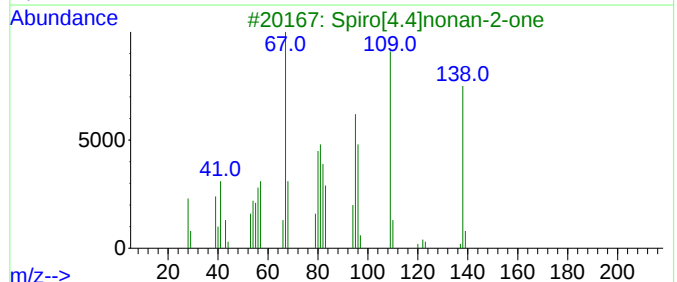
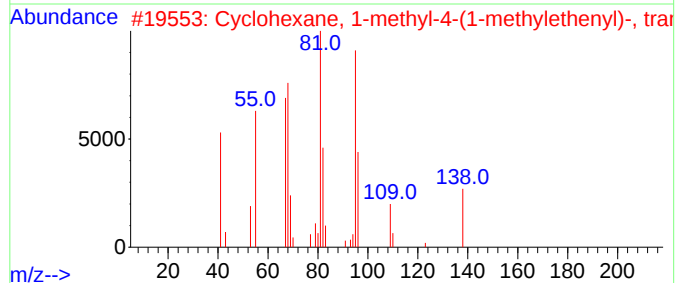
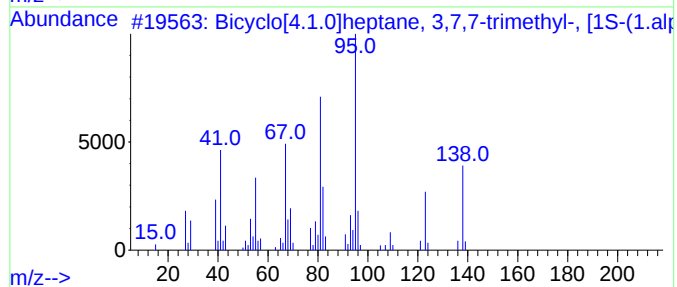
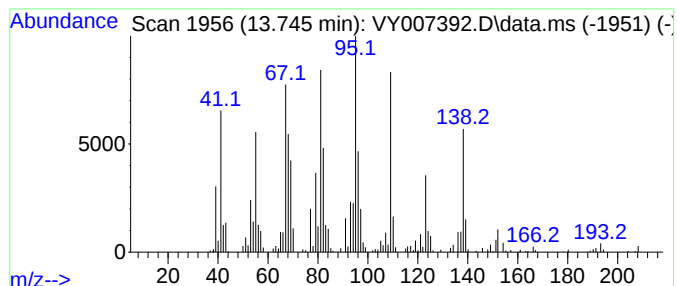
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y020222S.M
Quant Title : SW846 8260

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

Peak Number 1 Bicyclo[4.1.0]heptane, 3,7,... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.745	24.95 ug/l	264696	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	002778-68-9	70
2			Cyclohexane, 1-methyl-4-(1-methy...	138	C10H18	001124-25-0	64
3			Spiro[4.4]nonan-2-one	138	C9H14O	034177-18-9	64
4			Cyclooctene, 1,2-dimethyl-	138	C10H18	054299-96-6	62
5			Bicyclo[2.2.1]heptane, 1,7,7-tri...	138	C10H18	000464-15-3	60



