

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY071224\
 Data File : VY018802.D
 Acq On : 12 Jul 2024 17:05
 Operator : SY/MD
 Sample : P3207-01
 Misc : 5.01g/5.0mL/MSVOA_Y/SOIL/A
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 CHRT-26899

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\82Y070924S.M
 Title : SW846 8260

Signal : TIC: VY018802.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.205	59	63	66	rBV3	3319	4693	1.26%	0.137%
2	3.942	341	348	354	rBV3	1834	4563	1.22%	0.133%
3	4.692	461	471	486	rBV3	23193	73469	19.66%	2.138%
4	4.936	501	511	512	rBV3	5542	10598	2.84%	0.308%
5	5.728	631	641	651	rBV6	4996	15550	4.16%	0.453%
6	6.972	832	845	856	rBV2	7092	22880	6.12%	0.666%
7	7.710	956	966	971	rBV	58230	139110	37.23%	4.048%
8	7.777	971	977	987	rVB2	93868	216001	57.80%	6.286%
9	8.130	1025	1035	1047	rBV	50696	113810	30.46%	3.312%
10	8.685	1118	1126	1141	rVB	146406	293828	78.63%	8.551%
11	10.173	1363	1370	1378	rBV	216201	373680	100.00%	10.874%
12	10.575	1430	1436	1442	rBV3	12920	22593	6.05%	0.657%
13	10.721	1454	1460	1465	rVB3	9750	17631	4.72%	0.513%
14	10.941	1488	1496	1501	rBV	4969	7128	1.91%	0.207%
15	11.484	1578	1585	1596	rBV	197194	325358	87.07%	9.468%
16	12.331	1718	1724	1729	rVB4	17760	30669	8.21%	0.893%
17	12.477	1742	1748	1755	rBV2	144888	237948	63.68%	6.925%
18	12.739	1783	1791	1796	rVB7	2420	4593	1.23%	0.134%
19	12.806	1796	1802	1808	rBV9	4296	9160	2.45%	0.267%
20	13.002	1828	1834	1839	rBV3	8839	17118	4.58%	0.498%
21	13.117	1847	1853	1857	rBV7	2978	6969	1.86%	0.203%
22	13.178	1862	1863	1870	rVB5	4310	6272	1.68%	0.183%
23	13.245	1870	1874	1875	rBV3	3299	3738	1.00%	0.109%
24	13.422	1897	1903	1911	rVB	141814	225370	60.31%	6.559%
25	13.544	1921	1923	1931	rVB8	2488	5136	1.37%	0.149%
26	13.611	1931	1934	1936	rBV4	3122	4560	1.22%	0.133%
27	13.648	1936	1940	1950	rVB10	5704	14577	3.90%	0.424%
28	13.745	1950	1956	1959	rBV5	19299	33674	9.01%	0.980%
29	13.861	1969	1975	1981	rBV9	4347	12159	3.25%	0.354%
30	13.916	1981	1984	1986	rBV4	4568	6024	1.61%	0.175%
31	13.965	1987	1992	1997	rVB5	12108	22937	6.14%	0.667%
32	14.068	2007	2009	2013	rVB5	3363	4313	1.15%	0.126%
33	14.123	2013	2018	2026	rVB8	13629	30297	8.11%	0.882%
34	14.203	2026	2031	2035	rBV8	6800	15452	4.14%	0.450%
35	14.251	2035	2039	2042	rBV3	23965	43826	11.73%	1.275%
36	14.282	2042	2044	2050	rVV2	33023	54610	14.61%	1.589%

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37	14.331	2050	2052	2056	rVB3	8981	11061	2.96%	0.322%
38	14.392	2056	2062	2064	rBV2	24142	46067	12.33%	1.341%
39	14.422	2064	2067	2070	rVV4	25444	38758	10.37%	1.128%
40	14.465	2070	2074	2080	rVB6	15251	33842	9.06%	0.985%
41	14.568	2089	2091	2093	rBV3	4965	5243	1.40%	0.153%
42	14.617	2097	2099	2102	rVB4	9723	9881	2.64%	0.288%
43	14.678	2103	2109	2114	rBV7	20961	56391	15.09%	1.641%
44	14.727	2114	2117	2122	rVB6	23850	35905	9.61%	1.045%
45	14.776	2123	2125	2128	rBV4	7046	10399	2.78%	0.303%
46	14.873	2134	2141	2145	rBV4	40783	71623	19.17%	2.084%
47	14.940	2148	2152	2157	rVB4	43541	66701	17.85%	1.941%
48	15.001	2157	2162	2164	rBV3	29429	51189	13.70%	1.490%
49	15.269	2201	2206	2210	rBV3	54167	108893	29.14%	3.169%
50	15.343	2215	2218	2219	rBV2	18256	22800	6.10%	0.664%
51	16.470	2399	2403	2416	rVB7	99922	246296	65.91%	7.167%
52	16.598	2420	2424	2438	rVB7	52394	190957	51.10%	5.557%

