

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY061323\
 Data File : VY014142.D
 Acq On : 13 Jun 2023 16:16
 Operator : KP/MD
 Sample : 03154-01
 Misc : 5.08g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 CHRT-24051

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\82Y060923S.M
 Title : SW846 8260

Signal : TIC: VY014142.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.217	59	65	72	rBV3	7935	14756	2.18%	0.164%
2	4.710	461	474	489	rBV	21712	66311	9.78%	0.736%
3	5.740	634	643	651	rBV5	4607	14196	2.09%	0.158%
4	6.966	833	844	859	rBV	16025	53545	7.90%	0.594%
5	7.527	927	936	945	rBV5	2473	7070	1.04%	0.078%
6	7.710	954	966	972	rBV	109826	265068	39.10%	2.942%
7	7.783	972	978	995	rVB	172364	397369	58.61%	4.411%
8	8.136	1022	1036	1047	rBV	108908	252529	37.25%	2.803%
9	8.685	1117	1126	1141	rBV	276690	538763	79.46%	5.980%
10	10.173	1363	1370	1377	rBV	391261	677994	100.00%	7.526%
11	10.240	1377	1381	1388	rVB	55367	92943	13.71%	1.032%
12	10.368	1395	1402	1408	rBV2	9713	15933	2.35%	0.177%
13	10.575	1428	1436	1443	rBV	23259	40897	6.03%	0.454%
14	10.941	1490	1496	1502	rBV	25967	41551	6.13%	0.461%
15	11.313	1554	1557	1564	rVB3	5728	10250	1.51%	0.114%
16	11.483	1575	1585	1593	rBV	380354	624314	92.08%	6.930%
17	11.703	1615	1621	1631	rVB6	12699	28380	4.19%	0.315%
18	12.026	1671	1674	1682	rVB4	6317	11756	1.73%	0.130%
19	12.227	1705	1707	1713	rVB6	4862	8643	1.27%	0.096%
20	12.300	1713	1719	1720	rBV6	6678	11140	1.64%	0.124%
21	12.331	1720	1724	1730	rVB	28627	45191	6.67%	0.502%
22	12.477	1742	1748	1757	rBV2	307333	507748	74.89%	5.636%
23	12.575	1762	1764	1768	rVB3	7098	7599	1.12%	0.084%
24	12.642	1770	1775	1783	rVB9	10666	25923	3.82%	0.288%
25	12.751	1783	1793	1797	rBV7	21204	67475	9.95%	0.749%
26	12.800	1797	1801	1809	rVB2	83289	130173	19.20%	1.445%
27	12.947	1821	1825	1828	rBV4	5336	8392	1.24%	0.093%
28	13.038	1832	1840	1841	rBV8	7033	13535	2.00%	0.150%
29	13.068	1842	1845	1848	rVB5	11439	14272	2.11%	0.158%
30	13.123	1849	1854	1858	rBV6	22281	41157	6.07%	0.457%
31	13.184	1858	1864	1869	rVB2	37569	77882	11.49%	0.864%
32	13.245	1871	1874	1877	rBV5	10252	16730	2.47%	0.186%
33	13.312	1883	1885	1888	rVV2	8574	7531	1.11%	0.084%
34	13.367	1890	1894	1897	rVV	38213	52972	7.81%	0.588%
35	13.422	1898	1903	1911	rVB	279315	452725	66.77%	5.025%
36	13.489	1911	1914	1918	rBV5	12696	17279	2.55%	0.192%

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Sampling : 1

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Max Peaks: 100

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Peak Location: TOP

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

Peak separation: 5

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37	13.611	1930	1934	1937	rBV4	20580	35324	5.21%	0.392%
38	13.745	1950	1956	1960	rBV2	128358	234675	34.61%	2.605%
39	13.965	1987	1992	2005	rVB9	76308	196329	28.96%	2.179%
40	14.074	2005	2010	2013	rBV5	39191	70650	10.42%	0.784%
41	14.123	2014	2018	2025	rBV3	69779	156065	23.02%	1.732%
42	14.282	2035	2044	2054	rBV4	194757	546031	80.54%	6.061%
43	14.391	2057	2062	2064	rVV	134563	218269	32.19%	2.423%
44	14.422	2065	2067	2070	rVV3	114730	144037	21.24%	1.599%
45	14.465	2070	2074	2081	rVB7	89002	198576	29.29%	2.204%
46	14.580	2088	2093	2096	rBV	300968	398184	58.73%	4.420%
47	14.678	2103	2109	2114	rBV6	83686	218148	32.18%	2.421%
48	14.727	2114	2117	2123	rVB5	104182	169247	24.96%	1.879%
49	14.873	2134	2141	2146	rVB3	165859	323825	47.76%	3.594%
50	14.940	2148	2152	2156	rVB	149961	216185	31.89%	2.400%
51	15.001	2157	2162	2165	rBV	131881	245741	36.25%	2.728%
52	15.269	2202	2206	2215	rBV5	135843	366090	54.00%	4.064%
53	15.440	2230	2234	2237	rBV5	52439	89002	13.13%	0.988%
54	16.476	2399	2404	2419	rVB6	198211	522712	77.10%	5.802%

