

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY081523\
 Data File : VY015101.D
 Acq On : 15 Aug 2023 14:20
 Operator : SY/MD
 Sample : 03961-03
 Misc : 5.01g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 20071

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\82Y081423S.M
 Title : SW846 8260

Signal : TIC: VY015101.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.211	59	64	72	rBV3	8399	14441	1.84%	0.134%
2	3.948	338	349	359	rBV2	12536	34514	4.40%	0.321%
3	4.704	463	473	489	rBV	27795	87638	11.16%	0.814%
4	4.948	494	513	529	rBV3	40224	173430	22.09%	1.611%
5	5.741	632	643	654	rVB2	6637	21422	2.73%	0.199%
6	6.972	830	845	866	rBV	250641	738083	93.99%	6.854%
7	7.259	882	892	903	rVB2	30192	77835	9.91%	0.723%
8	7.710	955	966	972	rBV	112029	265850	33.85%	2.469%
9	7.783	972	978	989	rVB	186338	419313	53.40%	3.894%
10	8.136	1027	1036	1047	rBV	115538	250876	31.95%	2.330%
11	8.234	1047	1052	1060	rVV3	5624	12507	1.59%	0.116%
12	8.319	1060	1066	1074	rVB2	5072	11822	1.51%	0.110%
13	8.551	1096	1104	1114	rBV	6907	16187	2.06%	0.150%
14	8.685	1118	1126	1137	rBV	286948	564424	71.88%	5.241%
15	9.069	1183	1189	1193	rBV3	6728	13117	1.67%	0.122%
16	9.130	1193	1199	1206	rBV	24242	48873	6.22%	0.454%
17	9.270	1213	1222	1233	rVB5	3912	13693	1.74%	0.127%
18	9.447	1245	1251	1256	rBV	14763	28370	3.61%	0.263%
19	9.514	1256	1262	1272	rVB	29521	59532	7.58%	0.553%
20	9.612	1272	1278	1286	rBV4	4573	9869	1.26%	0.092%
21	9.746	1293	1300	1306	rVB3	5947	12781	1.63%	0.119%
22	9.972	1324	1337	1347	rBV3	11892	34708	4.42%	0.322%
23	10.069	1347	1353	1357	rBV2	11241	21299	2.71%	0.198%
24	10.179	1363	1371	1377	rBV	452029	785268	100.00%	7.292%
25	10.240	1377	1381	1386	rVB	21976	32928	4.19%	0.306%
26	10.368	1394	1402	1408	rVB5	4680	10315	1.31%	0.096%
27	10.490	1416	1422	1431	rVB8	4953	13001	1.66%	0.121%
28	10.715	1449	1459	1468	rVB3	25668	64682	8.24%	0.601%
29	10.831	1468	1478	1483	rBV	31656	57858	7.37%	0.537%
30	10.935	1490	1495	1500	rBV2	15717	27991	3.56%	0.260%
31	11.374	1564	1567	1576	rVB5	4256	9855	1.25%	0.092%
32	11.490	1576	1586	1596	rBV	451025	737323	93.89%	6.847%
33	11.587	1596	1602	1610	rBV2	23842	49066	6.25%	0.456%
34	11.697	1614	1620	1625	rBV	57315	109483	13.94%	1.017%
35	11.807	1631	1638	1642	rVB7	4828	8640	1.10%	0.080%
36	12.026	1669	1674	1682	rVB	41185	66550	8.47%	0.618%