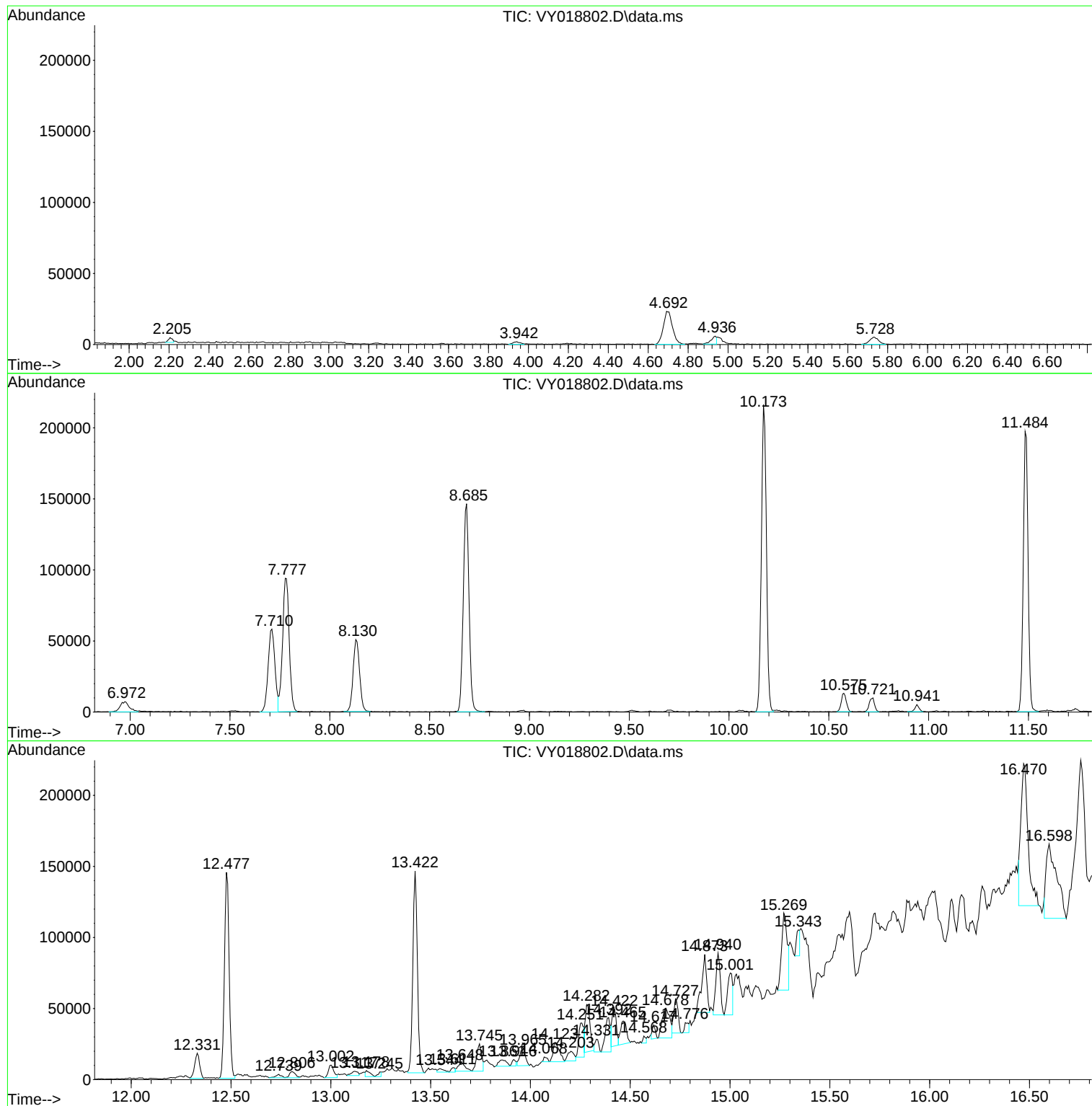
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y070924S.M
Quant Title : SW846 8260

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



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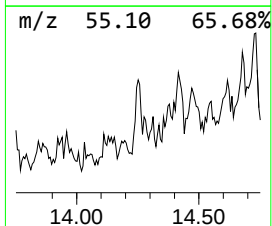
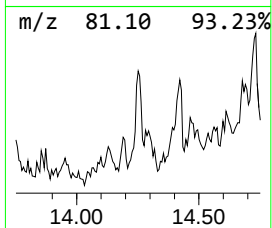
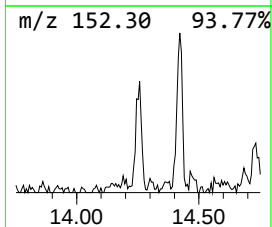
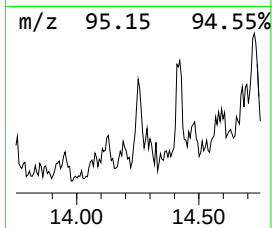
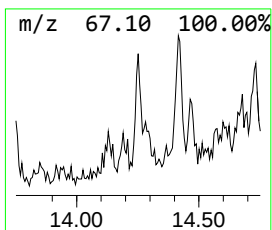
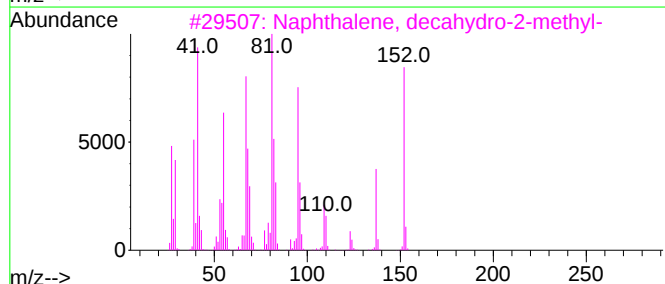
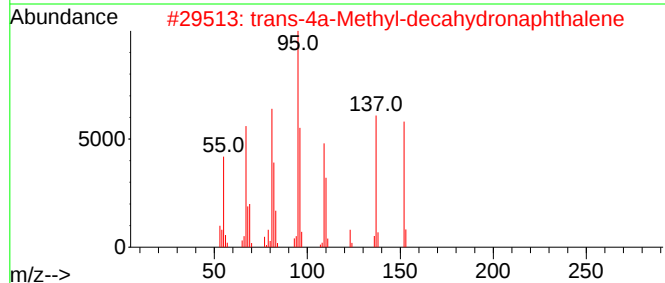
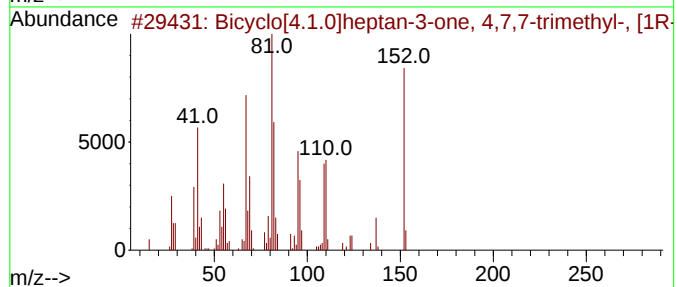
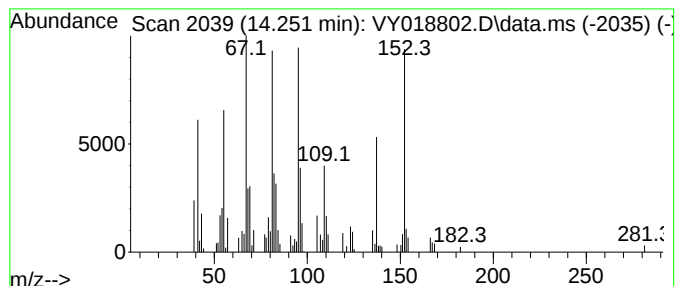
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y070924S.M
Quant Title : SW846 8260

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

Peak Number 1 Bicyclo[4.1.0]heptan-3-one,... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.251	9.72 ug/l	43826	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[4.1.0]heptan-3-one, 4,7,...	152	C10H16O	004176-04-9	81
2			trans-4a-Methyl-decahydronaphtha...	152	C11H20	002547-27-5	76
3			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	74
4			Pulegone	152	C10H16O	000089-82-7	60
5			trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	60