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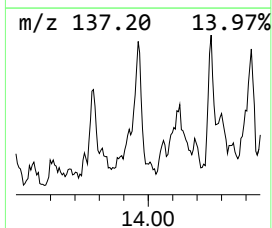
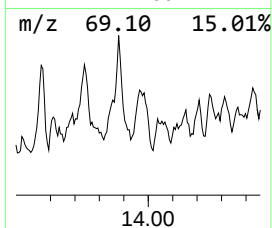
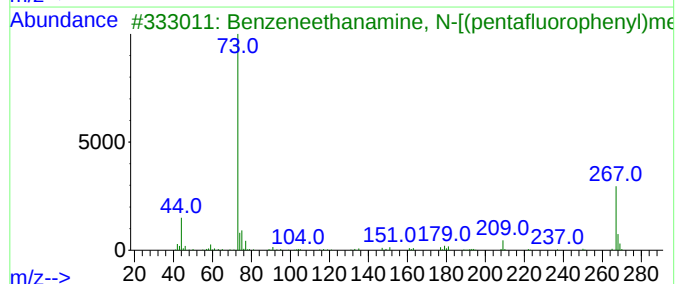
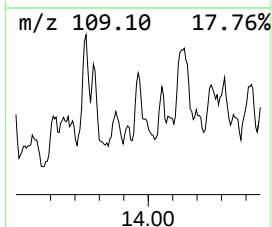
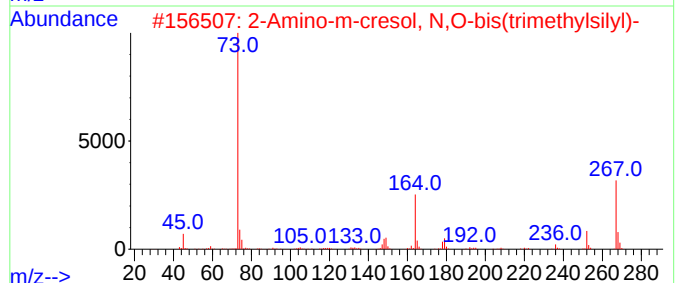
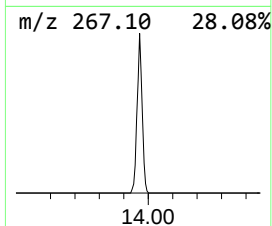
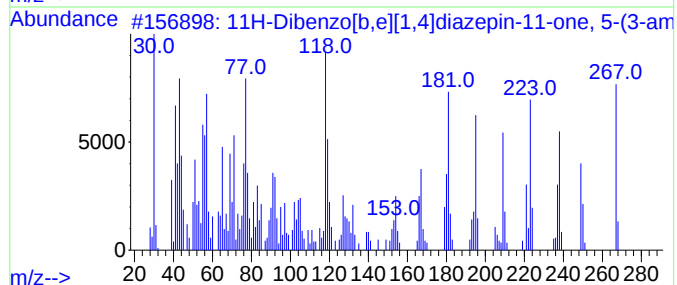
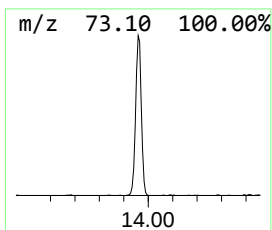
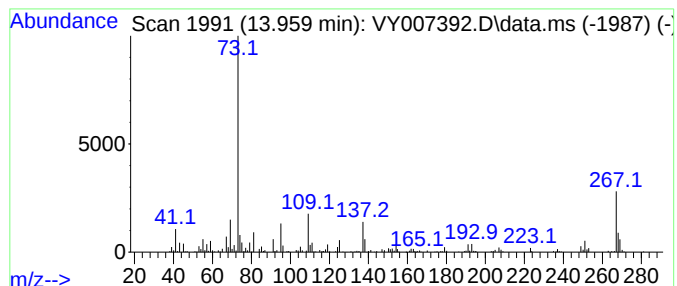
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y020222S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 11H-Dibenzo[b,e][1,4]diazep... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.959	23.80 ug/l	252546	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11H-Dibenzo[b,e][1,4]diazepin-11...	267	C16H17N3O	013450-73-2	53
2			2-Amino-m-cresol, N,O-bis(trimet...	267	C13H25NOSi2	1000449-77-1	43
3			Benzeneethanamine, N-[(pentaflu...	475	C21H26F5NO2Si2	055429-85-1	37
4			Acridone, TMS derivative	267	C16H17NOSi	1000478-16-0	32
5			Methoprene	310	C19H34O3	040596-69-8	28



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ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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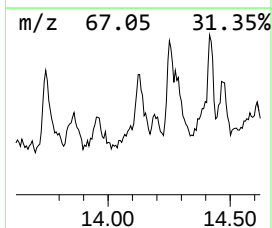
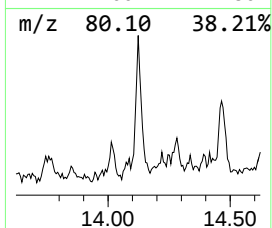
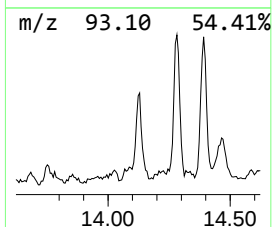
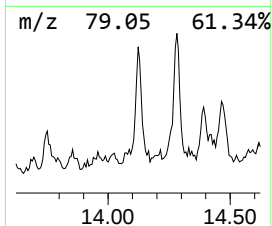
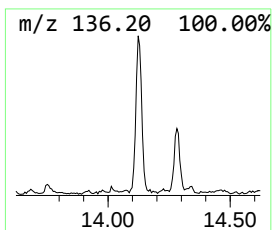
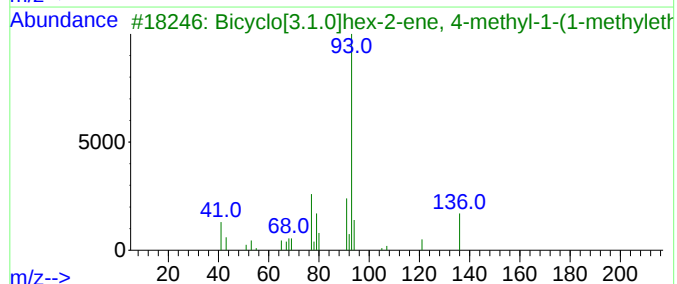
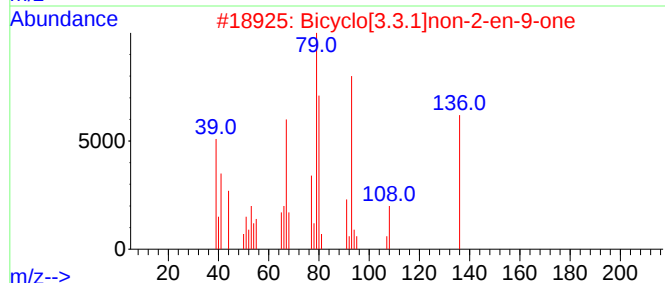
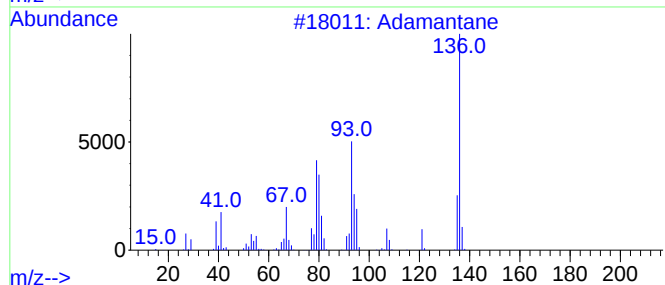
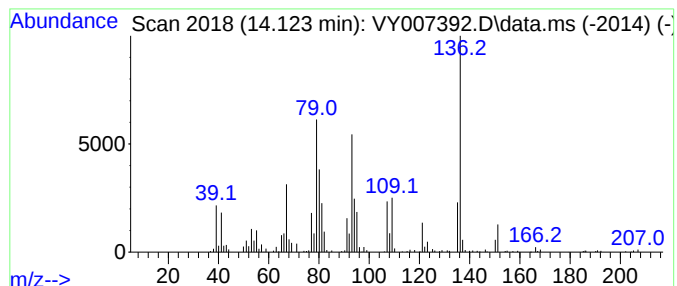
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y020222S.M
Quant Title : SW846 8260