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37	12.105	1682	1687	1693	rBV	22980	34783	4.43%	0.323%
38	12.203	1697	1703	1706	rBV5	10782	18478	2.35%	0.172%
39	12.416	1730	1738	1742	rBV7	9263	19102	2.43%	0.177%
40	12.477	1742	1748	1755	rVV	364185	582329	74.16%	5.408%
41	12.599	1764	1768	1776	rBV3	19336	36663	4.67%	0.340%
42	12.666	1777	1779	1784	rVB2	8210	11497	1.46%	0.107%
43	12.733	1784	1790	1793	rBV	31307	54294	6.91%	0.504%
44	12.806	1798	1802	1809	rVB2	61311	95263	12.13%	0.885%
45	12.971	1819	1829	1832	rBV5	11674	33989	4.33%	0.316%
46	13.117	1848	1853	1858	rBV	47436	75500	9.61%	0.701%
47	13.160	1858	1860	1864	rBV3	8354	11144	1.42%	0.103%
48	13.312	1872	1885	1890	rBV10	24456	70808	9.02%	0.658%
49	13.361	1890	1893	1895	rBV4	7200	9825	1.25%	0.091%
50	13.422	1896	1903	1912	rVV	446222	717164	91.33%	6.660%
51	13.526	1912	1920	1929	rVB3	46026	94405	12.02%	0.877%
52	13.617	1930	1935	1939	rBV4	20361	44382	5.65%	0.412%
53	13.751	1951	1957	1967	rBV4	91309	198833	25.32%	1.846%
54	13.855	1970	1974	1977	rBV4	16741	30645	3.90%	0.285%
55	13.965	1987	1992	1998	rVB6	43390	68637	8.74%	0.637%
56	14.081	2005	2011	2014	rBV5	40009	74887	9.54%	0.695%
57	14.129	2014	2019	2027	rVV7	59620	143695	18.30%	1.334%
58	14.209	2027	2032	2035	rBV6	32643	65767	8.38%	0.611%
59	14.282	2036	2044	2050	rBV2	145041	382512	48.71%	3.552%
60	14.391	2056	2062	2065	rBV	135279	254529	32.41%	2.364%
61	14.465	2070	2074	2081	rVB4	96252	212482	27.06%	1.973%
62	14.611	2095	2098	2103	rVB4	67319	98247	12.51%	0.912%
63	14.678	2103	2109	2114	rBV4	113419	310809	39.58%	2.886%
64	14.733	2114	2118	2123	rVB4	122060	211797	26.97%	1.967%
65	14.873	2138	2141	2147	rVB	159423	229291	29.20%	2.129%
66	14.940	2148	2152	2156	rVB2	176196	261294	33.27%	2.426%
67	15.001	2157	2162	2165	rBV	154204	300234	38.23%	2.788%
68	15.282	2203	2208	2214	rBV4	171157	480808	61.23%	4.465%
69	16.476	2399	2404	2410	rBV6	314799	631027	80.36%	5.860%

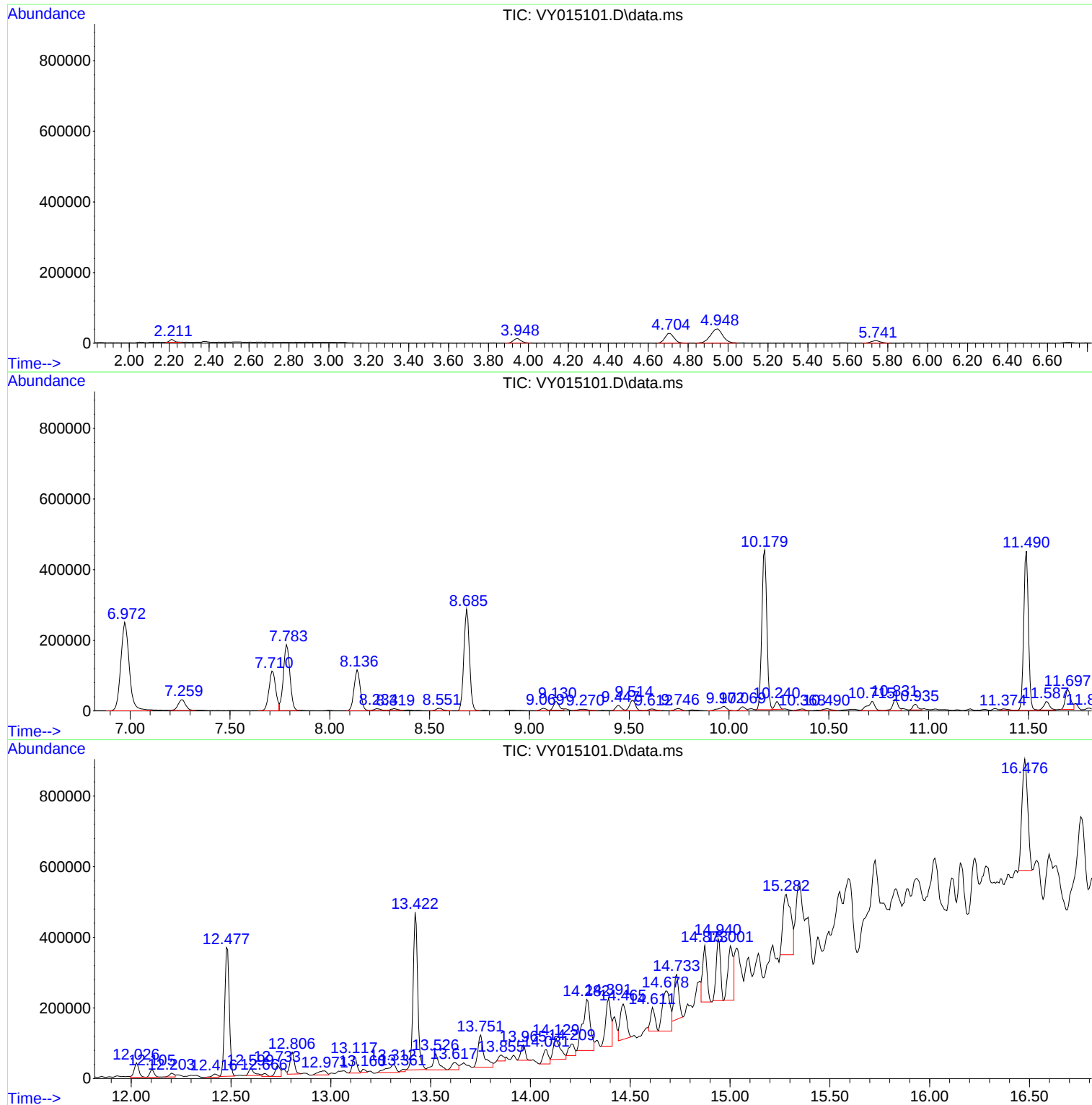
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y081423S.M
Quant Title : SW846 8260