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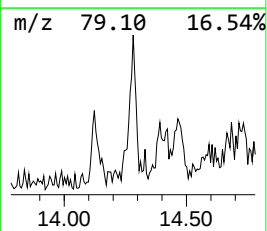
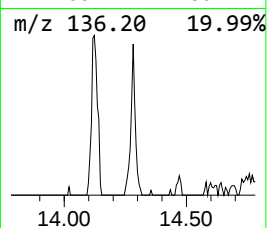
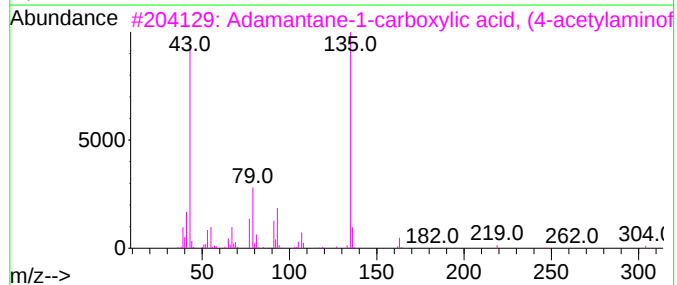
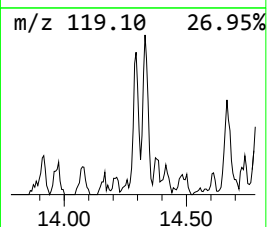
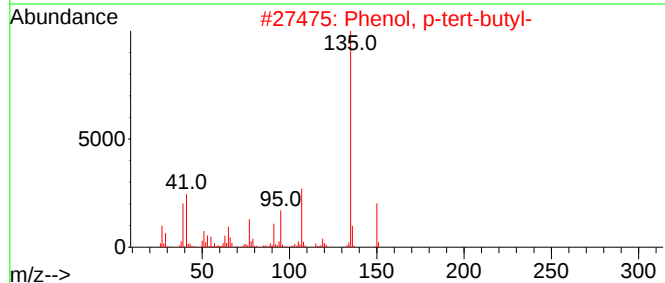
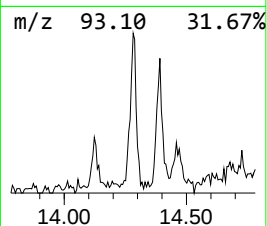
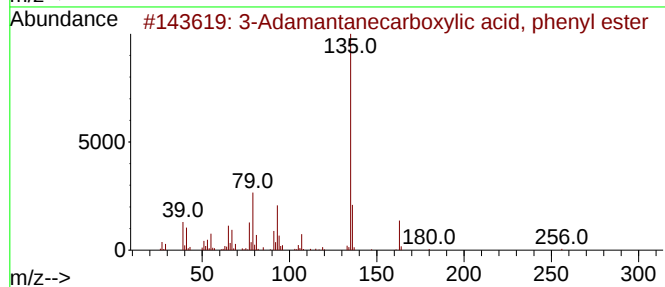
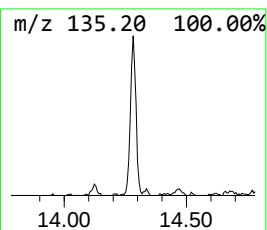
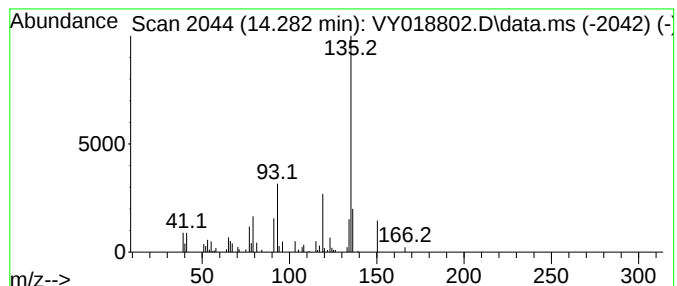
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y070924S.M
Quant Title : SW846 8260

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

Peak Number 2 3-Adamantanecarboxylic acid... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.282	12.12 ug/l	54610	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Adamantanecarboxylic acid, phe...	256	C17H20O2	035856-79-2	50
2			Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	46
3			Adamantane-1-carboxylic acid, (4...	304	C15H20N4O3	1000305-04-4	43
4			o-Anisic acid, dodec-9-ynyl ester	316	C20H28O3	1000299-95-2	43
5			5-(4-Trifluormethylsulfonylpheny...	372	C17H19F3N2O2S	187338-96-1	42



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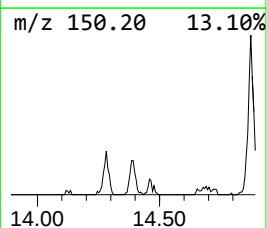
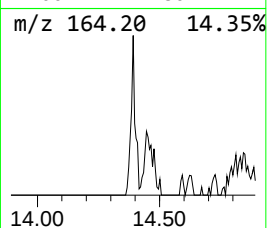
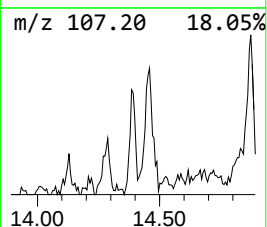
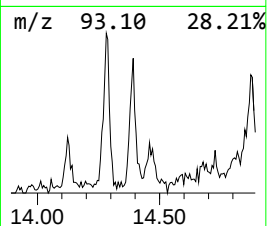
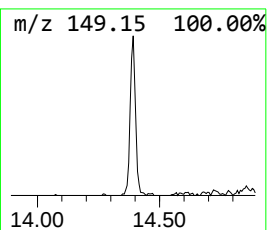
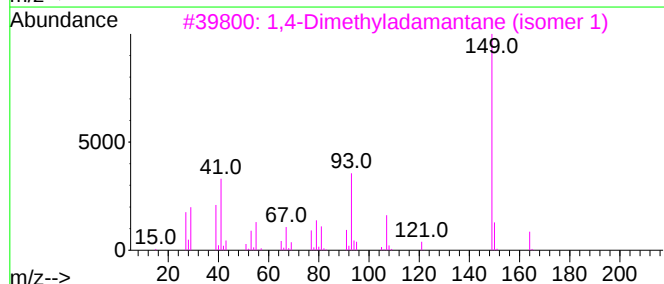
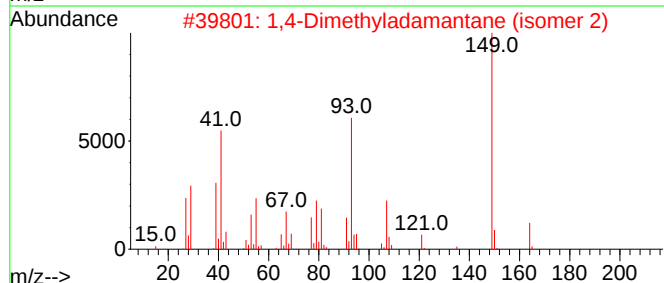
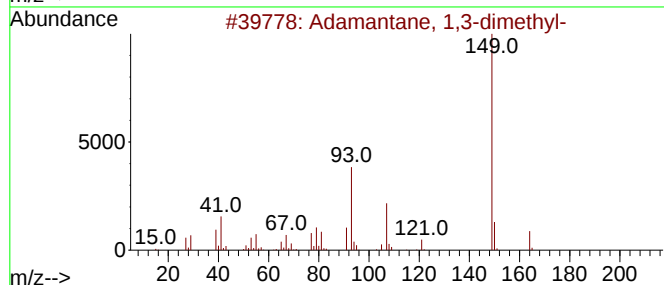
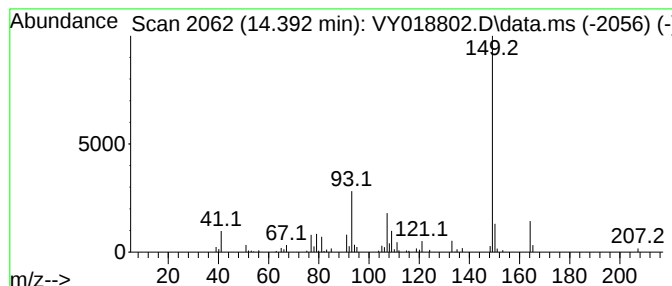
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Adamantane, 1,3-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.392	10.22 ug/l	46067	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	90
2			1,4-Dimethyladamantane (isomer 2)	164	C12H20	1000460-67-1	87
3			1,4-Dimethyladamantane (isomer 1)	164	C12H20	1000460-67-0	83
4			Added stereo to name	164	C12H20	024145-88-8	83
5			Adamantane, 1-isothiocyanato-3-m...	207	C12H17NS	136860-48-5	74