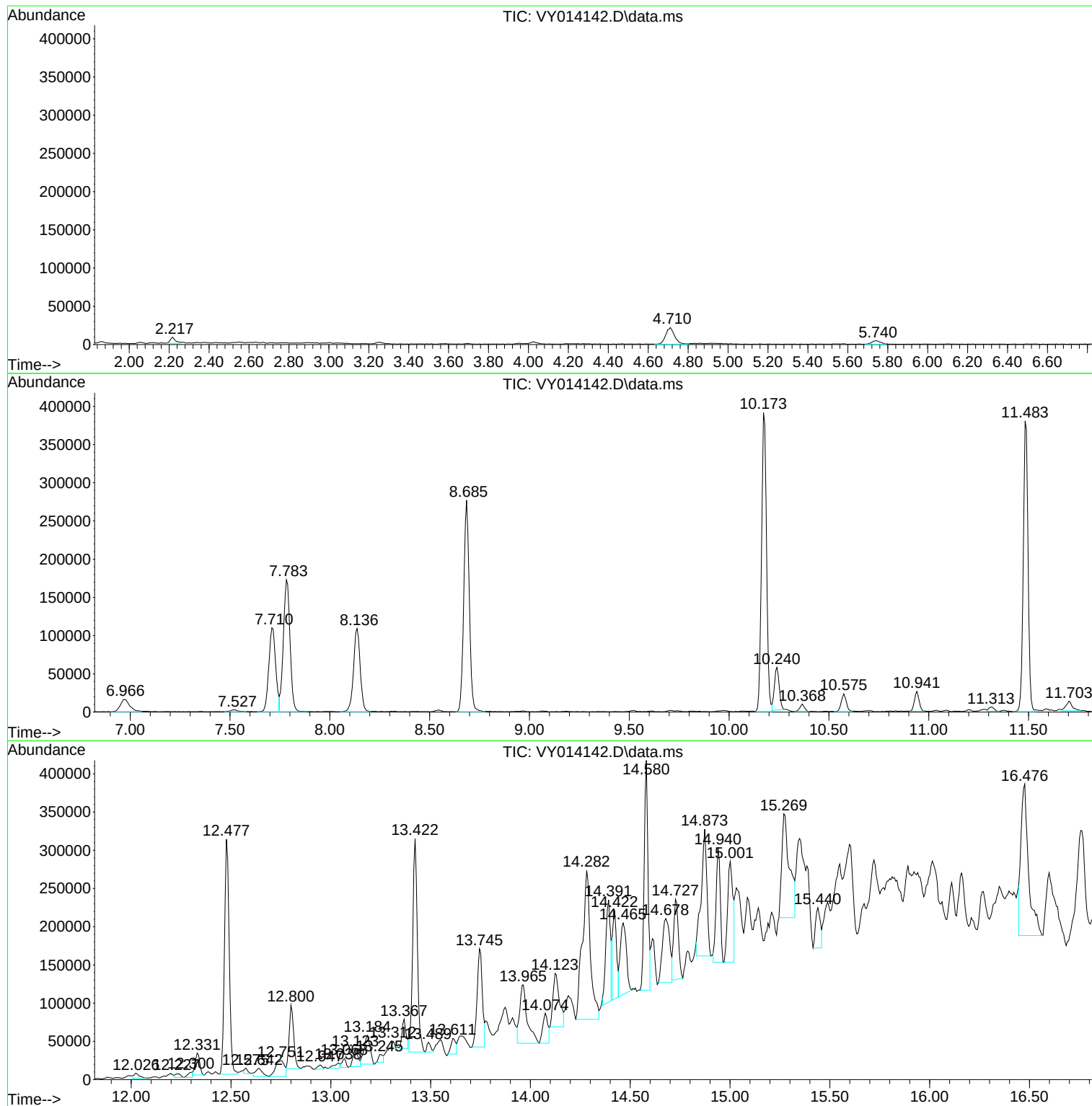
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060923S.M
Quant Title : SW846 8260

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



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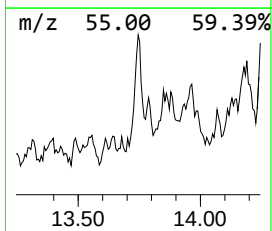
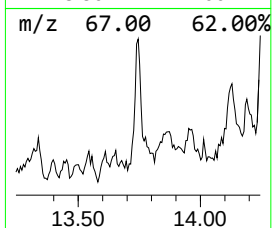
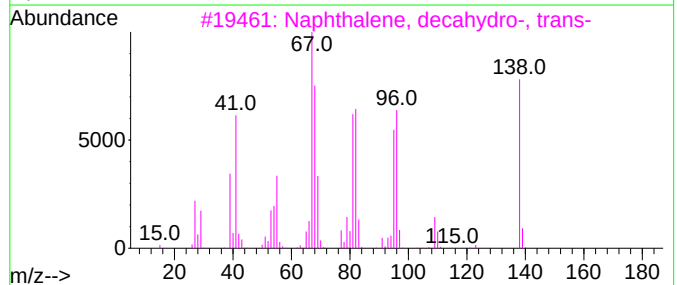
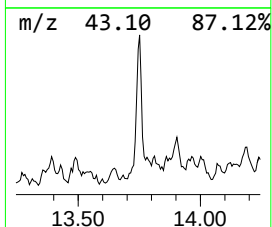
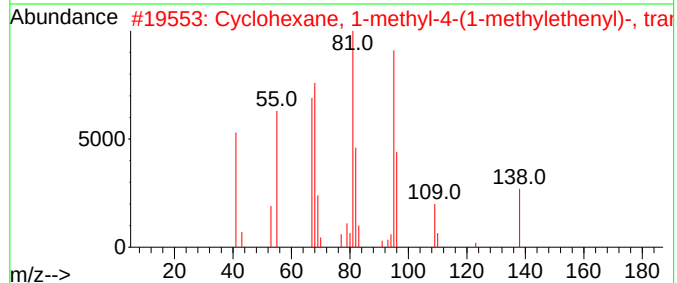
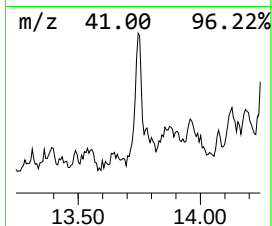
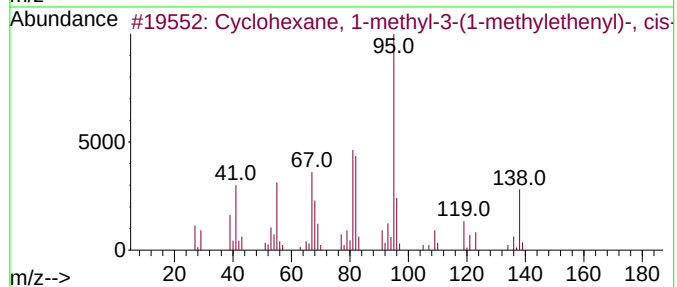
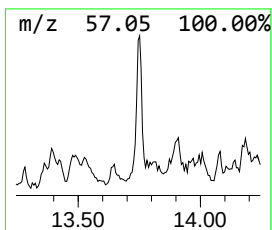
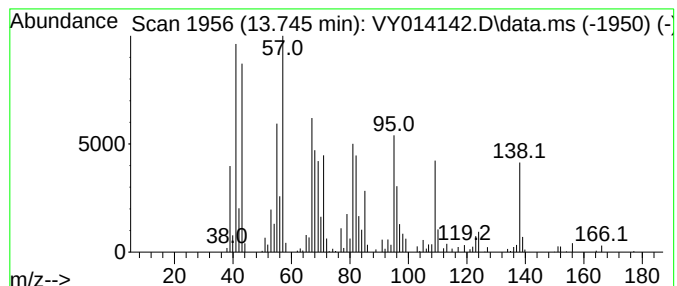
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060923S.M
Quant Title : SW846 8260

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

Peak Number 1 Cyclohexane, 1-methyl-3-(1-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.745	25.92 ug/l	234675	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1-methyl-3-(1-methy...	138	C10H18	024399-15-3	83
2			Cyclohexane, 1-methyl-4-(1-methy...	138	C10H18	001124-25-0	64
3			Naphthalene, decahydro-, trans-	138	C10H18	000493-02-7	60
4			Naphthalene, decahydro-	138	C10H18	000091-17-8	55
5			Cyclooctene, 3-methyl-	124	C9H16	013152-05-1	50



