

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY020525\
 Data File : VY021081.D
 Acq On : 05 Feb 2025 12:17
 Operator : SY/MD
 Sample : Q1261-01
 Misc : 5.01g/5.0mL/MSVOA_Y/SOIL/A
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 CHRT-20430

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\82Y020325S.M
 Title : SW846 8260

Signal : TIC: VY021081.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.178	68	75	85	rVB3	6195	10867	1.31%	0.122%
2	4.866	502	516	524	rBV2	4432	17437	2.11%	0.195%
3	5.659	634	646	659	rBV2	32343	102997	12.45%	1.153%
4	6.890	838	848	855	rBV2	4207	11900	1.44%	0.133%
5	7.640	960	971	977	rBV2	109253	259771	31.40%	2.907%
6	7.713	977	983	993	rVB	174960	406574	49.14%	4.550%
7	7.927	1008	1018	1026	rBV4	4555	11399	1.38%	0.128%
8	8.067	1031	1041	1052	rBV	93664	221545	26.78%	2.479%
9	8.481	1102	1109	1117	rVB3	5809	11765	1.42%	0.132%
10	8.622	1124	1132	1143	rBV	278034	543493	65.69%	6.082%
11	9.115	1203	1213	1219	rBV6	7160	16346	1.98%	0.183%
12	9.682	1298	1306	1312	rBV4	5072	10575	1.28%	0.118%
13	10.109	1369	1376	1382	rBV	332061	583846	70.57%	6.534%
14	10.176	1382	1387	1394	rVB	61347	106667	12.89%	1.194%
15	10.304	1400	1408	1416	rVB3	5723	12513	1.51%	0.140%
16	10.451	1424	1432	1437	rBV4	4941	8821	1.07%	0.099%
17	10.554	1444	1449	1457	rVB7	6583	15356	1.86%	0.172%
18	10.652	1459	1465	1470	rVB4	6064	10842	1.31%	0.121%
19	10.975	1513	1518	1522	rVV2	10423	18916	2.29%	0.212%
20	11.024	1522	1526	1531	rVB4	7175	11594	1.40%	0.130%
21	11.225	1549	1559	1568	rVB6	9682	25603	3.09%	0.287%
22	11.420	1584	1591	1601	rBV	199829	333997	40.37%	3.738%
23	11.524	1602	1608	1612	rBV	22860	37106	4.48%	0.415%
24	11.633	1617	1626	1636	rVV3	57869	157212	19.00%	1.759%
25	11.713	1636	1639	1643	rVB	7572	11314	1.37%	0.127%
26	11.938	1668	1676	1677	rBV4	20148	39972	4.83%	0.447%
27	11.956	1677	1679	1689	rVB2	26489	50858	6.15%	0.569%
28	12.097	1698	1702	1705	rBV2	17110	30103	3.64%	0.337%
29	12.133	1705	1708	1711	rVV5	17250	27639	3.34%	0.309%
30	12.176	1711	1715	1719	rVV4	17054	32189	3.89%	0.360%
31	12.231	1719	1724	1726	rVV4	20410	37525	4.54%	0.420%
32	12.267	1726	1730	1735	rVB	54431	86733	10.48%	0.971%
33	12.347	1740	1743	1749	rVB7	8771	14608	1.77%	0.163%
34	12.414	1749	1754	1759	rVB	101547	157298	19.01%	1.760%
35	12.487	1759	1766	1768	rBV6	10211	20860	2.52%	0.233%
36	12.542	1772	1775	1777	rBV4	7721	9882	1.19%	0.111%

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37	12.572	1777	1780	1788	rVB4	27424	57113	6.90%	0.639%
38	12.664	1788	1795	1801	rBV6	42580	114204	13.80%	1.278%
39	12.737	1802	1807	1812	rVB5	72389	115400	13.95%	1.291%
40	12.798	1814	1817	1824	rVB5	15411	31736	3.84%	0.355%
41	12.871	1826	1829	1836	rVB6	20658	37177	4.49%	0.416%
42	12.968	1837	1845	1853	rVB9	33204	97090	11.73%	1.087%
43	13.048	1853	1858	1863	rBV2	71482	134250	16.23%	1.502%
44	13.121	1863	1870	1875	rVB8	27406	64782	7.83%	0.725%
45	13.182	1875	1880	1883	rBV6	30010	60623	7.33%	0.678%
46	13.243	1884	1890	1894	rVV5	35520	73287	8.86%	0.820%
47	13.322	1901	1903	1905	rBV3	15387	14926	1.80%	0.167%
48	13.359	1906	1909	1910	rBV2	21250	24120	2.92%	0.270%
49	13.432	1917	1921	1922	rBV3	14820	19851	2.40%	0.222%
50	13.480	1925	1929	1934	rVB5	38074	72818	8.80%	0.815%
51	13.541	1934	1939	1943	rBV4	43704	87296	10.55%	0.977%
52	13.676	1955	1961	1971	rBV4	202923	428163	51.75%	4.792%
53	13.846	1986	1989	1991	rBV4	26723	35314	4.27%	0.395%
54	13.889	1992	1996	2002	rVB6	77502	140672	17.00%	1.574%
55	14.005	2010	2015	2018	rBV4	65951	107867	13.04%	1.207%
56	14.054	2018	2023	2030	rVB2	139983	243779	29.46%	2.728%
57	14.133	2031	2036	2040	rBV5	50891	117314	14.18%	1.313%
58	14.206	2040	2048	2060	rBV2	314815	827365	100.00%	9.259%
59	14.316	2061	2066	2069	rBV	237200	387665	46.86%	4.339%
60	14.389	2074	2078	2084	rVB3	128375	294884	35.64%	3.300%
61	14.602	2107	2113	2118	rBV4	105182	273081	33.01%	3.056%
62	14.657	2118	2122	2128	rVB4	106662	180237	21.78%	2.017%
63	14.797	2141	2145	2151	rVB	173464	267048	32.28%	2.989%
64	14.864	2152	2156	2161	rVB	163850	240580	29.08%	2.692%
65	14.919	2161	2165	2168	rBV	105549	181956	21.99%	2.036%
66	15.194	2205	2210	2217	rBV4	153467	401029	48.47%	4.488%
67	15.626	2279	2281	2288	rVB4	52730	80040	9.67%	0.896%
68	16.370	2398	2403	2412	rVB4	112714	257661	31.14%	2.884%