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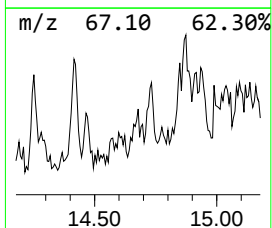
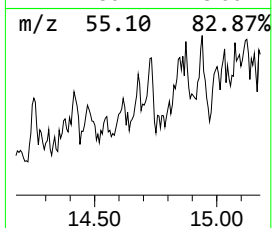
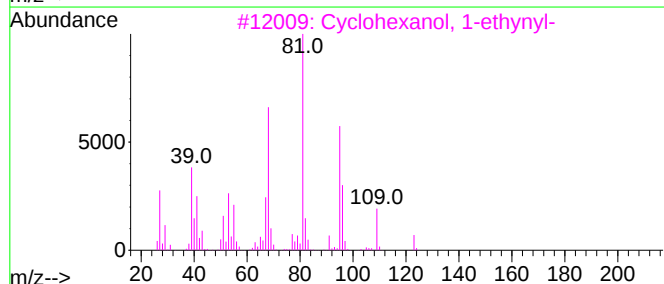
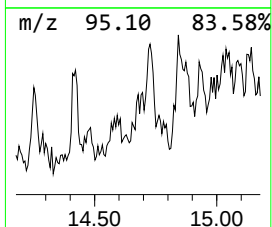
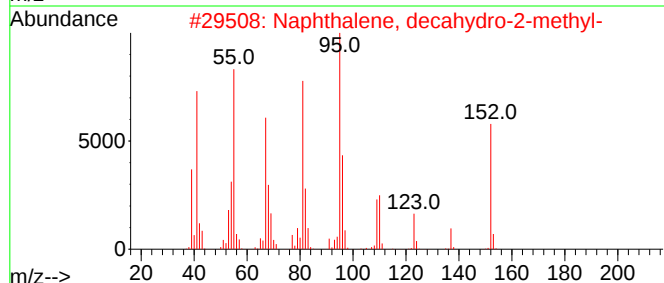
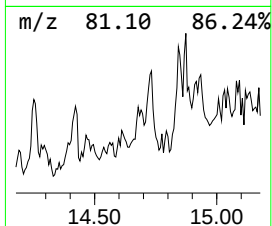
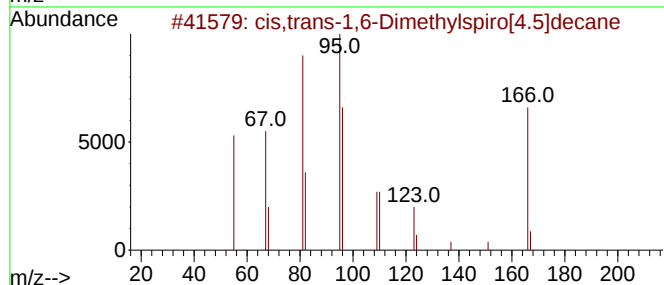
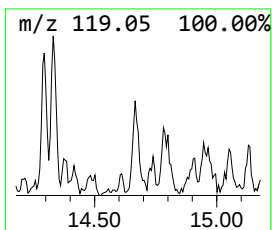
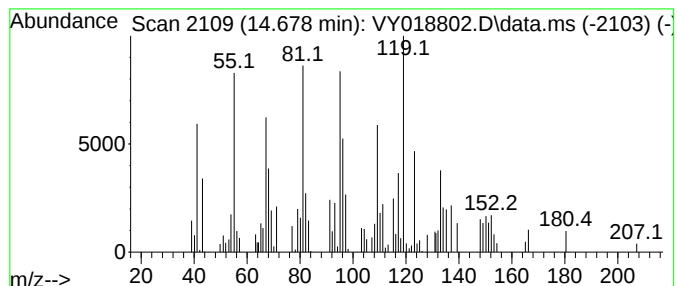
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 unknown14.678 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.678	12.51 ug/l	56391	1,4-Dichlorobenzene-d4	13.422	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis,trans-1,6-Dimethylspiro[4.5]...	166	C12H22	1000111-72-3	45
2	Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	43
3	Cyclohexanol, 1-ethynyl-	124	C8H12O	000078-27-3	38
4	cis,cis-1,6-Dimethylspiro[4.5]de...	166	C12H22	1000111-72-4	38
5	1H-Indene, 1-ethyloctahydro-7a-m...	166	C12H22	056324-71-1	38