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Instrument :
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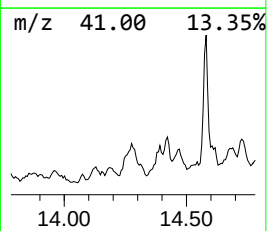
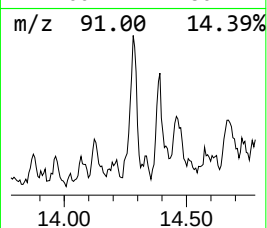
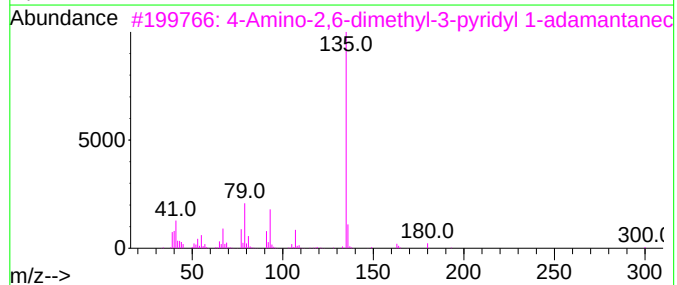
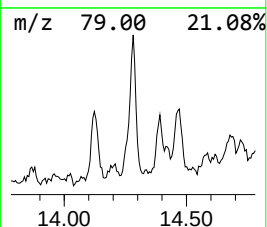
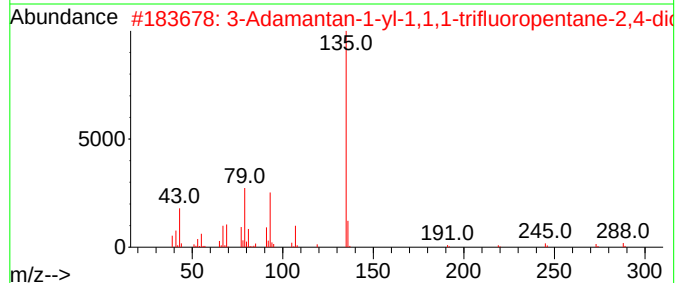
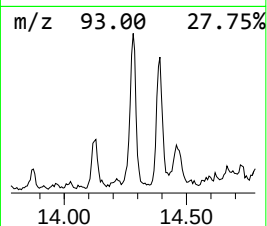
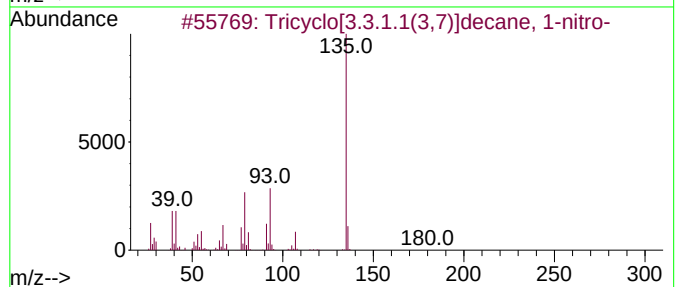
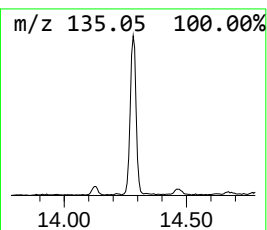
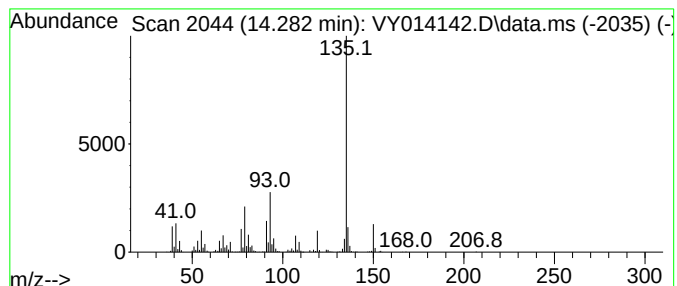
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060923S.M
Quant Title : SW846 8260

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

Peak Number 2 Tricyclo[3.3.1.1(3,7)]decan... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.282	60.30 ug/l	546031	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tricyclo[3.3.1.1(3,7)]decane, 1-...	181	C10H15NO2	007575-82-8	72
2			3-Adamantan-1-yl-1,1,1-trifluoro...	288	C15H19F3O2	1000311-44-8	72
3			4-Amino-2,6-dimethyl-3-pyridyl 1...	300	C18H24N2O2	1000260-99-2	64
4			N-(3-Hydroxy-2,6-dimethyl-4-pyri...	300	C18H24N2O2	1000260-99-3	64
5			1-Adamantyl bromomethyl ketone	256	C12H17BrO	005122-82-7	59



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Instrument :
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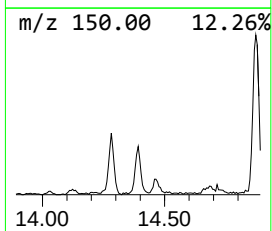
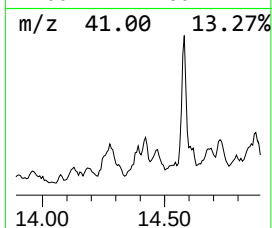
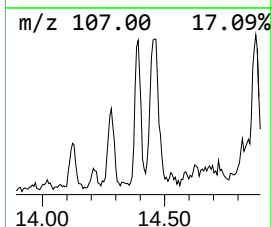
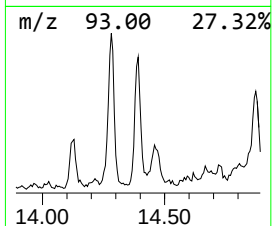
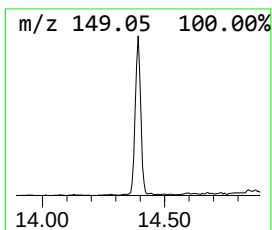
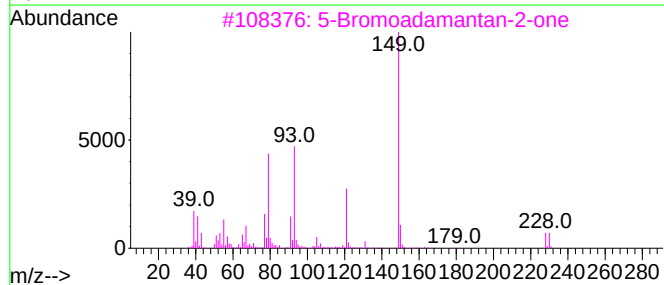
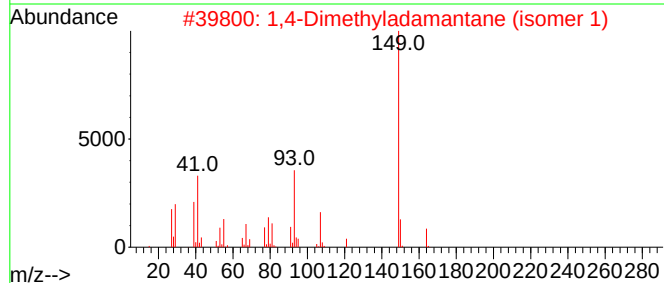
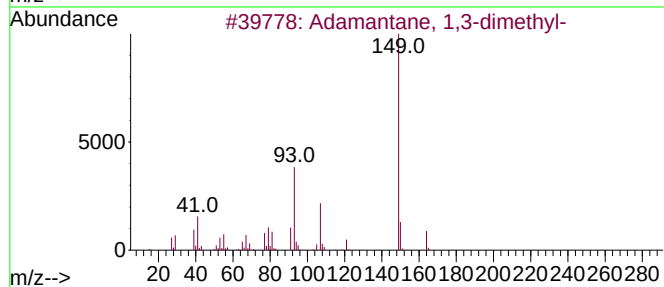
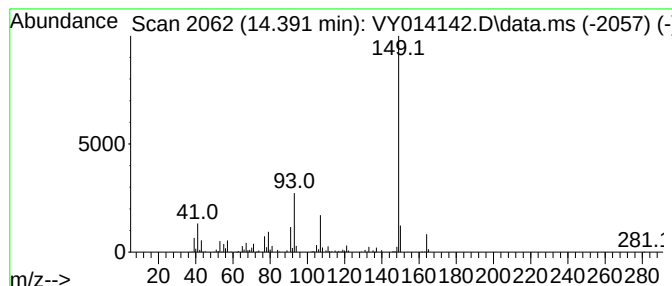
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060923S.M
Quant Title : SW846 8260