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

Peak Number 3 Adamantane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.123	23.07 ug/l	244803	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Adamantane	136	C10H16	000281-23-2	91
2			Bicyclo[3.3.1]non-2-en-9-one	136	C9H12O	004844-11-5	70
3			Bicyclo[3.1.0]hex-2-ene, 4-methy...	136	C10H16	028634-89-1	43
4			Cyclooctene, 3-(1-methylethenyl)-	150	C11H18	061233-78-1	43
5			1-Methyl-6-methylenebicyclo[3.2....	122	C9H14	1000210-90-0	27



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ClientSampleId :
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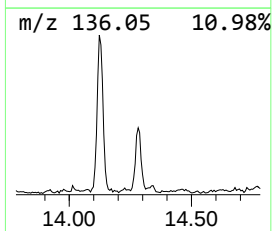
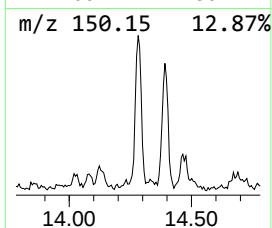
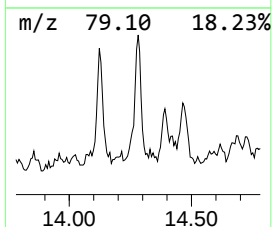
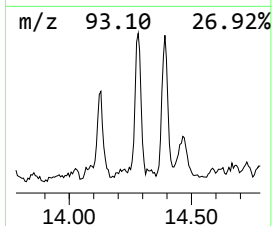
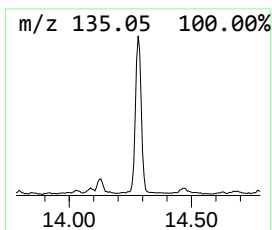
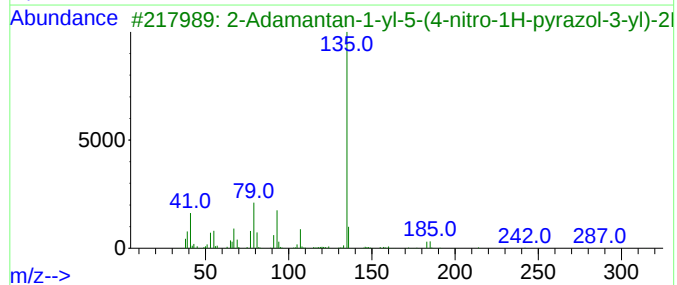
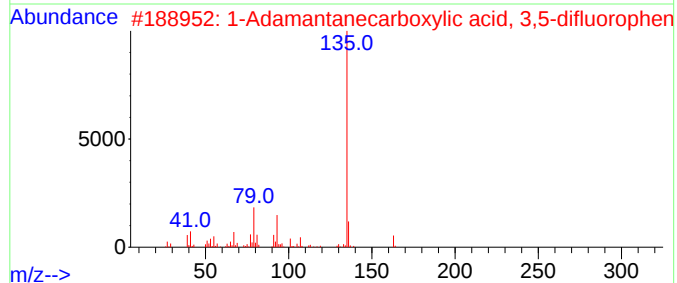
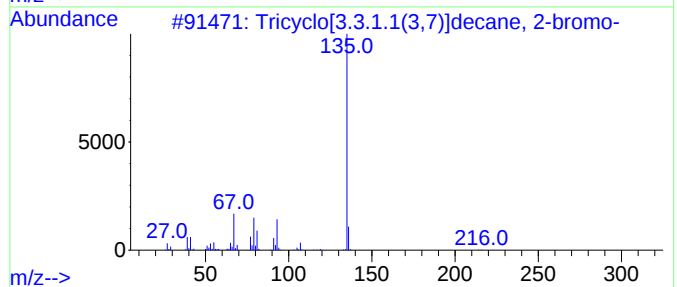
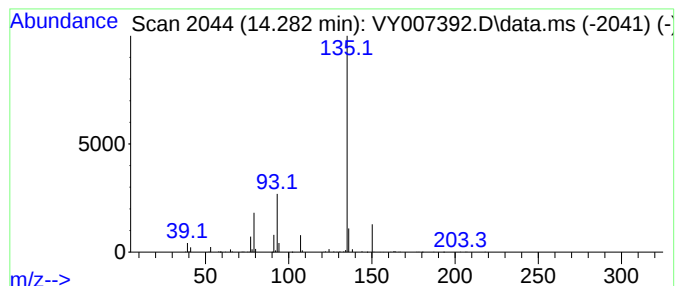
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Quant Title : SW846 8260