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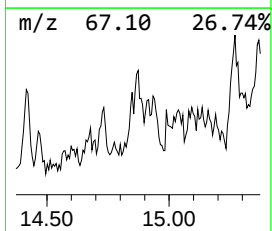
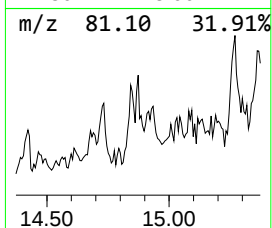
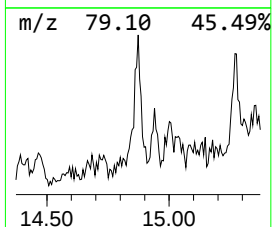
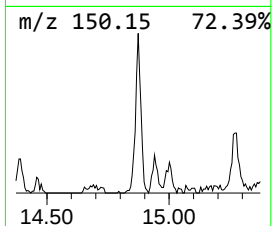
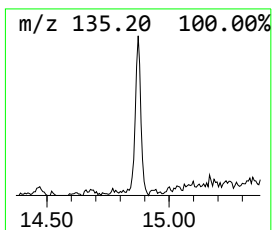
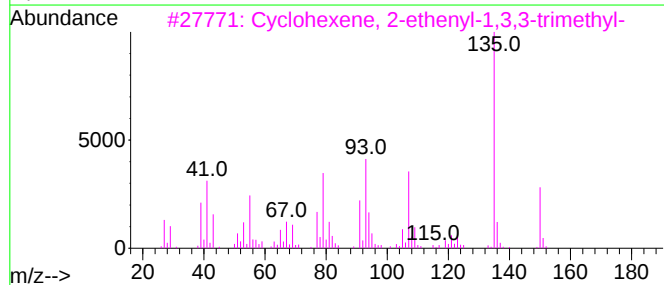
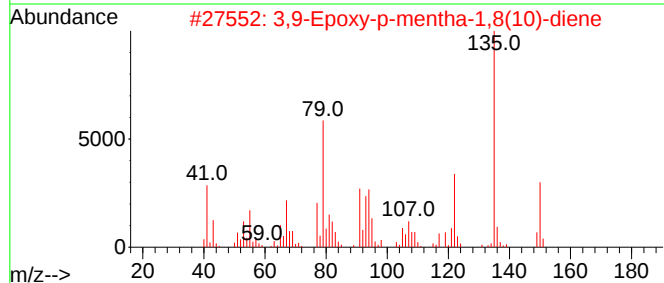
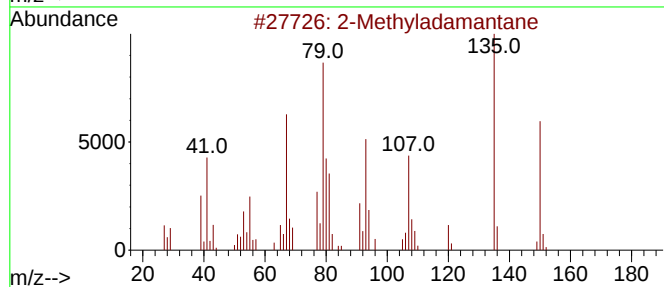
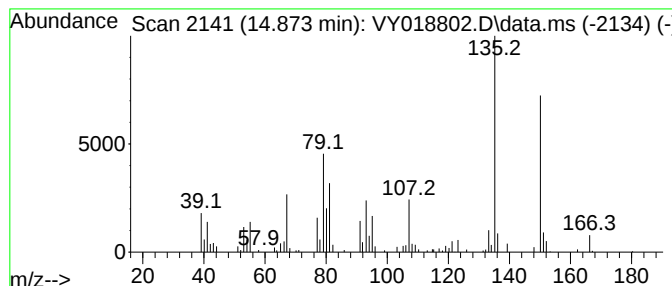
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Quant Title : SW846 8260

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

Peak Number 5 2-Methyladamantane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.873	15.89 ug/l	71623	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methyladamantane	150	C11H18	000700-56-1	90
2			3,9-Epoxy-p-mentha-1,8(10)-diene	150	C10H14O	1000111-14-8	76
3			Cyclohexene, 2-ethenyl-1,3,3-tri...	150	C11H18	005293-90-3	70
4			Y-Methylbicyclo(4.3.0)non-6-en-8...	150	C10H14O	1000424-65-9	58
5			Ethanone, 1-(2-hydroxy-5-methylp...	150	C9H10O2	001450-72-2	55



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY071224\
Data File : VY018802.D
Acq On : 12 Jul 2024 17:05
Operator : SY/MD
Sample : P3207-01
Misc : 5.01g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
CHRT-26899

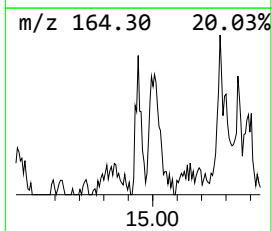
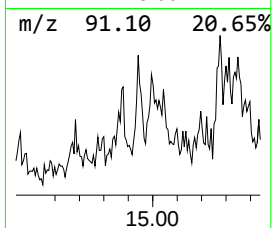
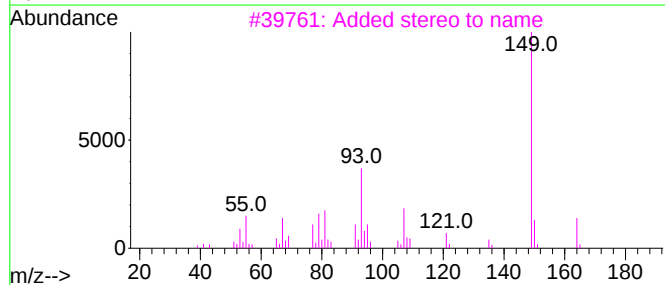
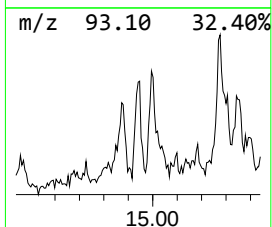
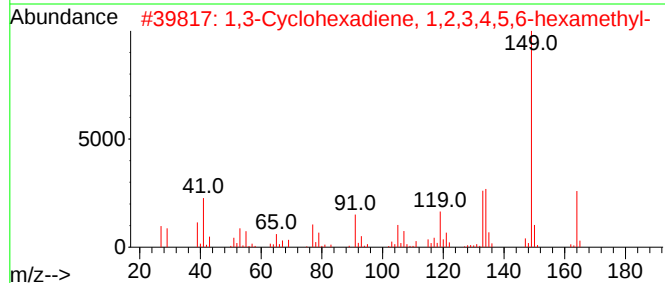
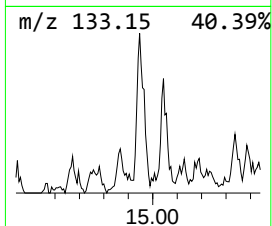
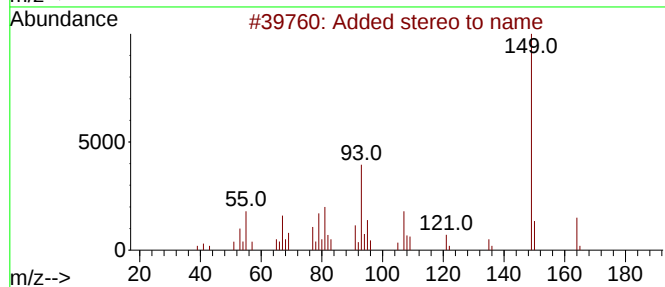
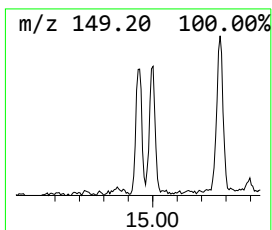
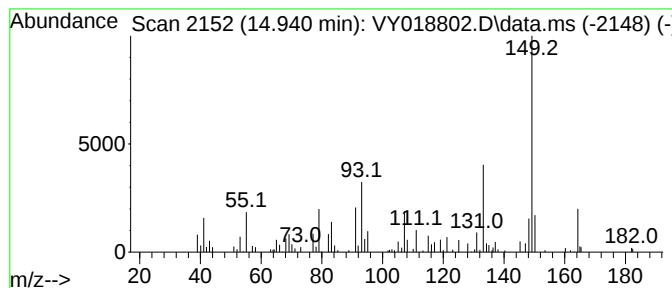
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Quant Title : SW846 8260