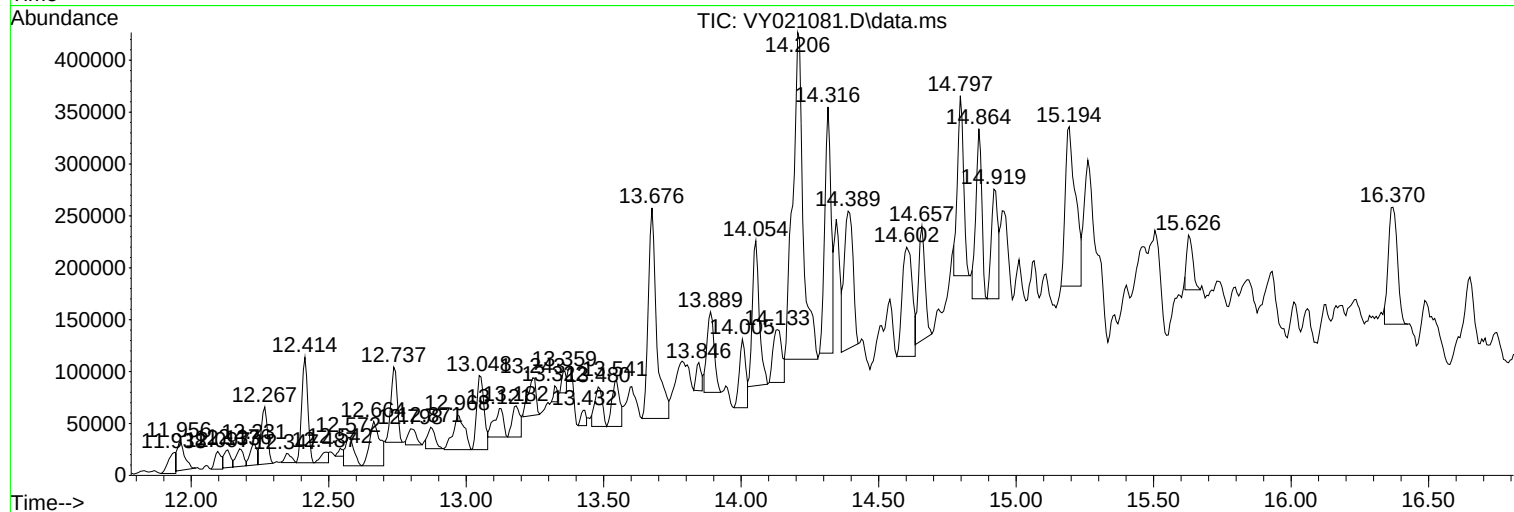
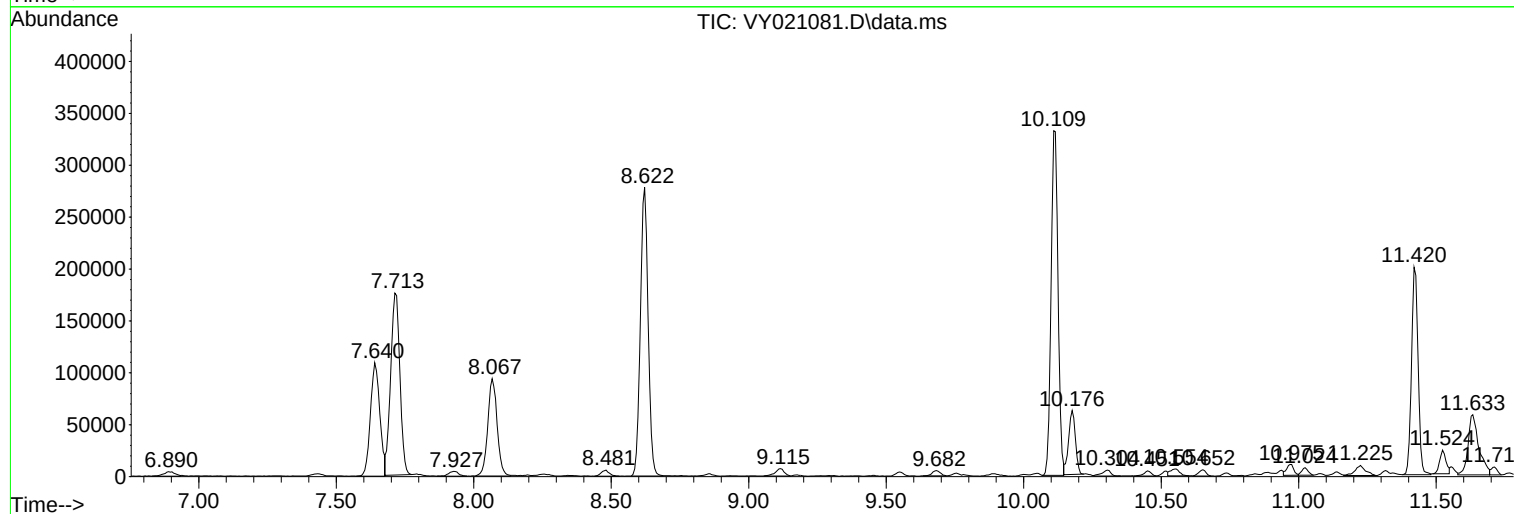
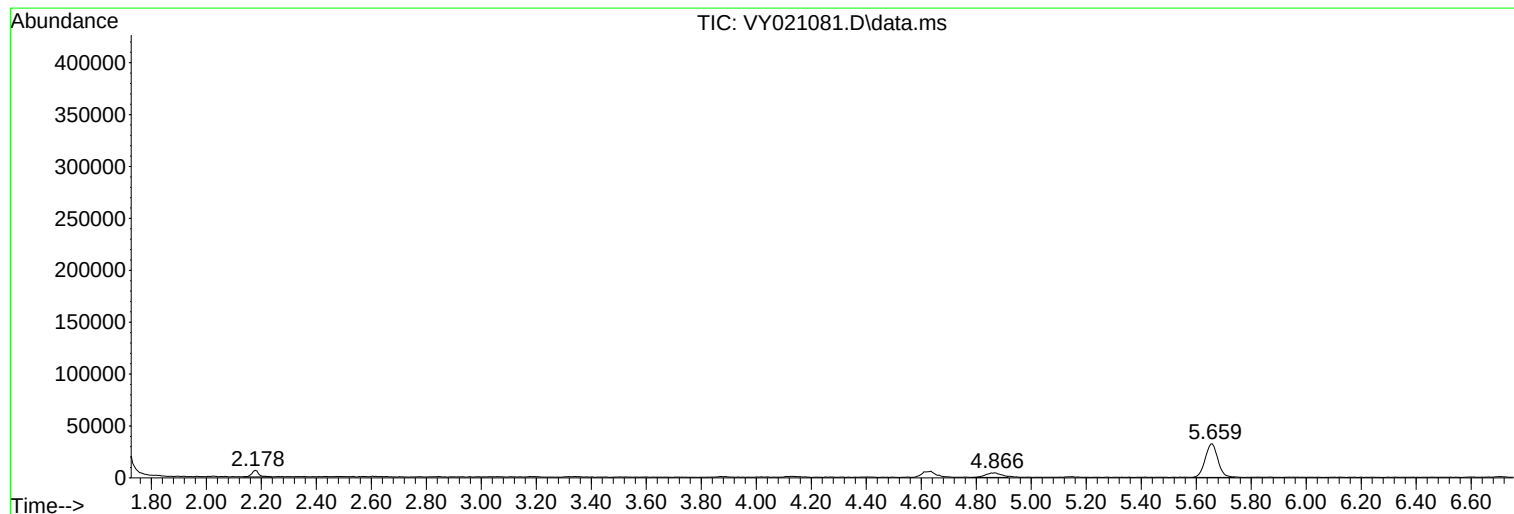
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ClientSampleId :
CHRT-20430