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



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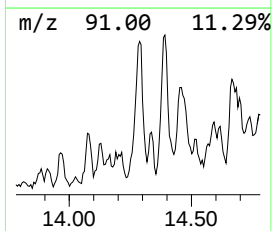
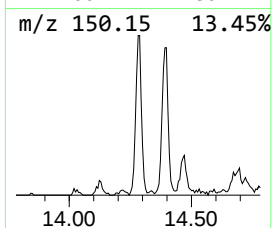
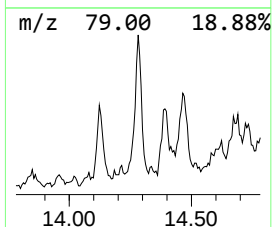
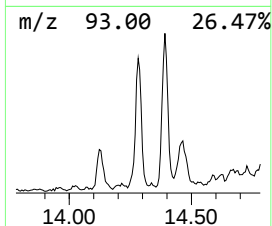
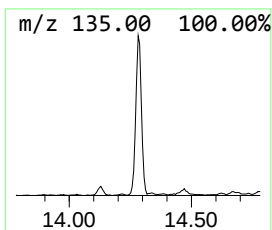
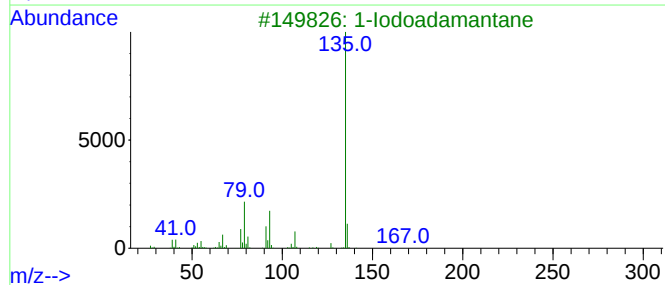
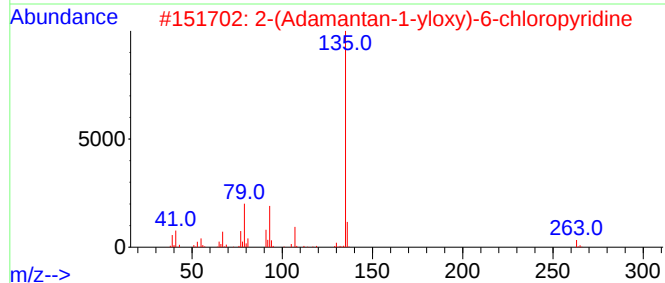
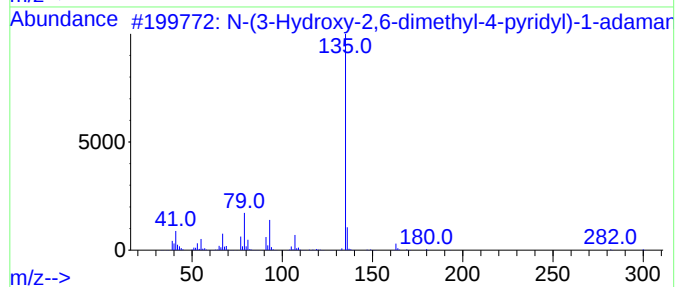
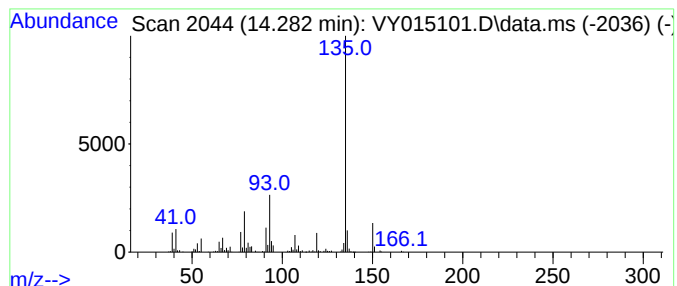
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y081423S.M
Quant Title : SW846 8260