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

Peak Number 3 Adamantane, 1,3-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.391	24.11 ug/l	218269	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	91
2			1,4-Dimethyladamantane (isomer 1)	164	C12H20	1000460-67-0	91
3			5-Bromoadamantan-2-one	228	C10H13BrO	020098-20-8	72
4			Tricyclo[4.3.1.1(3,8)]undecane-1...	208	C13H20O2	031083-60-0	72
5			Benzaldehyde, 4-methoxy-3-(2,6-d...	270	C17H18O3	1000273-78-6	50



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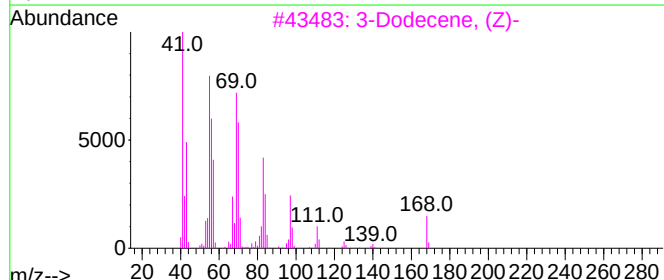
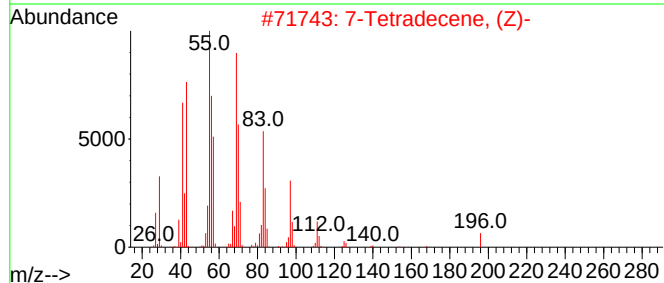
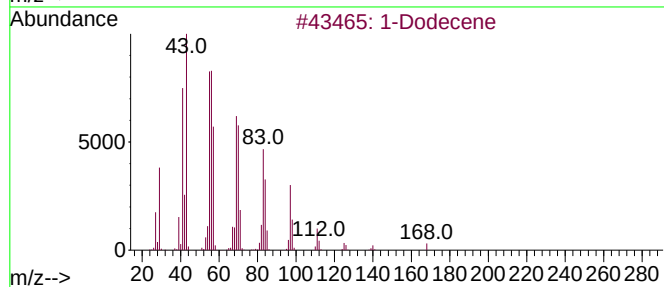
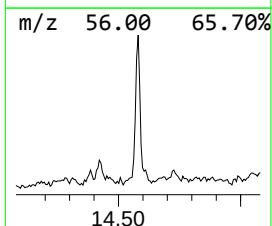
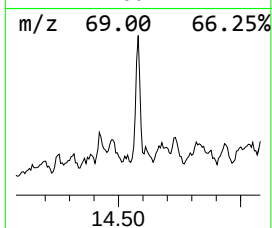
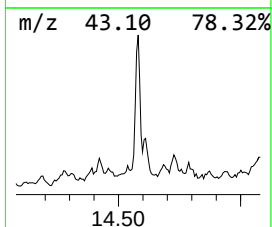
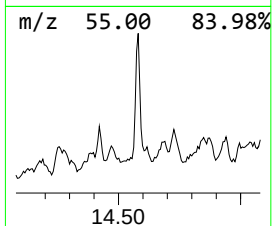
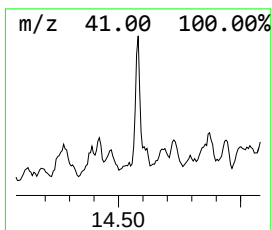
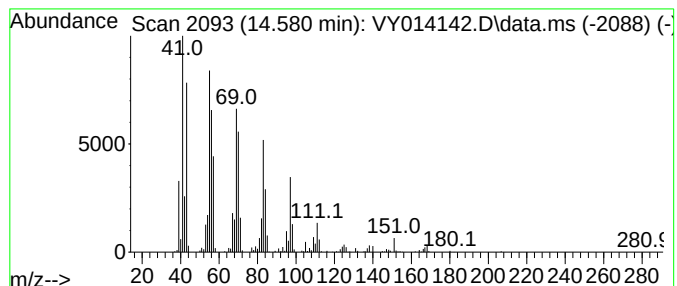
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060923S.M
Quant Title : SW846 8260

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

Peak Number 4 1-Dodecene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.580	43.98 ug/l	398184	1,4-Dichlorobenzene-d4	13.422

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Dodecene	168	C12H24	000112-41-4	97
2		7-Tetradecene, (Z)-	196	C14H28	041446-60-0	91
3		3-Dodecene, (Z)-	168	C12H24	007239-23-8	91
4		Cyclopropane, nonyl-	168	C12H24	074663-85-7	91
5		Cyclododecane	168	C12H24	000294-62-2	87