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y020325S.M
Quant Title : SW846 8260

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



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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
CHRT-20430

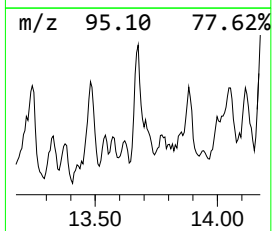
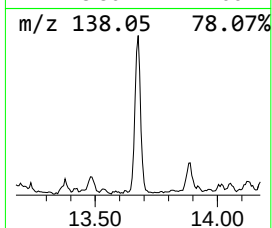
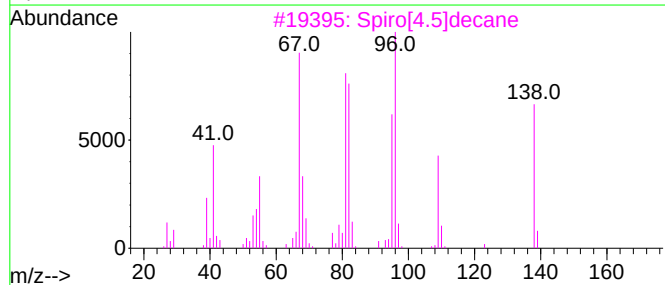
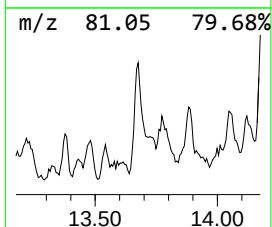
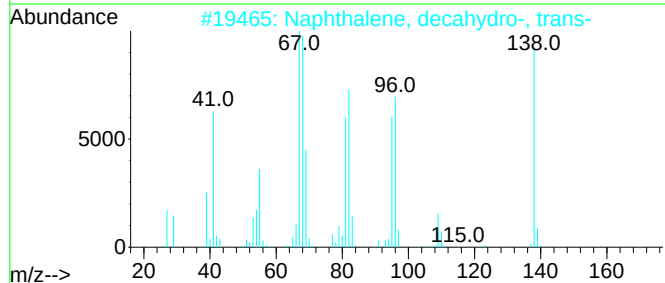
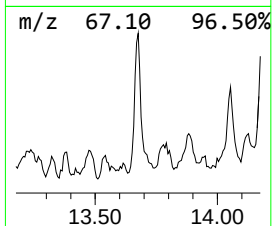
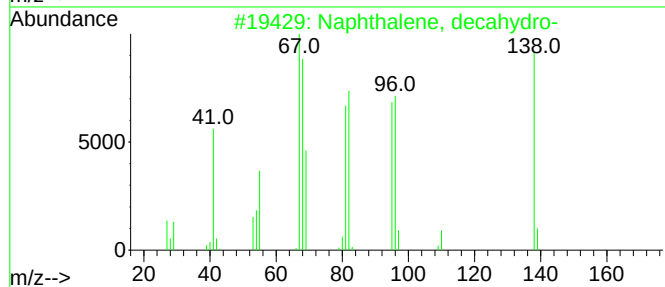
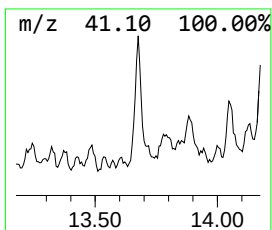
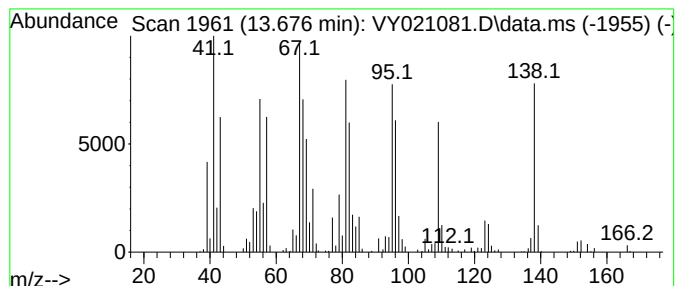
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y020325S.M
Quant Title : SW846 8260

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

Peak Number 1 Naphthalene, decahydro- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.676	887.57 ug/l	428163	1,4-Dichlorobenzene-d4	13.352

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-	138	C10H18	000091-17-8	96
2			Naphthalene, decahydro-, trans-	138	C10H18	000493-02-7	94
3			Spiro[4.5]decane	138	C10H18	000176-63-6	76
4			Cyclohexene, 3-methyl-6-(1-methy...	138	C10H18	005256-65-5	76
5			Cyclohexane, 1-methyl-4-(1-methy...	138	C10H18	001124-25-0	76



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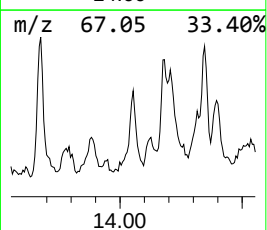
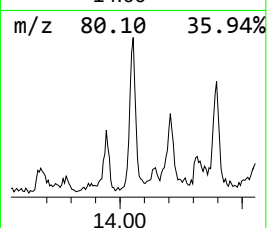
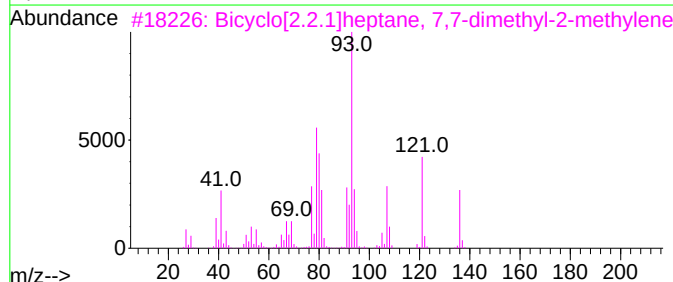
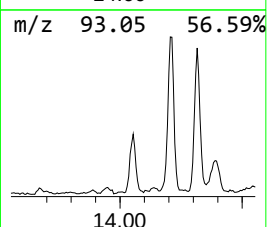
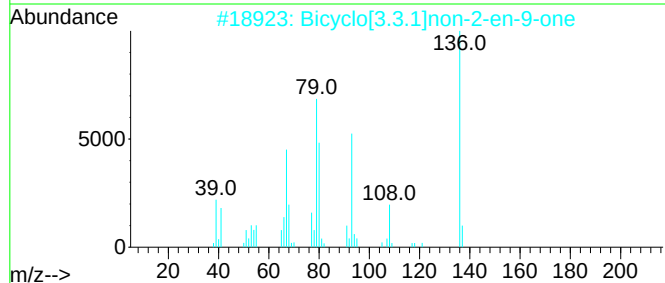
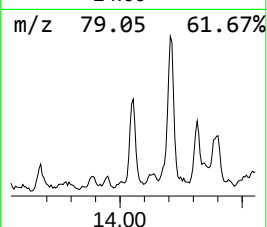
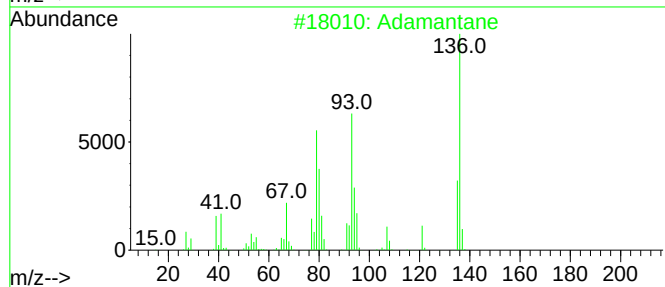
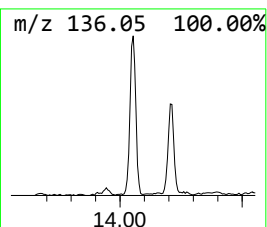
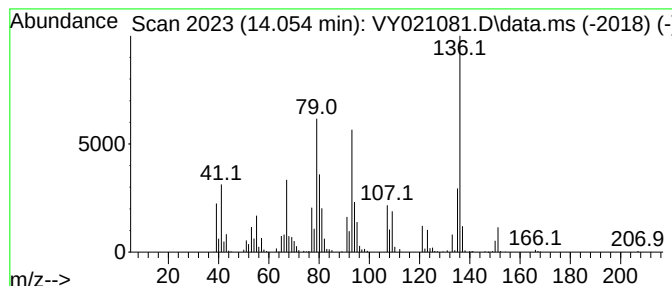
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y020325S.M
Quant Title : SW846 8260