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

Peak Number 6 unknown14.940 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.940	14.80 ug/l	66701	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Added stereo to name			164	C12H20	024145-88-8	53
2	1,3-Cyclohexadiene, 1,2,3,4,5,6-...			164	C12H20	1000152-09-6	49
3	Added stereo to name			164	C12H20	024145-89-9	47
4	1,4-Dimethyladamantane (isomer 2)			164	C12H20	1000460-67-1	47
5	Benzenemethanol, 4-(1,1-dimethyl...			164	C11H16O	000877-65-6	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY071224\
Data File : VY018802.D
Acq On : 12 Jul 2024 17:05
Operator : SY/MD
Sample : P3207-01
Misc : 5.01g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
CHRT-26899

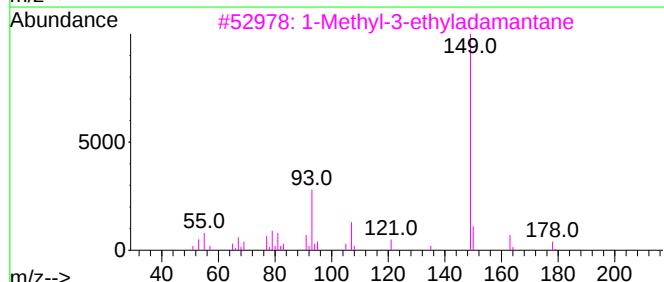
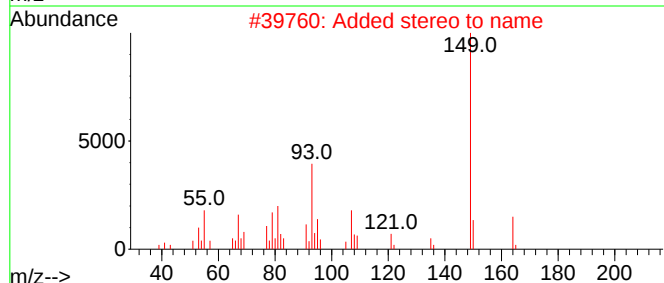
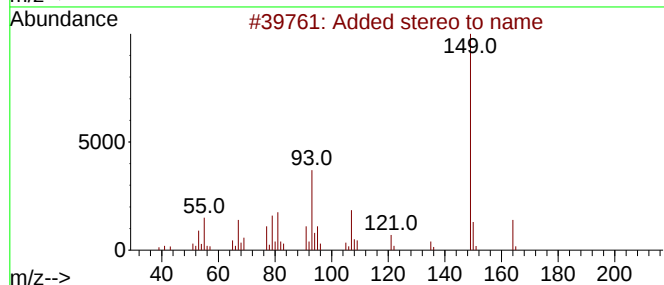
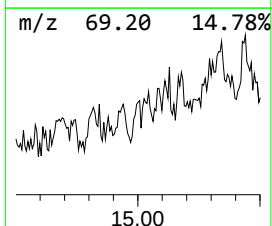
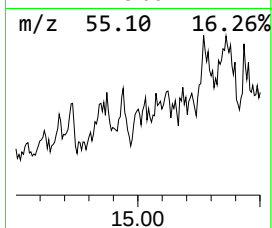
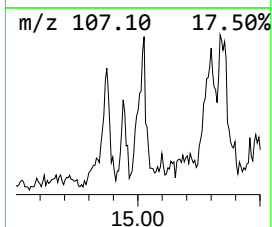
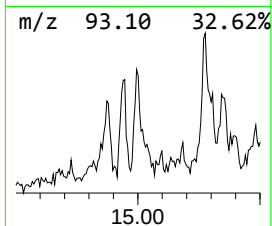
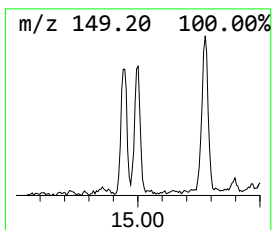
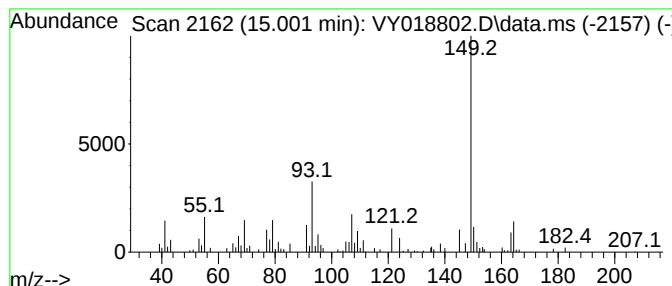
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Quant Title : SW846 8260

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.
15.001	11.36 ug/l	51189	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	Added stereo to name			164	C12H20	024145-88-8	80
3	1-Methyl-3-ethyladamantane			178	C13H22	001687-34-9	74
4	1,3-Cyclohexadiene, 1,3,5,5,6,6-...			164	C12H20	1000150-39-4	68
5	1,4-Dimethyladamantane (isomer 1)			164	C12H20	1000460-67-0	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY071224\
Data File : VY018802.D
Acq On : 12 Jul 2024 17:05
Operator : SY/MD
Sample : P3207-01
Misc : 5.01g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
CHRT-26899