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

Peak Number 4 Tricyclo[3.3.1.1(3,7)]decan... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.282	29.89 ug/l	317088	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tricyclo[3.3.1.1(3,7)]decane, 2-...	214	C10H15Br	007314-85-4	72
2			1-Adamantanecarboxylic acid, 3,5...	292	C17H18F2O2	1000293-75-1	72
3			2-Adamantan-1-yl-5-(4-nitro-1H-p...	315	C14H17N7O2	1000301-14-4	72
4			1-(Adamantan-1-yl)-2-chloroethanone	212	C12H17ClO	023532-68-5	72
5			1-Adamantanemethanol	166	C11H18O	000770-71-8	72



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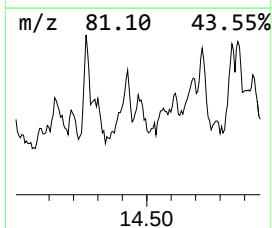
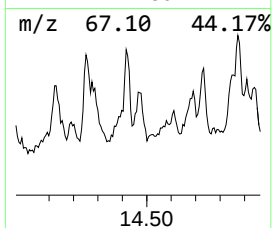
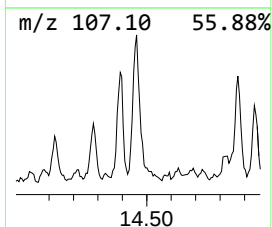
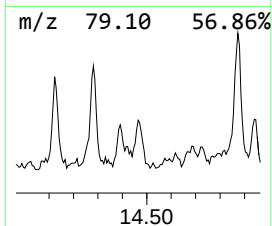
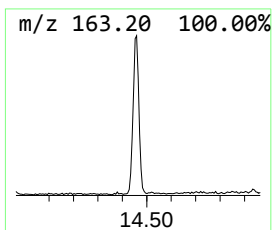
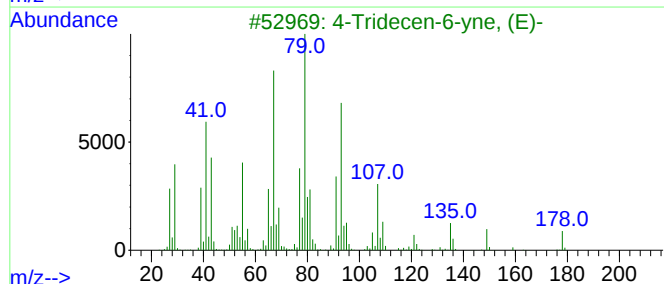
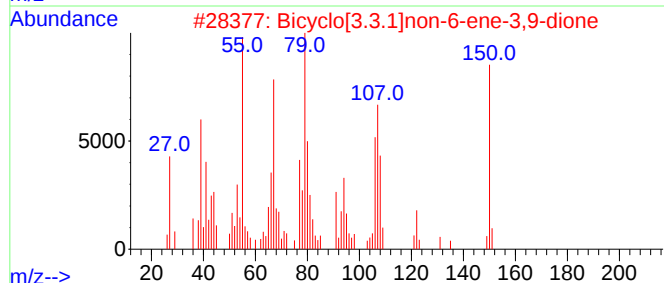
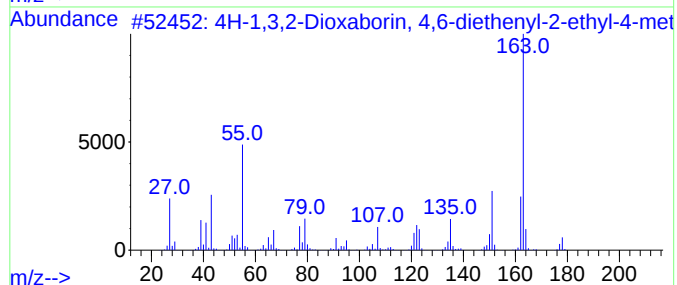
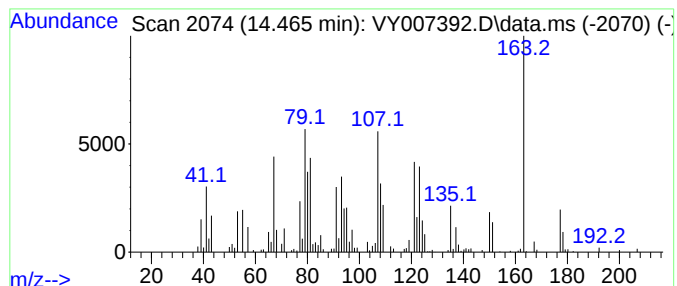
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Quant Title : SW846 8260