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

Peak Number 2 Adamantane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.054	505.35 ug/l	243779	1,4-Dichlorobenzene-d4	13.352

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Adamantane	136	C10H16	000281-23-2	95
2			Bicyclo[3.3.1]non-2-en-9-one	136	C9H12O	004844-11-5	64
3			Bicyclo[2.2.1]heptane, 7,7-dimet...	136	C10H16	000471-84-1	64
4			Bicyclo[3.3.0]oct-2-en-7-one, 6-...	136	C9H12O	1000150-43-7	62
5			2,5-Methano-1H-indene, octahydro-	136	C10H16	019026-94-9	58



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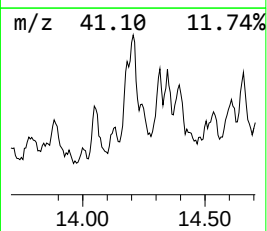
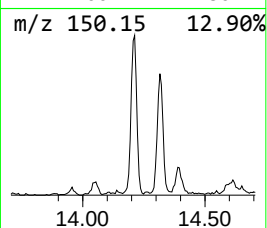
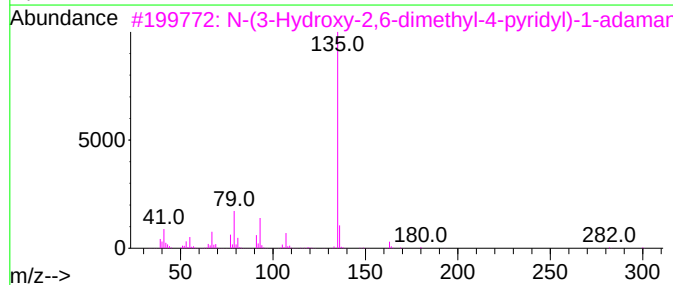
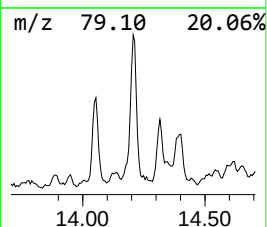
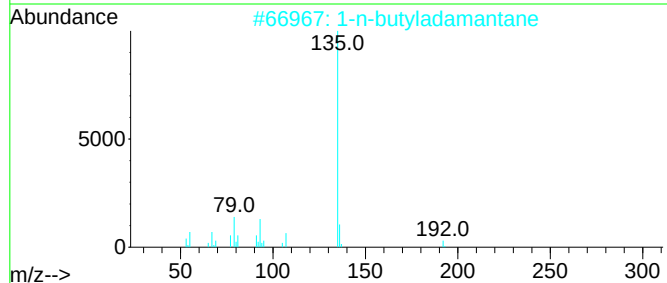
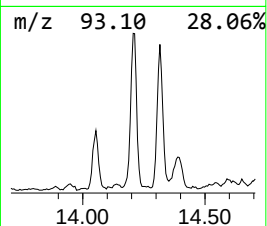
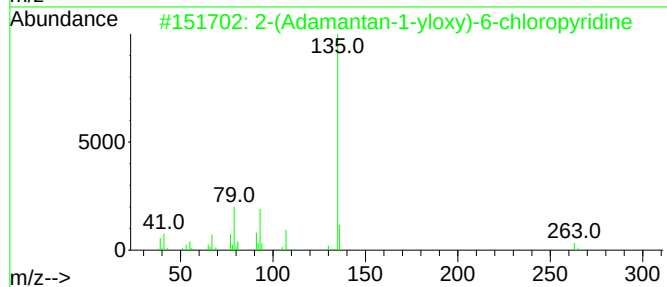
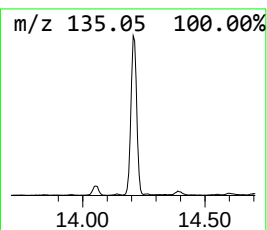
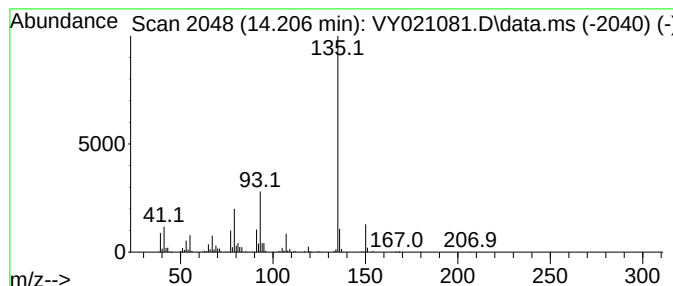
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 2-(Adamantan-1-yloxy)-6-chl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.206	1715.10 ug/l	827365	1,4-Dichlorobenzene-d4	13.352

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(Adamantan-1-yloxy)-6-chloropy...	263	C15H18ClNO	1000411-33-6	80		
2	1-n-butyladamantane	192	C14H24	014449-41-3	80		
3	N-(3-Hydroxy-2,6-dimethyl-4-pyri...	300	C18H24N2O2	1000260-99-3	72		
4	Phosphonic dichloride, 1-adamantyl-	252	C10H15Cl2OP	1000294-15-7	72		
5	1-Iodoadamantane	262	C10H15I	000768-93-4	72		