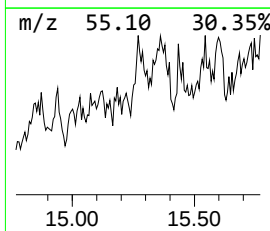
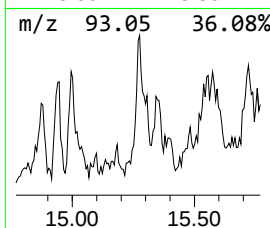
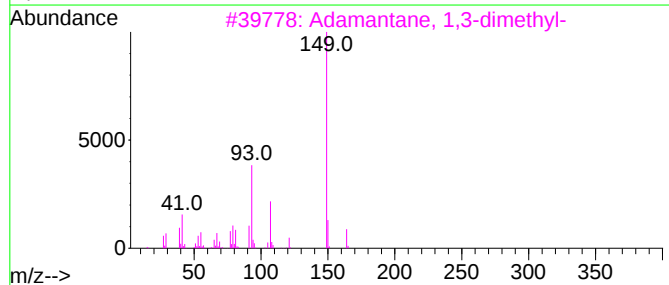
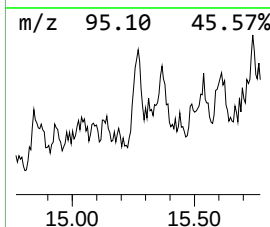
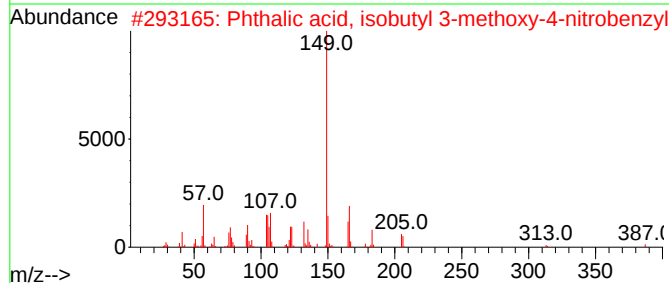
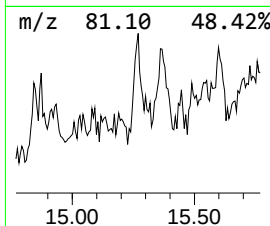
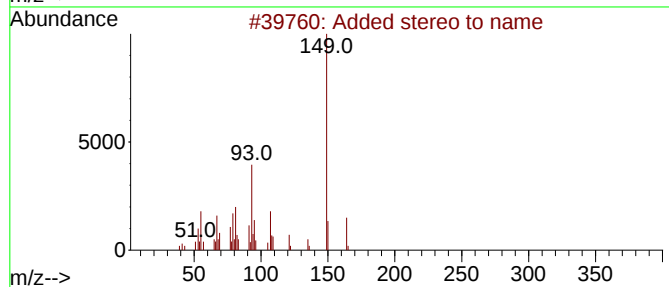
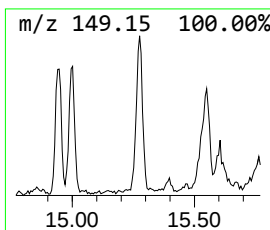
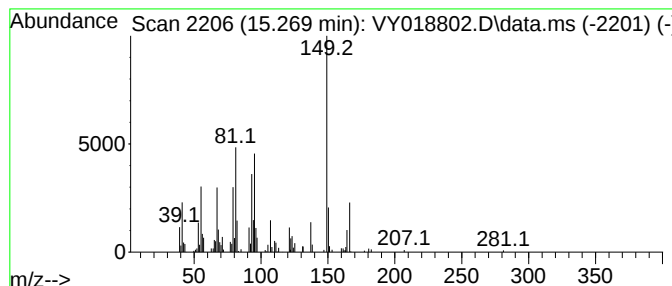
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Quant Title : SW846 8260

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

Peak Number 8 unknown15.269 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.269	24.16 ug/l	108893	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Added stereo to name			164	C12H20	024145-88-8	49
2	Phthalic acid, isobutyl 3-methox...			387	C20H21NO7	1000382-53-1	47
3	Adamantane, 1,3-dimethyl-			164	C12H20	000702-79-4	43
4	Added stereo to name			164	C12H20	024145-89-9	43
5	1-Methyl-3-ethyladamantane			178	C13H22	001687-34-9	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY071224\
Data File : VY018802.D
Acq On : 12 Jul 2024 17:05
Operator : SY/MD
Sample : P3207-01
Misc : 5.01g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
CHRT-26899

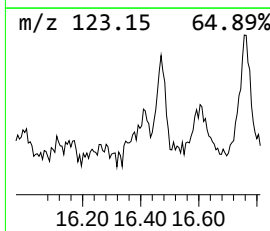
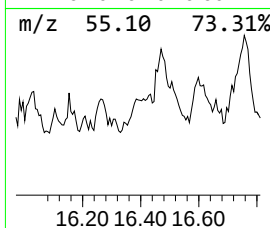
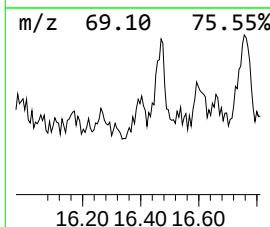
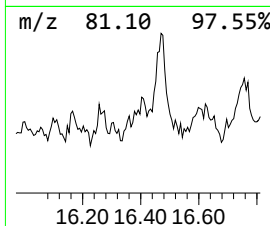
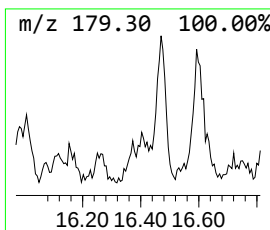
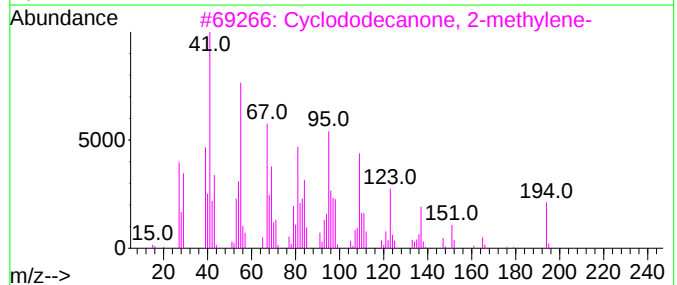
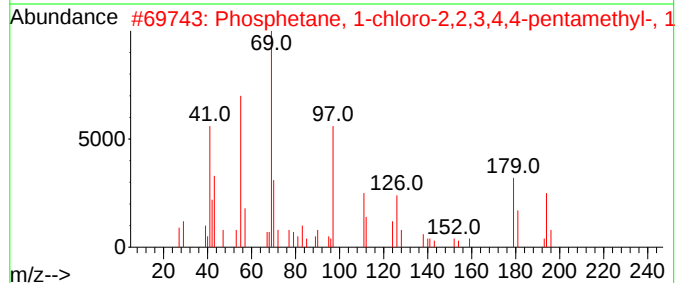
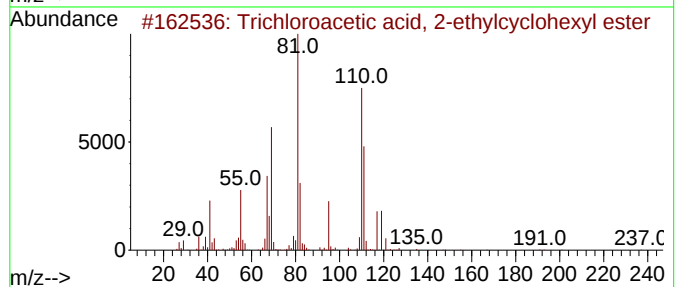
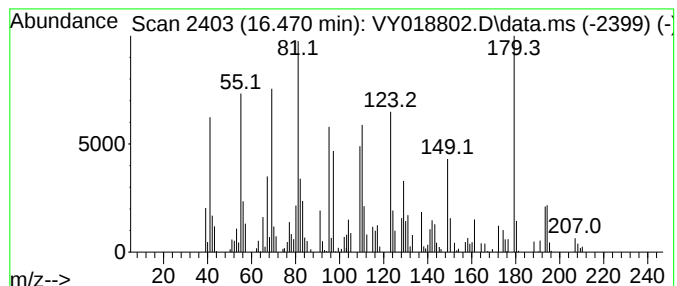
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Quant Title : SW846 8260