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

Peak Number 5 unknown14.464 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.464	17.66 ug/l	187410	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-1,3,2-Dioxaborin, 4,6-diethen...	178	C10H15B02	074630-03-8	38		
2	Bicyclo[3.3.1]non-6-ene-3,9-dione	150	C9H10O2	1000193-44-0	30		
3	4-Tridecen-6-yne, (E)-	178	C13H22	074744-43-7	25		
4	(11Z,14Z,17Z)-Methyl icoso-11,14...	320	C21H36O2	062472-96-2	22		
5	2-Methyl-2-bornene	150	C11H18	072540-93-3	14		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY020422\
Data File : VY007392.D
Acq On : 04 Feb 2022 14:15
Operator : SY/MD
Sample : N1381-07
Misc : 6.09g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
DB-07(13.5-15)-02-02-22

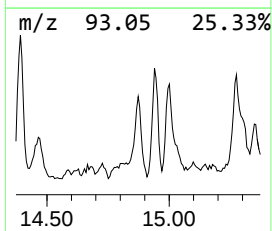
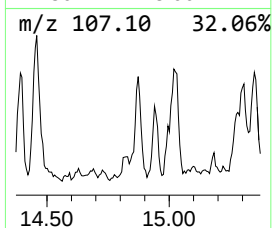
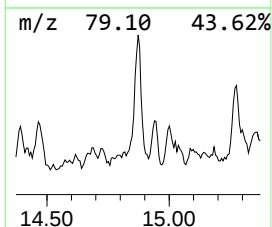
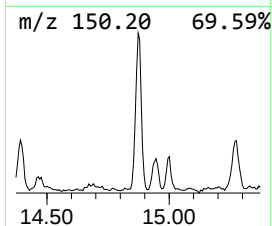
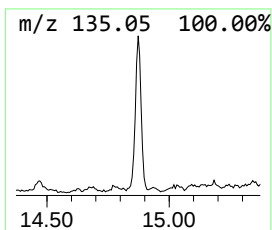
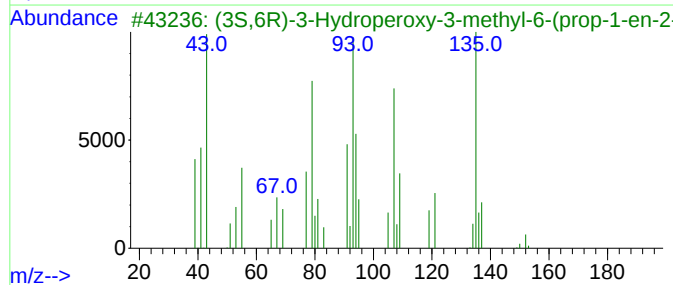
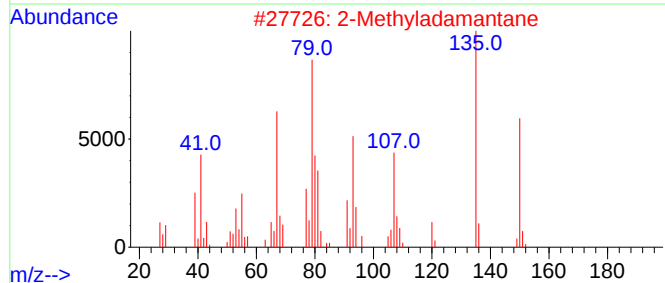
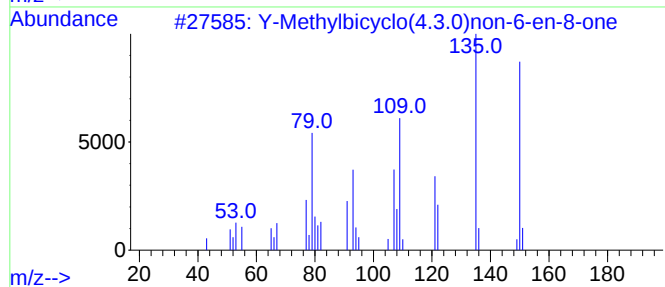
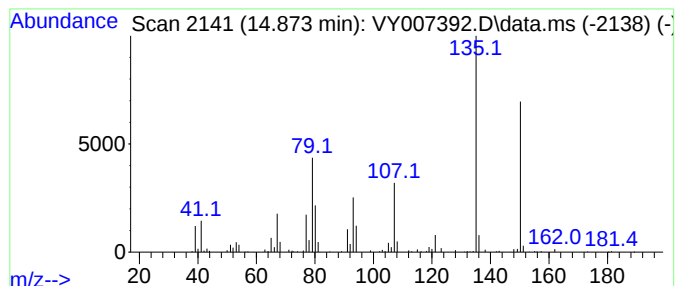
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Quant Title : SW846 8260