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MSVOA_Y
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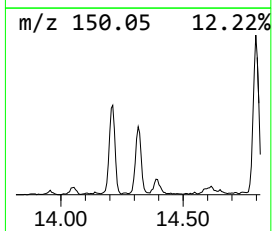
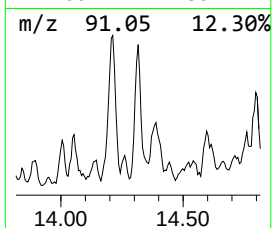
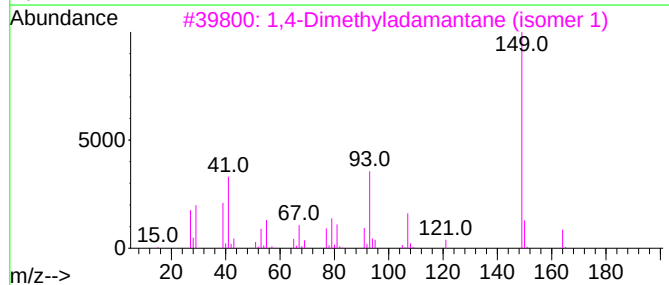
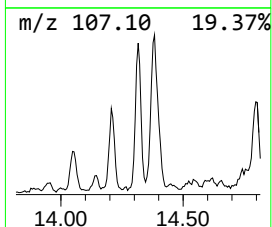
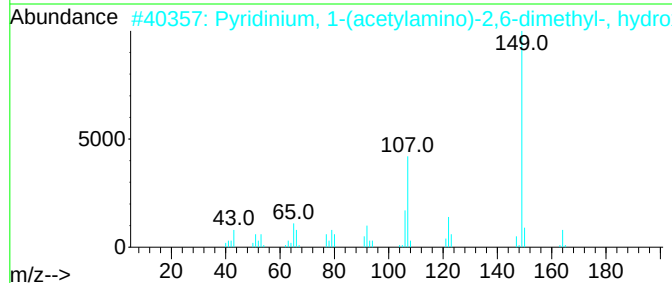
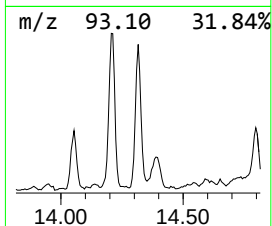
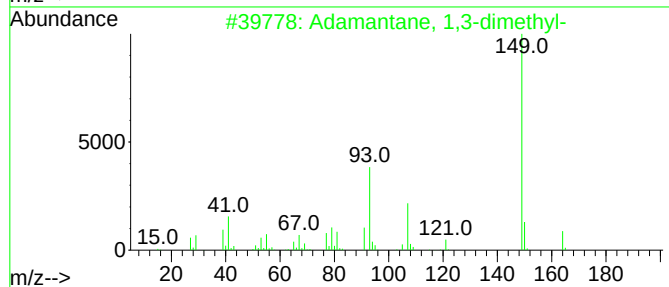
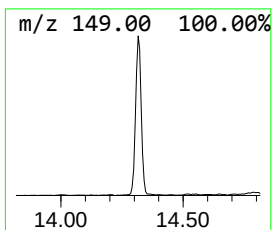
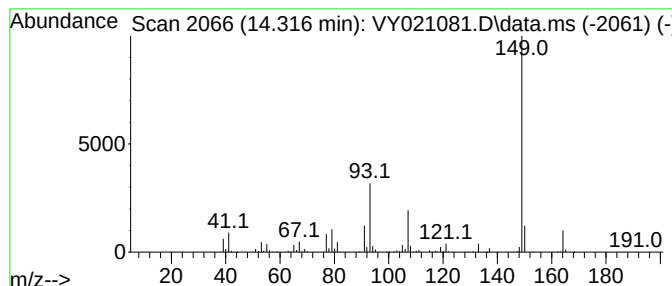
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y020325S.M
Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.316	803.62 ug/l	387665	1,4-Dichlorobenzene-d4	13.352

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	91
2			Pyridinium, 1-(acetylamino)-2,6-...	164	C9H12N2O	031020-35-6	53
3			1,4-Dimethyladamantane (isomer 1)	164	C12H20	1000460-67-0	50
4			1,4-Dimethyladamantane (isomer 2)	164	C12H20	1000460-67-1	49
5			1H-S-Triazolo[1,5-a]pyridin-4-iu...	149	C7H7N3O	013980-64-8	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY020525\
Data File : VY021081.D
Acq On : 05 Feb 2025 12:17
Operator : SY/MD
Sample : Q1261-01
Misc : 5.01g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
CHRT-20430

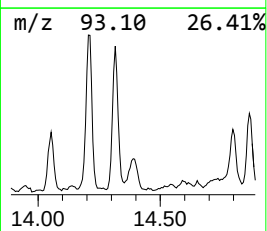
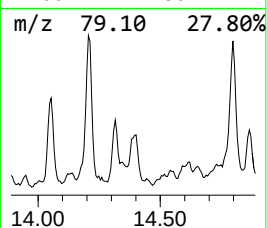
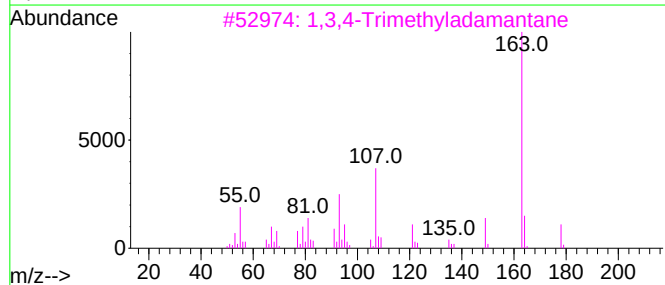
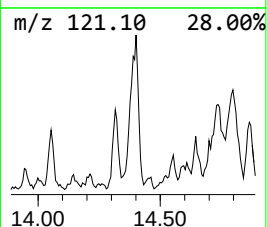
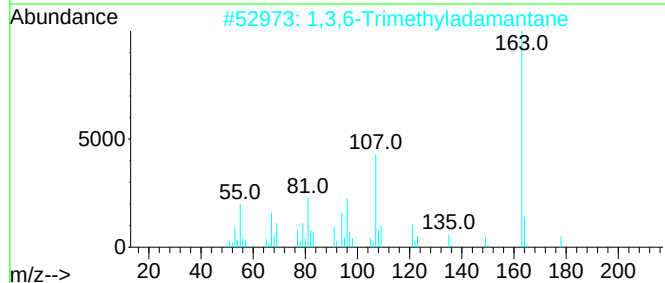
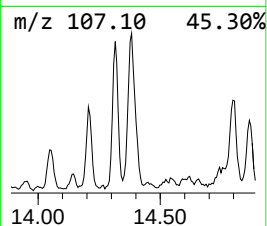
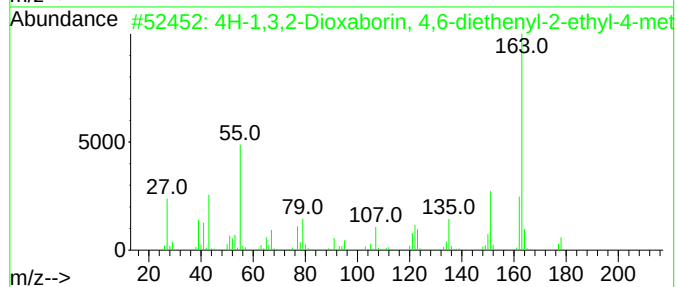
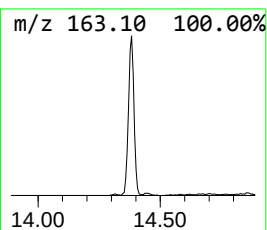
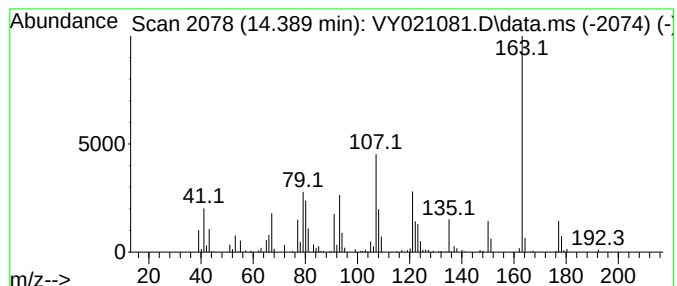
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Quant Title : SW846 8260