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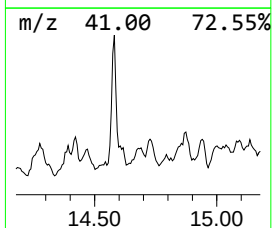
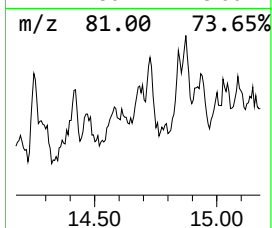
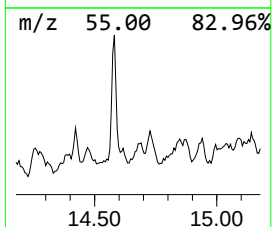
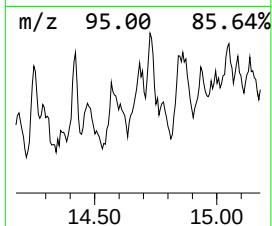
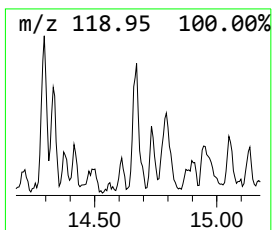
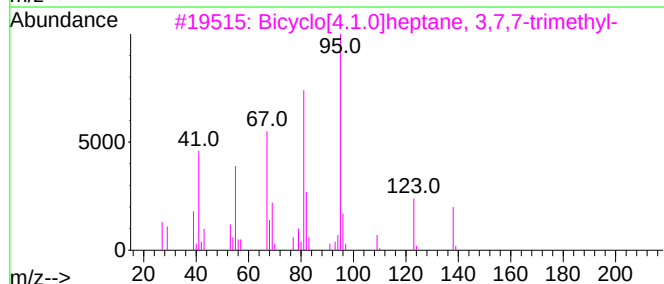
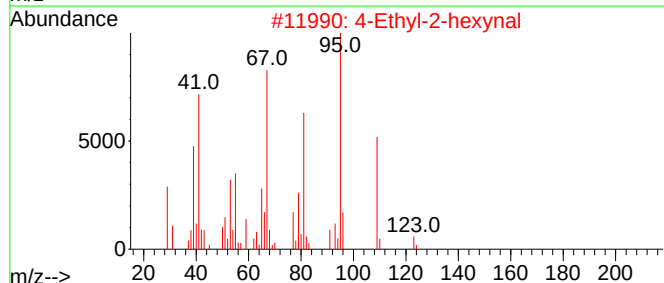
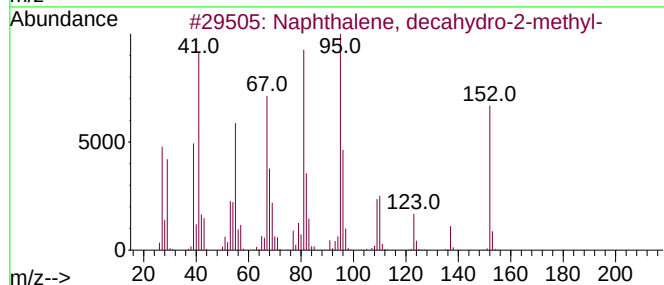
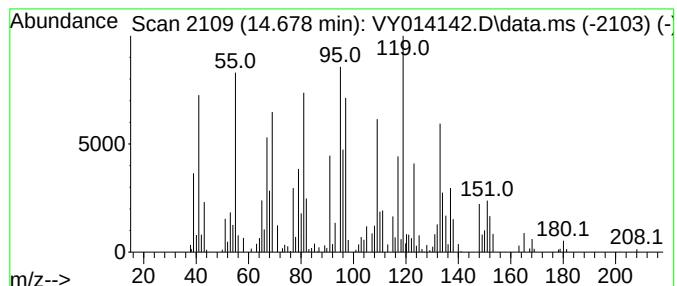
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Quant Title : SW846 8260

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

Peak Number 5 unknown14.678 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.678	24.09 ug/l	218148	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	38
2			4-Ethyl-2-hexynal	124	C8H12O	071932-97-3	25
3			Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	000554-59-6	25
4			2,6-Dimethylbicyclo[3.2.1]octane	138	C10H18	1000215-28-2	25
5			Cyclohexane, 1-methyl-4-(1-methy...	138	C10H18	001124-27-2	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY061323\
Data File : VY014142.D
Acq On : 13 Jun 2023 16:16
Operator : KP/MD
Sample : 03154-01
Misc : 5.08g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
CHRT-24051

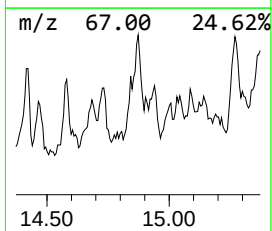
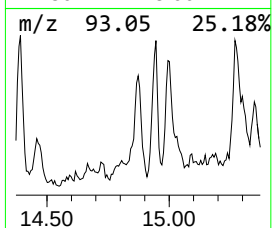
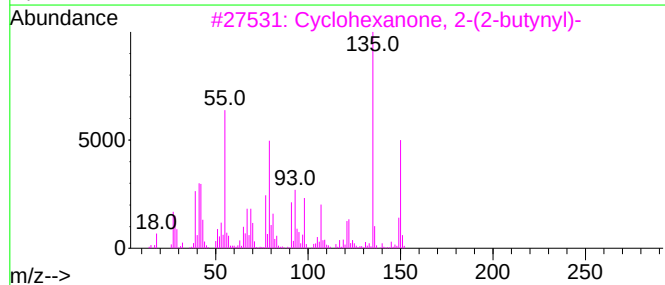
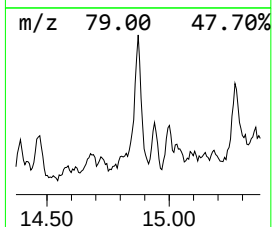
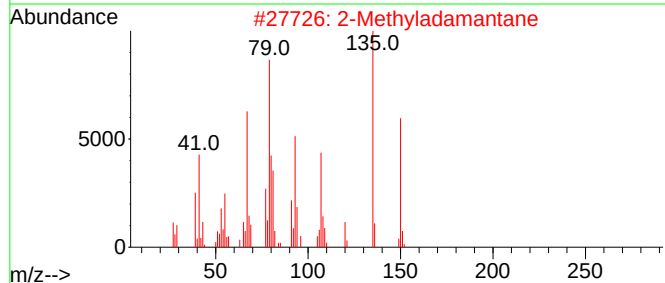
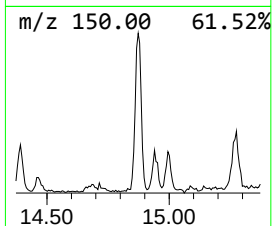
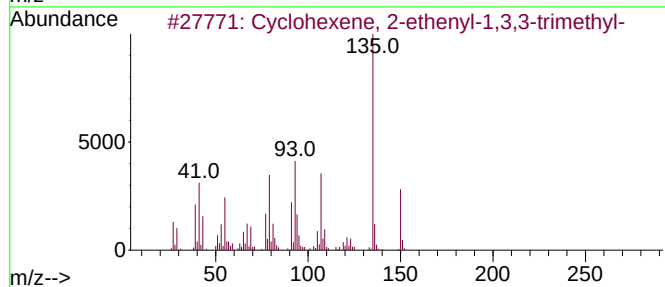
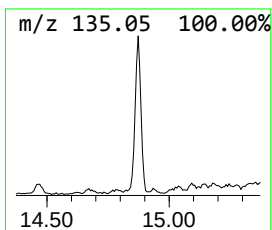
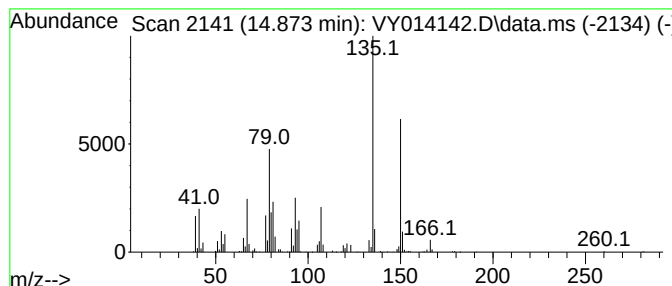
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Quant Title : SW846 8260