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

Peak Number 6 Y-Methylbicyclo(4.3.0)non-6... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.873	21.92 ug/l	232525	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Y-Methylbicyclo(4.3.0)non-6-en-8...	150	C10H14O	1000424-65-9	86
2			2-Methyladamantane	150	C11H18	000700-56-1	64
3			(3S,6R)-3-Hydroperoxy-3-methyl-6...	168	C10H16O2	077026-87-0	53
4			Cyclohexene, 2-ethenyl-1,3,3-tri...	150	C11H18	005293-90-3	53
5			4-Hydroxy-2-methylacetophenone	150	C9H10O2	000875-59-2	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY020422\
Data File : VY007392.D
Acq On : 04 Feb 2022 14:15
Operator : SY/MD
Sample : N1381-07
Misc : 6.09g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
DB-07(13.5-15)-02-02-22

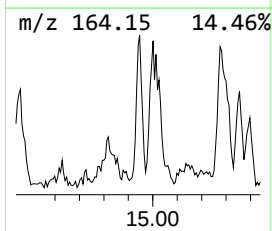
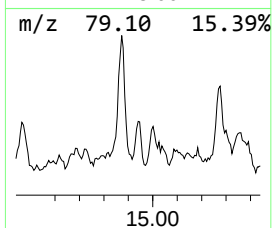
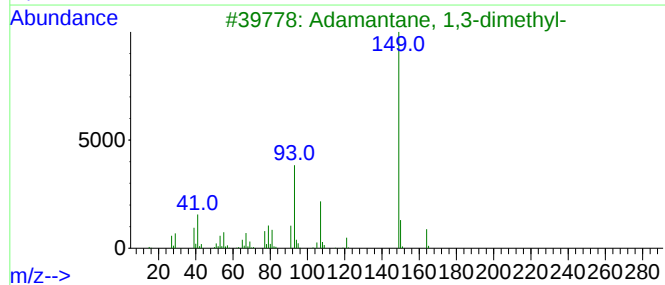
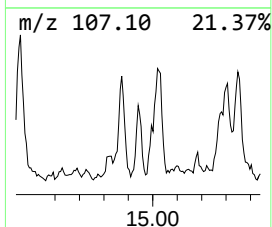
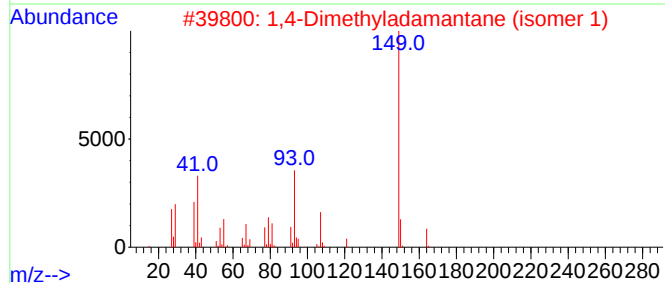
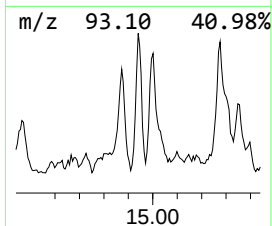
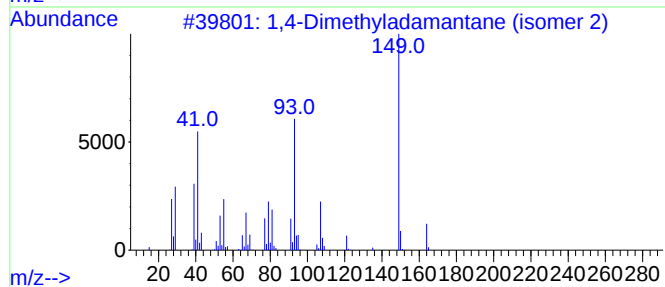
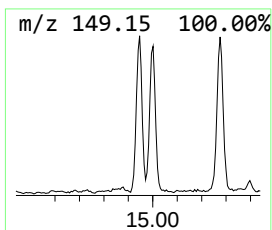
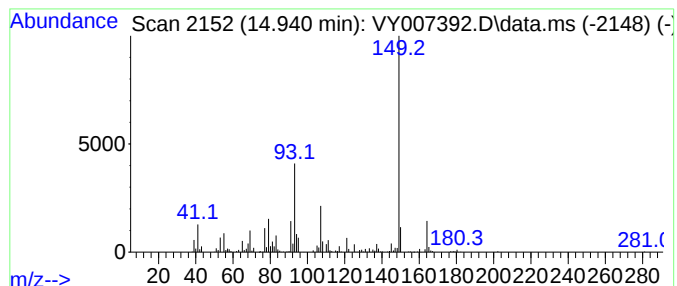
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Quant Title : SW846 8260

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

Peak Number 7 1,4-Dimethyladamantane (iso... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.940	19.95 ug/l	211660	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Dimethyladamantane (isomer 2)	164	C12H20	1000460-67-1	93
2			1,4-Dimethyladamantane (isomer 1)	164	C12H20	1000460-67-0	90
3			Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	86
4			Added stereo to name	164	C12H20	024145-88-8	74
5			Added stereo to name	164	C12H20	024145-89-9	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY020422\
Data File : VY007392.D
Acq On : 04 Feb 2022 14:15
Operator : SY/MD
Sample : N1381-07
Misc : 6.09g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
DB-07(13.5-15)-02-02-22