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

Peak Number 5 unknown14.389 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.389	611.28 ug/l	294884	1,4-Dichlorobenzene-d4	13.352

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-1,3,2-Dioxaborin, 4,6-diethen...	178	C10H15B02	074630-03-8	46		
2	1,3,6-Trimethyladamantane	178	C13H22	024139-37-5	40		
3	1,3,4-Trimethyladamantane	178	C13H22	1000214-98-3	40		
4	1,3,5-Trimethyladamantane	178	C13H22	000707-35-7	38		
5	1-Tyrophanamide	180	C9H12N2O2	1000131-25-3	37		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY020525\
Data File : VY021081.D
Acq On : 05 Feb 2025 12:17
Operator : SY/MD
Sample : Q1261-01
Misc : 5.01g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
CHRT-20430

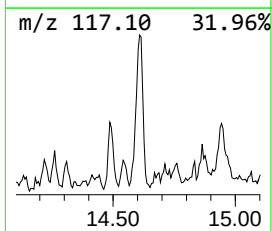
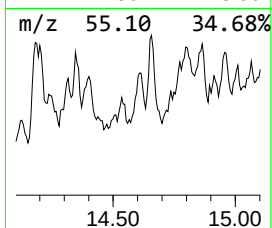
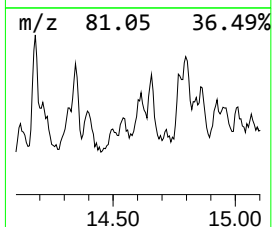
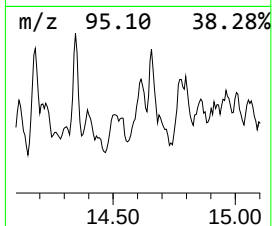
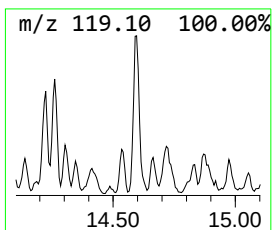
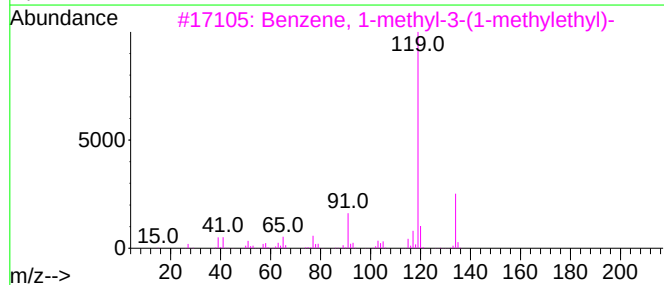
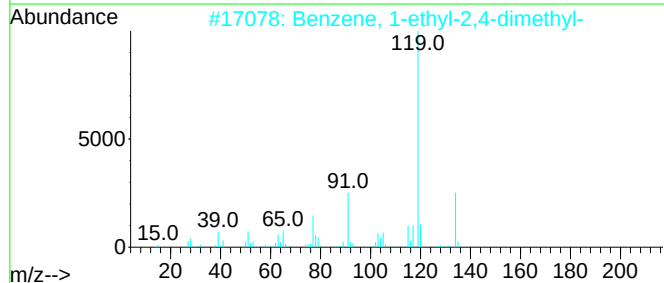
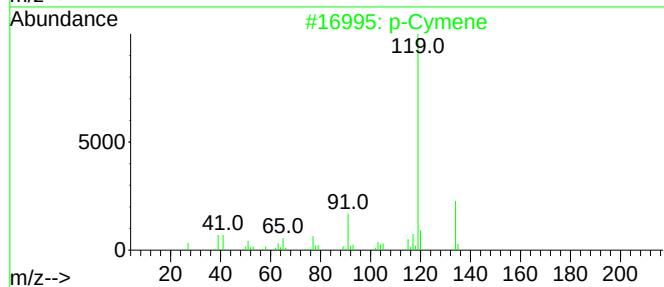
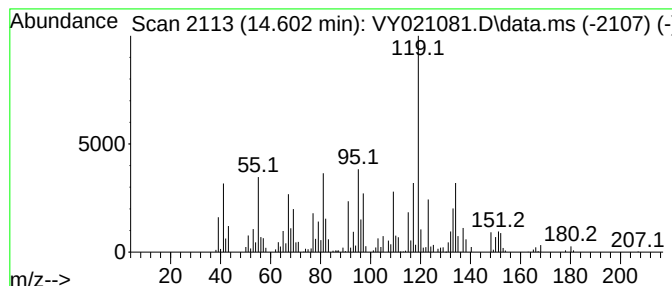
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Quant Title : SW846 8260

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

Peak Number 6 unknown14.602 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.602	566.09 ug/l	273081	1,4-Dichlorobenzene-d4	13.352

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			p-Cymene	134	C10H14	000099-87-6	42
2			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	42
3			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	38
4			o-Cymene	134	C10H14	000527-84-4	38
5			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY020525\
Data File : VY021081.D
Acq On : 05 Feb 2025 12:17
Operator : SY/MD
Sample : Q1261-01
Misc : 5.01g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
CHRT-20430