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

Peak Number 6 Cyclohexene, 2-ethenyl-1,3,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.873	35.76 ug/l	323825	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexene, 2-ethenyl-1,3,3-tri...	150	C11H18	005293-90-3	93
2			2-Methyladamantane	150	C11H18	000700-56-1	91
3			Cyclohexanone, 2-(2-butyryl)-	150	C10H14O	054166-48-2	87
4			3,9-Epoxy-p-mentha-1,8(10)-diene	150	C10H14O	1000111-14-8	81
5			p-Cymen-7-ol	150	C10H14O	000536-60-7	70



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY061323\
Data File : VY014142.D
Acq On : 13 Jun 2023 16:16
Operator : KP/MD
Sample : 03154-01
Misc : 5.08g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
CHRT-24051

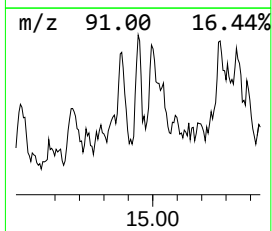
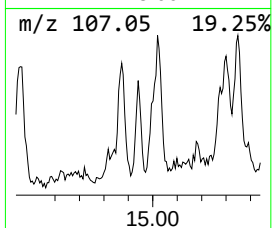
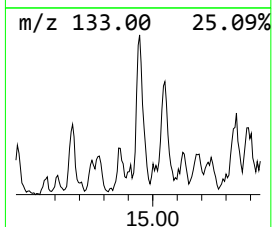
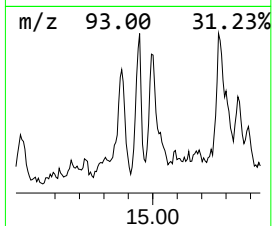
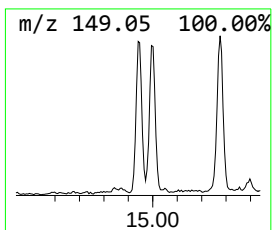
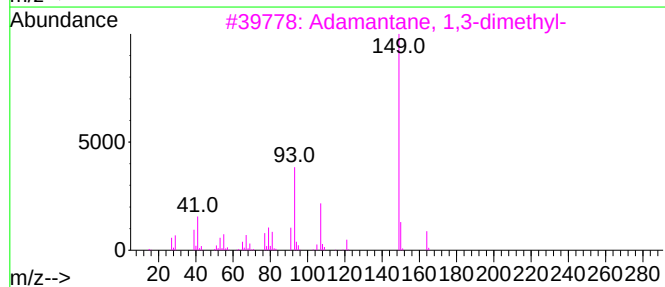
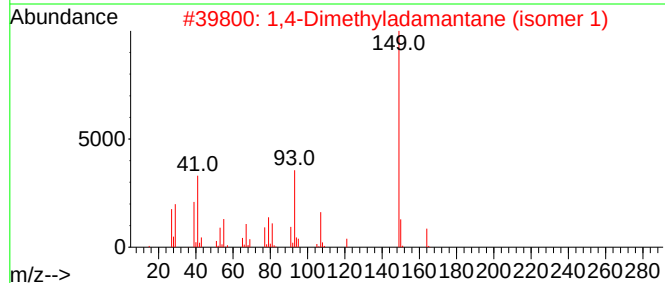
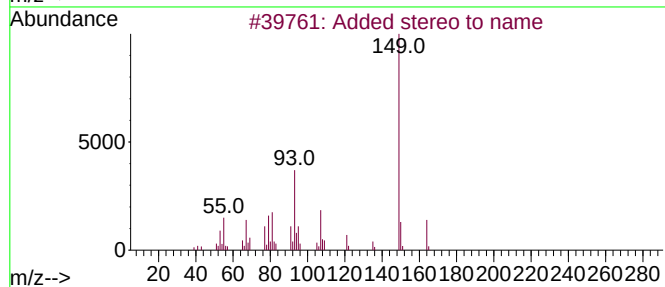
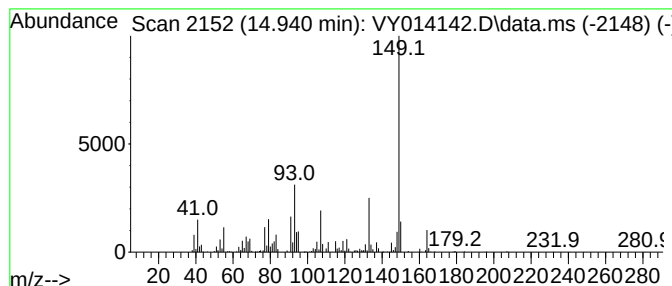
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Quant Title : SW846 8260

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

Peak Number 7 1,4-Dimethyladamantane (iso... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.940	23.88 ug/l	216185	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Added stereo to name			164	C12H20	024145-89-9	81
2	1,4-Dimethyladamantane (isomer 1)			164	C12H20	1000460-67-0	76
3	Adamantane, 1,3-dimethyl-			164	C12H20	000702-79-4	76
4	1,4-Dimethyladamantane (isomer 2)			164	C12H20	1000460-67-1	53
5	3-Methyl-1-adamantanecarboxylic ...			194	C12H18O2	1000504-38-9	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY061323\
Data File : VY014142.D
Acq On : 13 Jun 2023 16:16
Operator : KP/MD
Sample : 03154-01
Misc : 5.08g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
CHRT-24051