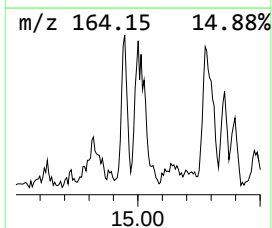
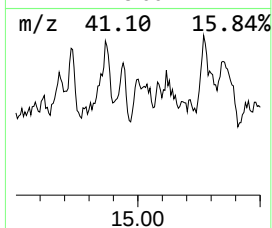
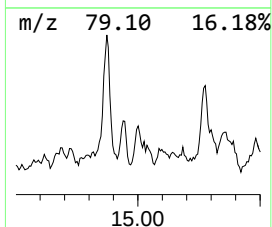
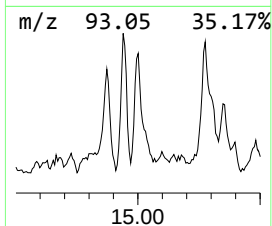
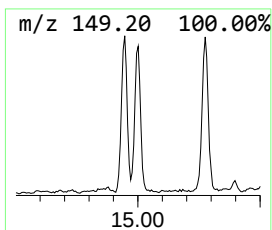
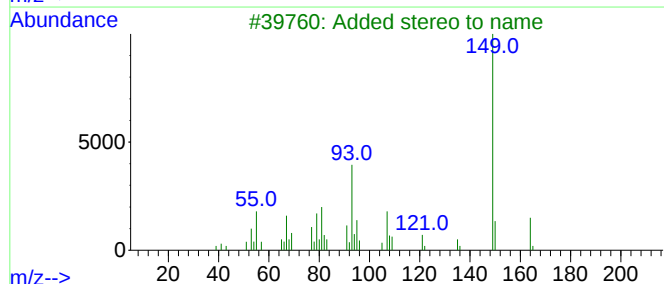
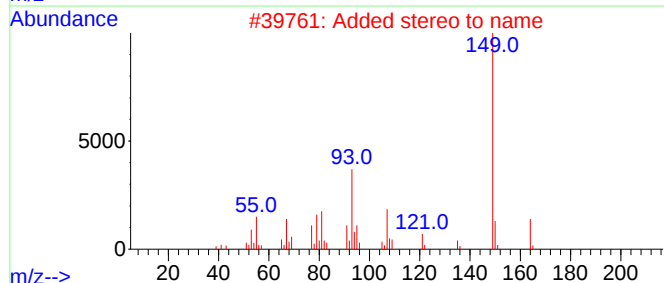
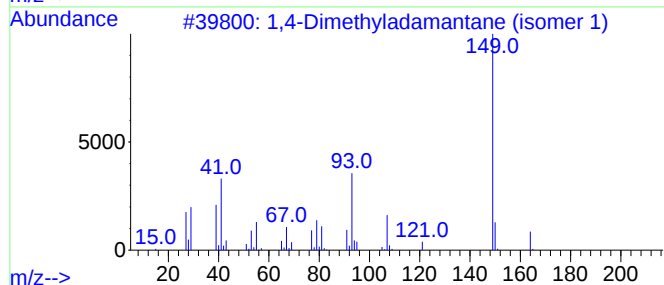
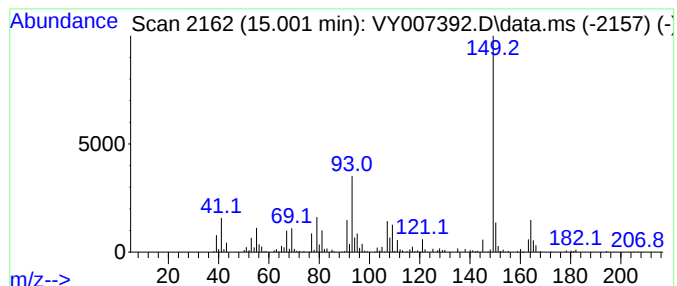
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y020222S.M
Quant Title : SW846 8260

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

Peak Number 8 1,4-Dimethyladamantane (iso... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.001	18.60 ug/l	197358	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	94
2			Added stereo to name	164	C12H20	024145-89-9	91
3			Added stereo to name	164	C12H20	024145-88-8	87
4			1,4-Dimethyladamantane (isomer 2)	164	C12H20	1000460-67-1	83
5			1-Methyl-3-ethyladamantane	178	C13H22	001687-34-9	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY020422\
Data File : VY007392.D
Acq On : 04 Feb 2022 14:15
Operator : SY/MD
Sample : N1381-07
Misc : 6.09g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
DB-07(13.5-15)-02-02-22