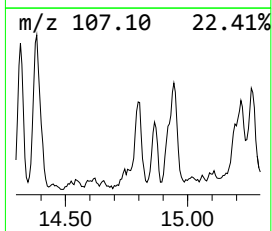
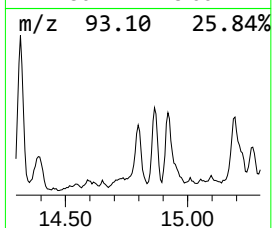
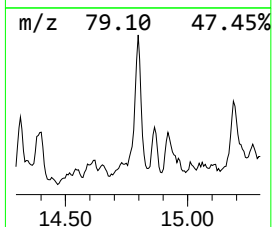
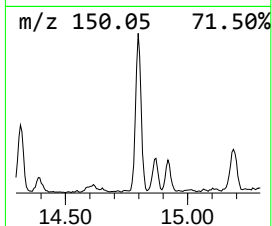
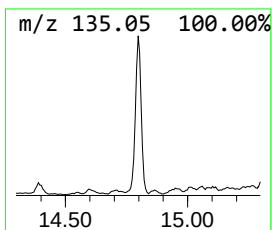
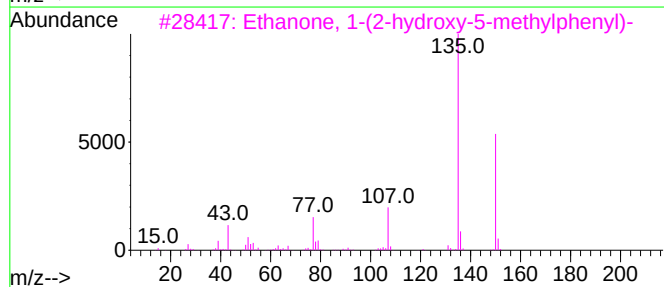
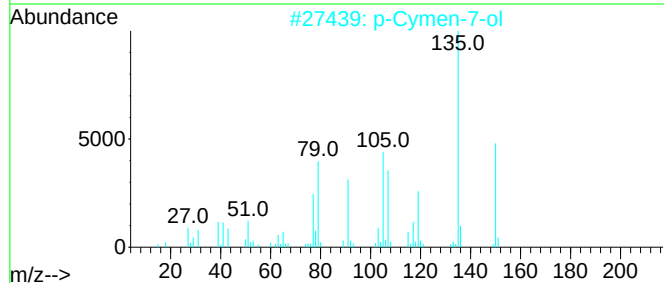
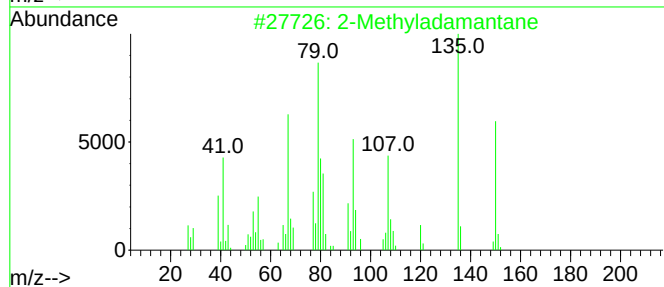
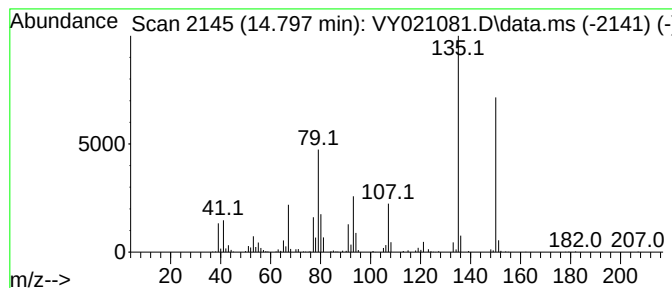
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 2-Methyladamantane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.797	553.58 ug/l	267048	1,4-Dichlorobenzene-d4	13.352

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methyladamantane	150	C11H18	000700-56-1	78
2			p-Cymen-7-ol	150	C10H14O	000536-60-7	50
3			Ethanone, 1-(2-hydroxy-5-methylp...	150	C9H10O2	001450-72-2	50
4			4-Hydroxy-3-methylacetophenone	150	C9H10O2	000876-02-8	47
5			Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY020525\
Data File : VY021081.D
Acq On : 05 Feb 2025 12:17
Operator : SY/MD
Sample : Q1261-01
Misc : 5.01g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
CHRT-20430

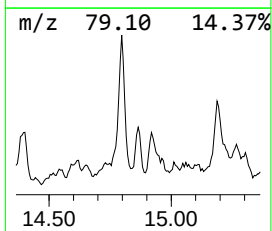
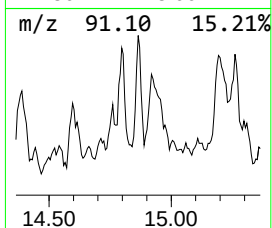
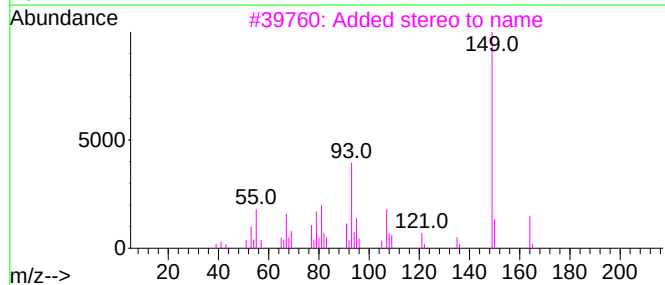
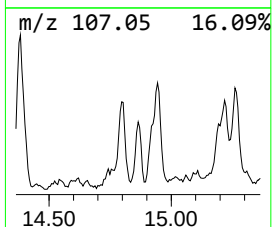
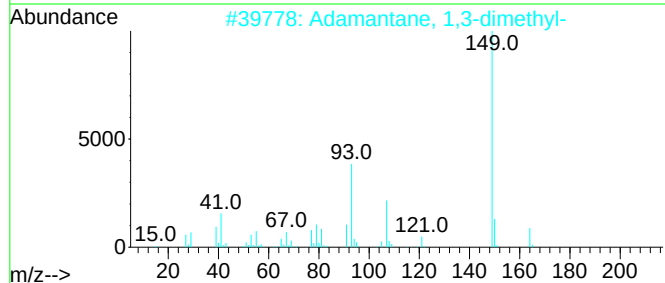
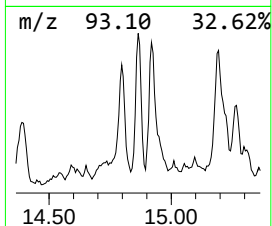
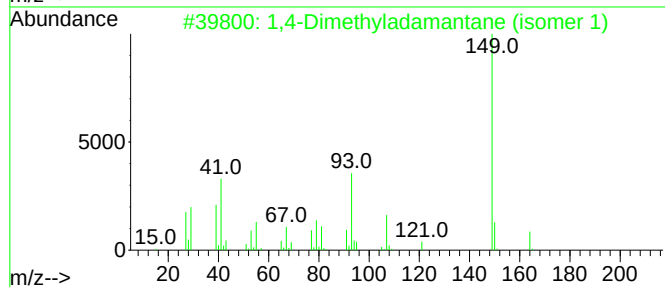
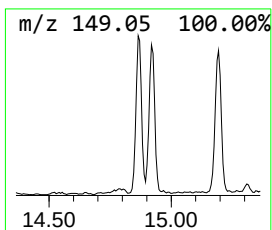
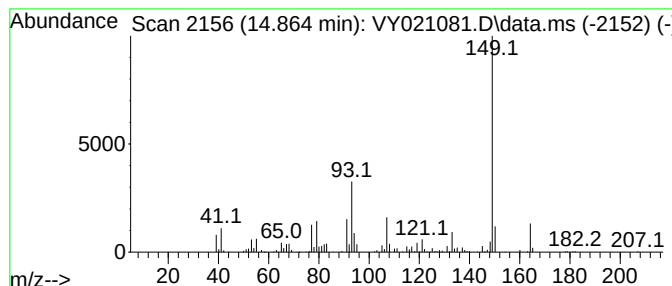
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Quant Title : SW846 8260