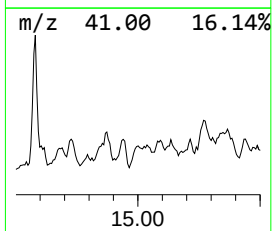
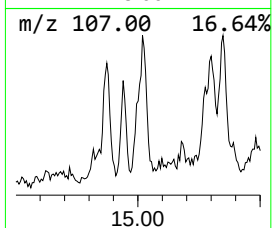
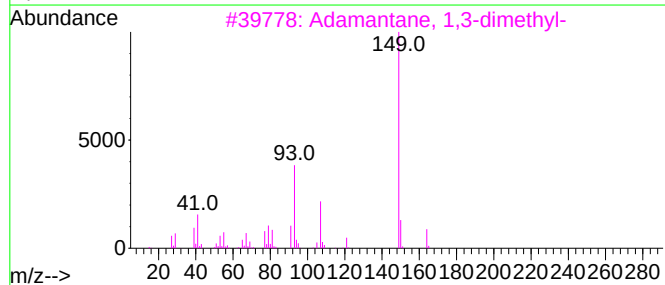
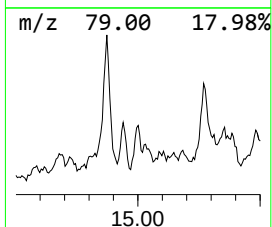
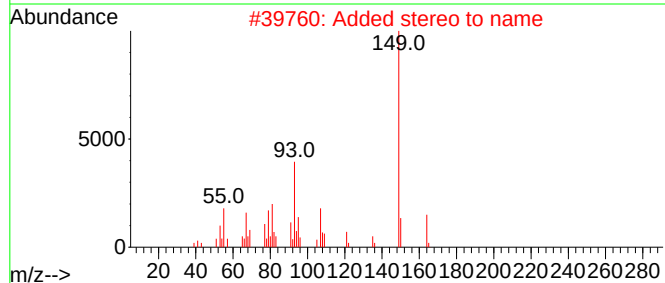
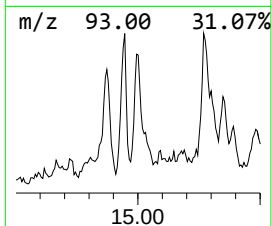
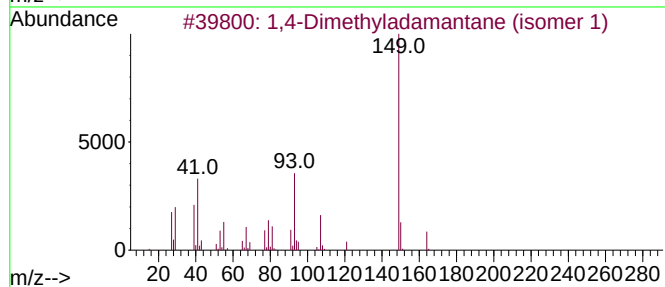
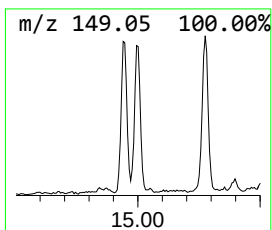
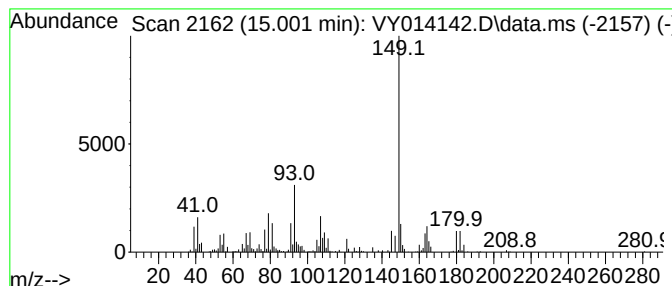
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Quant Title : SW846 8260

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

Peak Number 8 Methyl (1s,3s,5R,7S)-3-meth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.001	27.14 ug/l	245741	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	93
2			Added stereo to name	164	C12H20	024145-88-8	74
3			Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	68
4			Added stereo to name	164	C12H20	024145-89-9	68
5			Methyl (1s,3s,5R,7S)-3-methylada...	208	C13H20O2	1010504-39-1	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY061323\
Data File : VY014142.D
Acq On : 13 Jun 2023 16:16
Operator : KP/MD
Sample : 03154-01
Misc : 5.08g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
CHRT-24051

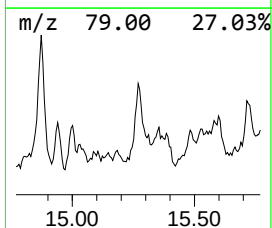
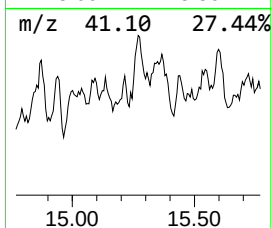
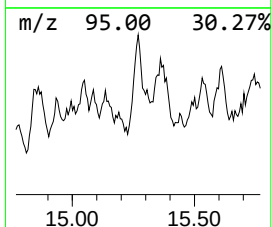
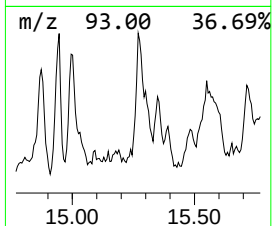
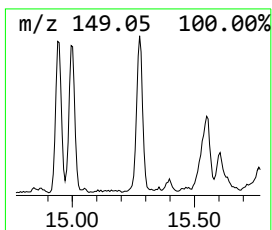
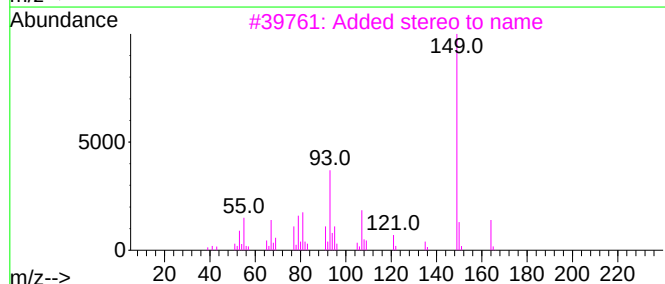
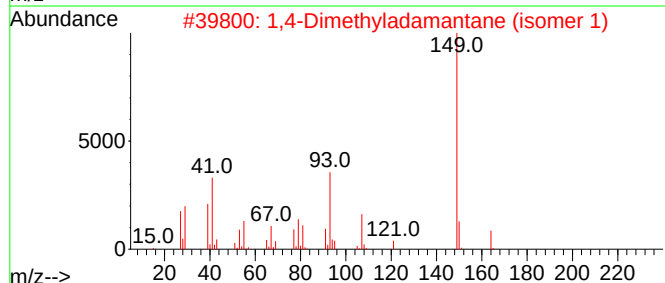
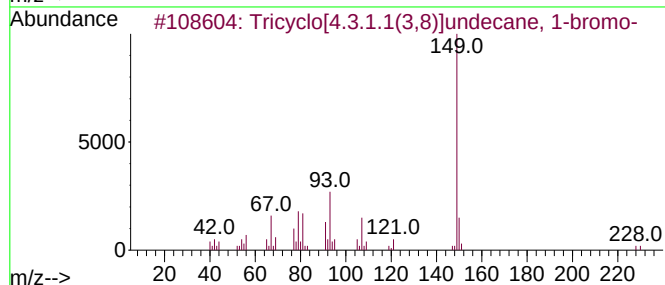
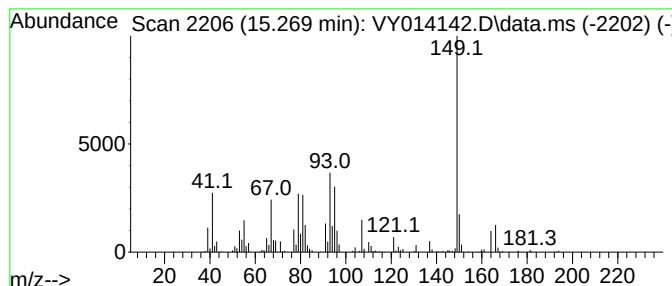
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Quant Title : SW846 8260