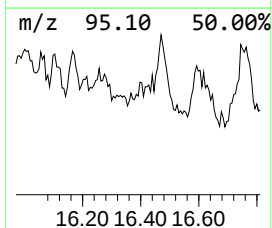
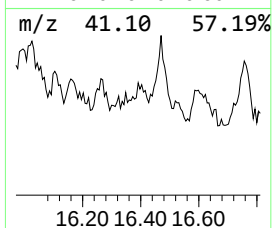
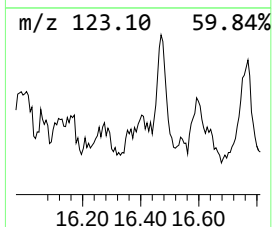
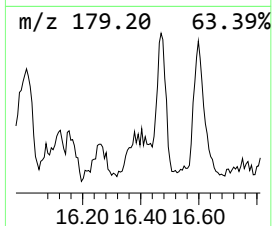
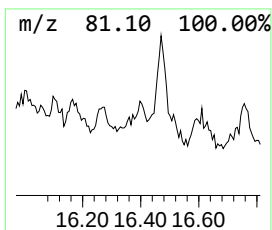
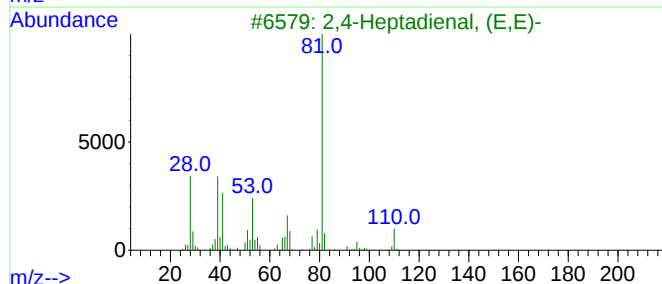
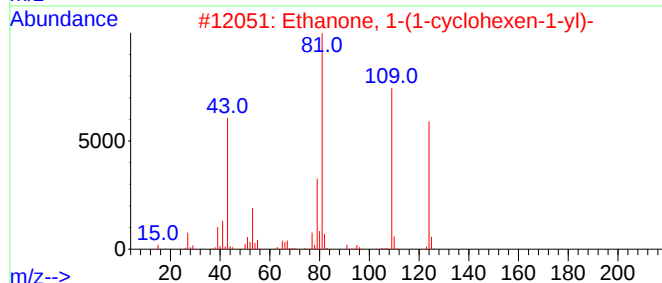
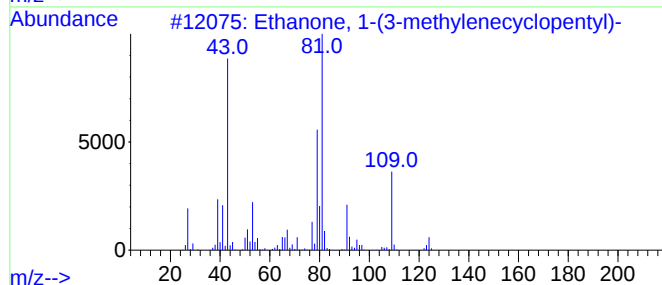
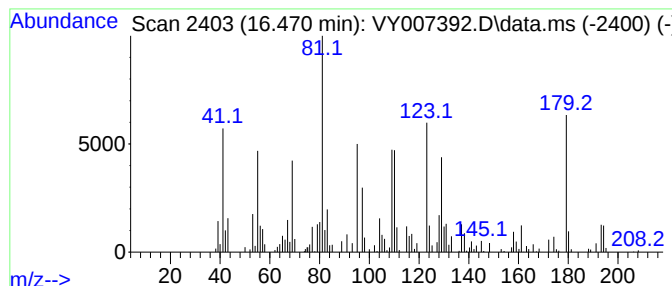
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Quant Title : SW846 8260

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

Peak Number 10 unknown16.470 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.470	23.17 ug/l	245802	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanone, 1-(3-methylenecyclopentyl)-	124	C8H12O	054829-98-0	22
2			Ethanone, 1-(1-cyclohexen-1-yl)-	124	C8H12O	000932-66-1	22
3			2,4-Heptadienal, (E,E)-	110	C7H10O	004313-03-5	22
4			1H-Pyrrole, 1-butyl-	123	C8H13N	000589-33-3	22
5			Cyclopropane, 1,1-dibromo-2-hexyl-	282	C9H16Br2	041848-90-2	22



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY020422\
Data File : VY007392.D
Acq On : 04 Feb 2022 14:15
Operator : SY/MD
Sample : N1381-07
Misc : 6.09g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
DB-07(13.5-15)-02-02-22

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y020222S.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
Bicyclo[4.1.0]h...	13.745	24.9	ug/l	264696	4	13.422	530468	50.0
11H-Dibenzo[b,e...	13.959	23.8	ug/l	252546	4	13.422	530468	50.0
Adamantane	14.123	23.1	ug/l	244803	4	13.422	530468	50.0
Tricyclo[3.3.1....	14.282	29.9	ug/l	317088	4	13.422	530468	50.0
unknown14.464	14.464	17.7	ug/l	187410	4	13.422	530468	50.0
Y-Methylbicyclo...	14.873	21.9	ug/l	232525	4	13.422	530468	50.0
1,4-Dimethylada...	14.940	19.9	ug/l	211660	4	13.422	530468	50.0
1,4-Dimethylada...	15.001	18.6	ug/l	197358	4	13.422	530468	50.0
unknown16.470	16.470	23.2	ug/l	245802	4	13.422	530468	50.0