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.
14.864	498.71 ug/l	240580	1,4-Dichlorobenzene-d4	13.352

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,4-Dimethyladamantane (isomer 1)	164	C12H20	1000460-67-0	91
2		Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	87
3		Added stereo to name	164	C12H20	024145-88-8	83
4		Added stereo to name	164	C12H20	024145-89-9	80
5		Adamantane, 1-isothiocyanato-3-m...	207	C12H17NS	136860-48-5	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY020525\
Data File : VY021081.D
Acq On : 05 Feb 2025 12:17
Operator : SY/MD
Sample : Q1261-01
Misc : 5.01g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
CHRT-20430

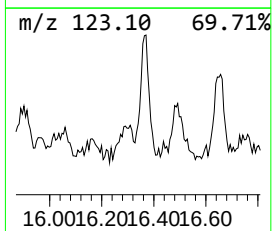
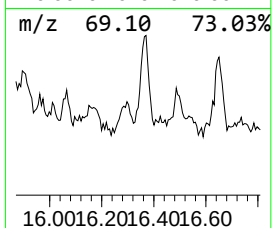
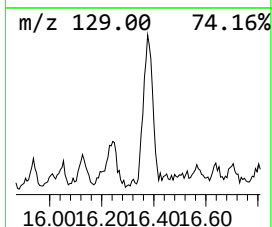
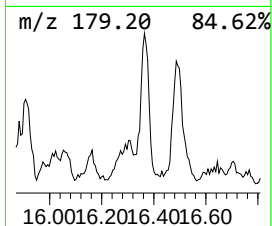
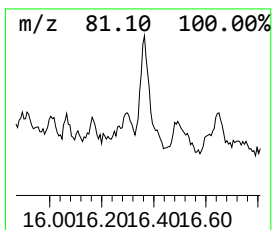
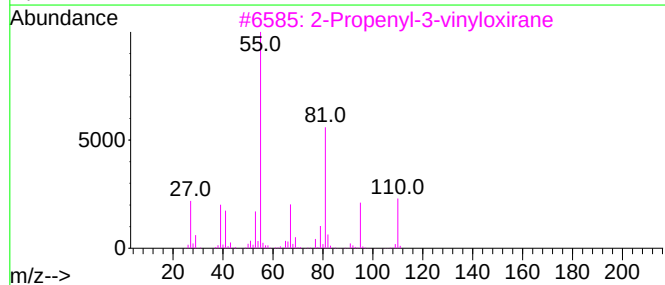
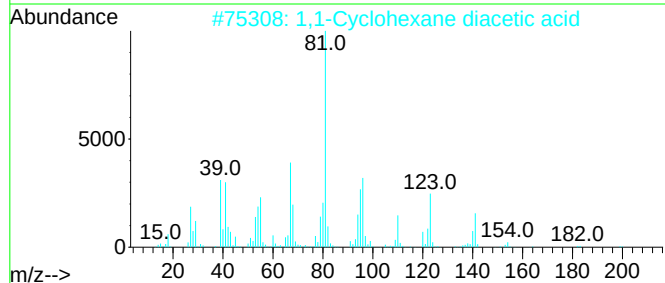
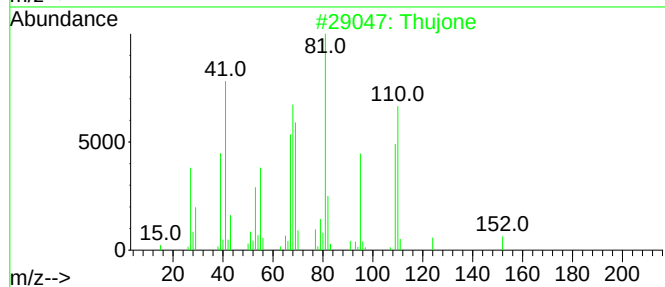
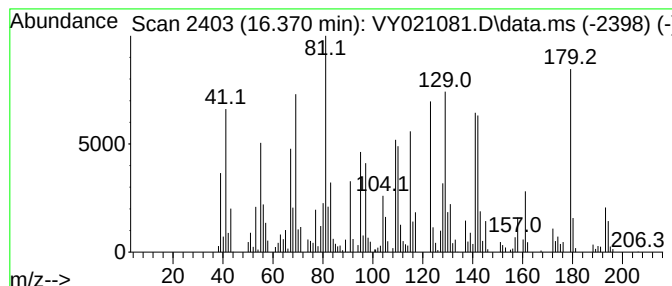
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Quant Title : SW846 8260

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

Peak Number 10 unknown16.370 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.370	534.12 ug/l	257661	1,4-Dichlorobenzene-d4	13.352

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thujone	152	C10H16O	000546-80-5	30
2			1,1-Cyclohexane diacetic acid	200	C10H16O4	009355-11-7	16
3			2-Propenyl-3-vinyloxirane	110	C7H10O	070597-49-8	14
4			Cyclopentane, 1-ethenyl-3-ethyl-...	138	C10H18	055170-98-4	14
5			trans-Chrysanthemal	152	C10H16O	020104-05-6	11



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY020525\
Data File : VY021081.D
Acq On : 05 Feb 2025 12:17
Operator : SY/MD
Sample : Q1261-01
Misc : 5.01g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
CHRT-20430

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y020325S.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
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Adamantane	14.054	505.4	ug/l	243779	4	13.352	24120	50.0
2-(Adamantan-1-...	14.206	1715.1	ug/l	827365	4	13.352	24120	50.0
Adamantane, 1,3...	14.316	803.6	ug/l	387665	4	13.352	24120	50.0
unknown14.389	14.389	611.3	ug/l	294884	4	13.352	24120	50.0
unknown14.602	14.602	566.1	ug/l	273081	4	13.352	24120	50.0
2-Methyladamantane	14.797	553.6	ug/l	267048	4	13.352	24120	50.0
1,4-Dimethylada...	14.864	498.7	ug/l	240580	4	13.352	24120	50.0
unknown16.370	16.370	534.1	ug/l	257661	4	13.352	24120	50.0