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

Peak Number 9 Tricyclo[4.3.1.1(3,8)]undec... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.269	40.43 ug/l	366090	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tricyclo[4.3.1.1(3,8)]undecane, ...	228	C11H17Br	021898-96-4	64
2			1,4-Dimethyladamantane (isomer 1)	164	C12H20	1000460-67-0	64
3			Added stereo to name	164	C12H20	024145-89-9	58
4			Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	52
5			Tricyclo[4.3.1.1(3,8)]undecane, ...	184	C11H17Cl	027011-46-7	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY061323\
Data File : VY014142.D
Acq On : 13 Jun 2023 16:16
Operator : KP/MD
Sample : 03154-01
Misc : 5.08g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
CHRT-24051

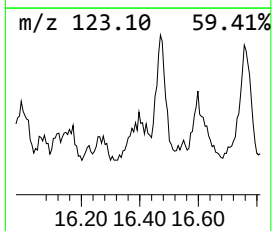
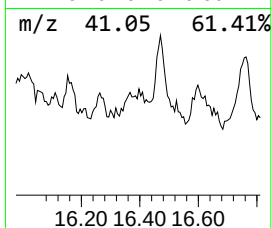
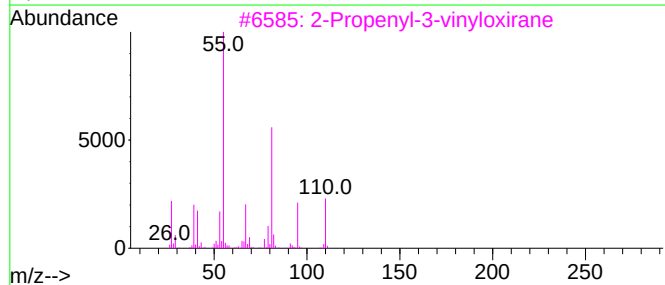
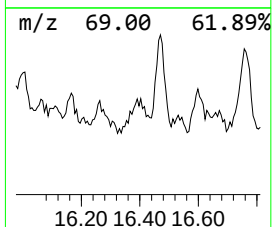
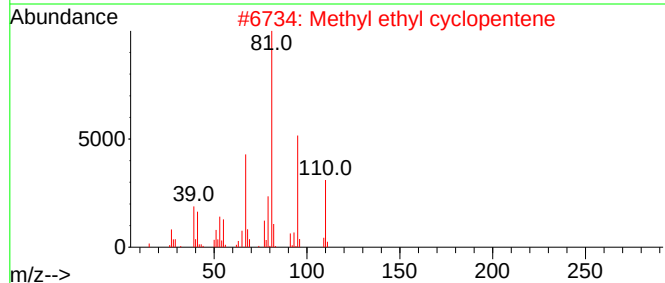
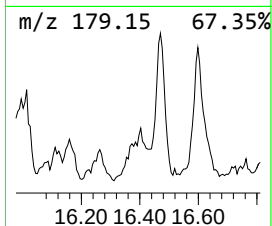
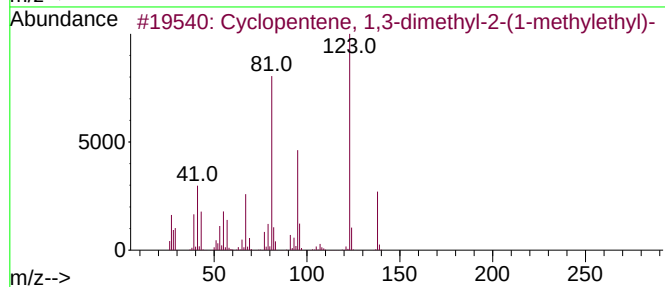
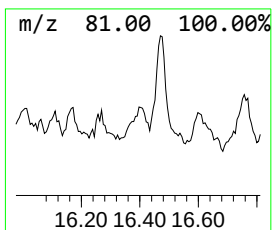
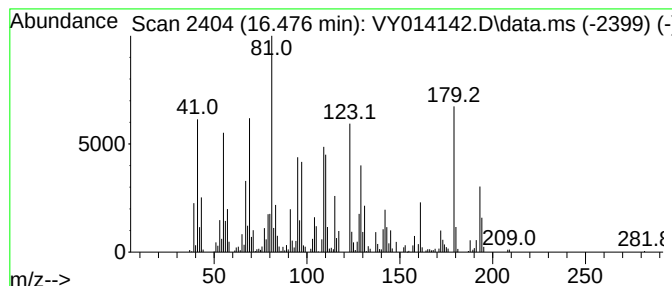
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Quant Title : SW846 8260

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

Peak Number 10 unknown16.476 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.476	57.73 ug/l	522712	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentene, 1,3-dimethyl-2-(1-...	138	C10H18	061142-32-3	38
2			Methyl ethyl cyclopentene	110	C8H14	019780-56-4	38
3			2-Propenyl-3-vinyloxirane	110	C7H10O	070597-49-8	30
4			2(1H)-Pentalenone, hexahydro-4-i...	250	C8H11IO	077070-56-5	27
5			2-Cyclohexene-1-carboxaldehyde, ...	152	C10H16O	000432-24-6	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY061323\
Data File : VY014142.D
Acq On : 13 Jun 2023 16:16
Operator : KP/MD
Sample : 03154-01
Misc : 5.08g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
CHRT-24051

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060923S.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
Cyclohexane, 1-...	13.745	25.9	ug/l	234675	4	13.422	452725	50.0
Tricyclo[3.3.1....	14.282	60.3	ug/l	546031	4	13.422	452725	50.0
Adamantane, 1,3...	14.391	24.1	ug/l	218269	4	13.422	452725	50.0
1-Dodecene	14.580	44.0	ug/l	398184	4	13.422	452725	50.0
unknown14.678	14.678	24.1	ug/l	218148	4	13.422	452725	50.0
Cyclohexene, 2-...	14.873	35.8	ug/l	323825	4	13.422	452725	50.0
1,4-Dimethylada...	14.940	23.9	ug/l	216185	4	13.422	452725	50.0
Methyl (1s,3s,5...	15.001	27.1	ug/l	245741	4	13.422	452725	50.0
Tricyclo[4.3.1....	15.269	40.4	ug/l	366090	4	13.422	452725	50.0
unknown16.476	16.476	57.7	ug/l	522712	4	13.422	452725	50.0