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

Peak Number 9 unknown16.470 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.470	54.64 ug/l	246296	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, 2-ethylcyc...	272	C10H15Cl3O2	1000282-57-3	35
2			Phosphetane, 1-chloro-2,2,3,4,4-...	194	C8H16ClOP	029276-11-7	35
3			Cyclododecanone, 2-methylene-	194	C13H22O	003045-76-9	18
4			Methyl ethyl cyclopentene	110	C8H14	019780-56-4	14
5			4-Ethylcyclohexanol	128	C8H16O	004534-74-1	14



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY071224\
Data File : VY018802.D
Acq On : 12 Jul 2024 17:05
Operator : SY/MD
Sample : P3207-01
Misc : 5.01g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
CHRT-26899

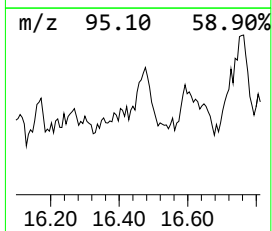
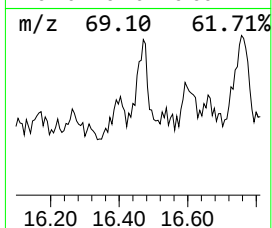
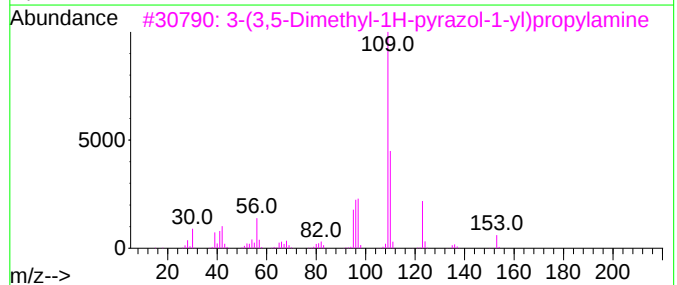
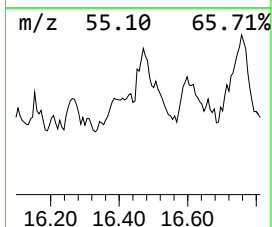
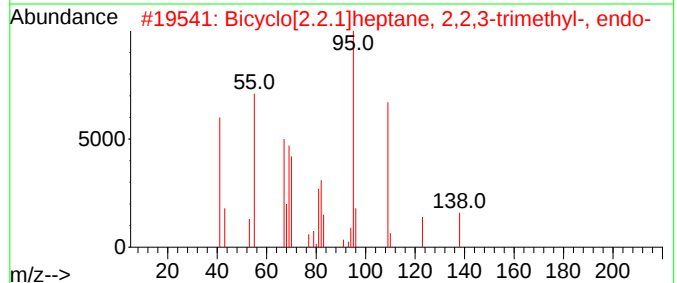
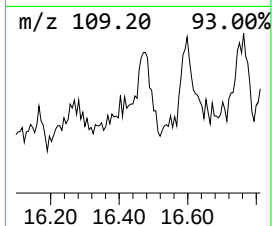
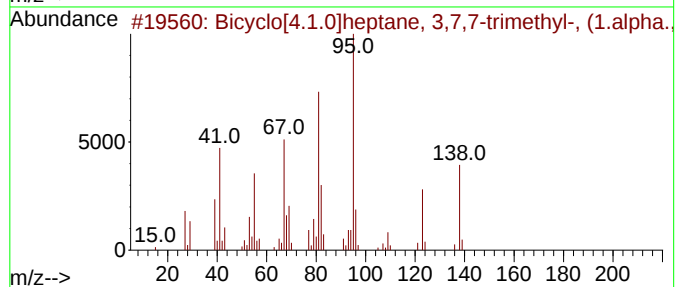
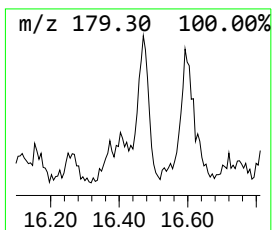
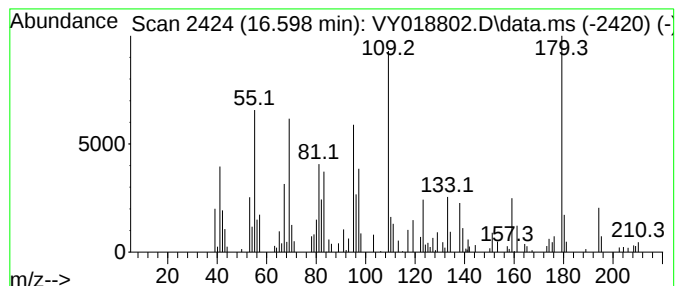
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Quant Title : SW846 8260

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

Peak Number 10 unknown16.599 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.599	42.37 ug/l	190957	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	018968-23-5	25
2			Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-40-7	25
3			3-(3,5-Dimethyl-1H-pyrazol-1-yl)...	153	C8H15N3	062821-89-0	22
4			Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-41-8	22
5			Furan-2-carboxaldehyde, 5-(1-pip...	179	C10H13NO2	022868-60-6	11



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY071224\
Data File : VY018802.D
Acq On : 12 Jul 2024 17:05
Operator : SY/MD
Sample : P3207-01
Misc : 5.01g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
CHRT-26899

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y070924S.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...	14.251	9.7	ug/l	43826	4	13.422	225370	50.0
3-Adamantanecar...	14.282	12.1	ug/l	54610	4	13.422	225370	50.0
Adamantane, 1,3...	14.392	10.2	ug/l	46067	4	13.422	225370	50.0
unknown14.678	14.678	12.5	ug/l	56391	4	13.422	225370	50.0
2-Methyladamantane	14.873	15.9	ug/l	71623	4	13.422	225370	50.0
unknown14.940	14.940	14.8	ug/l	66701	4	13.422	225370	50.0
1-Methyl-3-ethy...	15.001	11.4	ug/l	51189	4	13.422	225370	50.0
unknown15.269	15.269	24.2	ug/l	108893	4	13.422	225370	50.0
unknown16.470	16.470	54.6	ug/l	246296	4	13.422	225370	50.0
unknown16.599	16.599	42.4	ug/l	190957	4	13.422	225370	50.0