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

Peak Number 1 N-(3-Hydroxy-2,6-dimethyl-4... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.282	26.67 ug/l	382512	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N-(3-Hydroxy-2,6-dimethyl-4-pyri...	300	C18H24N2O2	1000260-99-3	72
2			2-(Adamantan-1-yloxy)-6-chloropy...	263	C15H18ClNO	1000411-33-6	72
3			1-Iodoadamantane	262	C10H15I	000768-93-4	72
4			Phosphonic dichloride, 1-adamantyl-	252	C10H15Cl2OP	1000294-15-7	72
5			Heptafluorobutanoic acid, 1-adam...	362	C15H17F7O2	1000282-96-9	72



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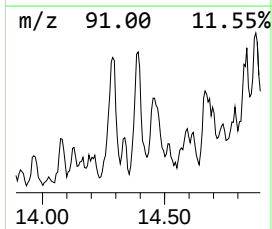
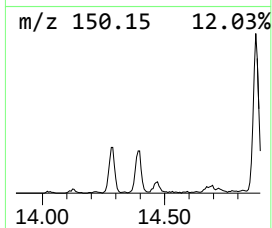
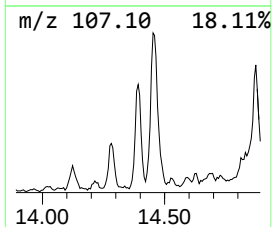
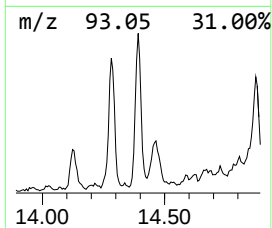
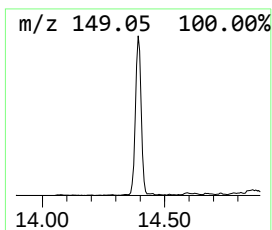
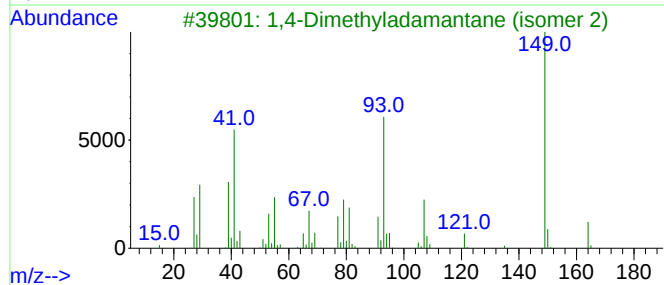
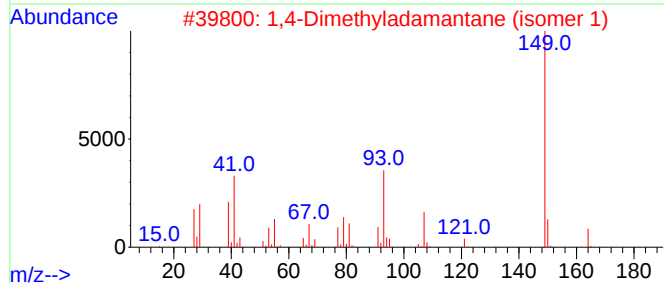
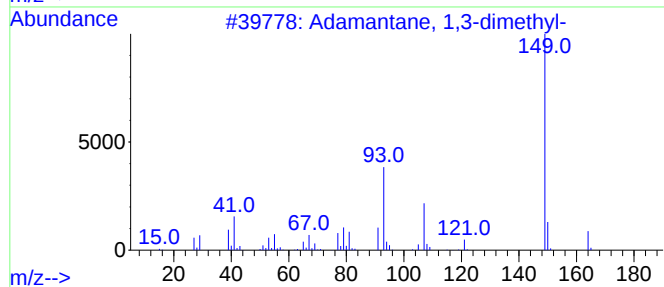
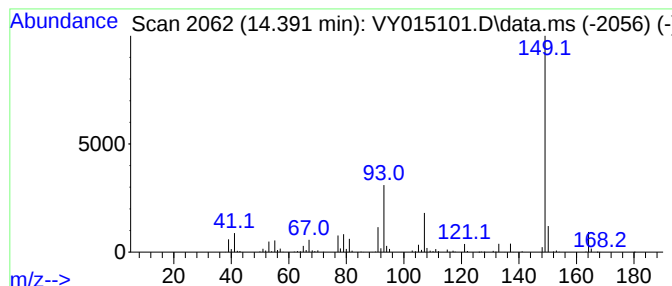
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y081423S.M
Quant Title : SW846 8260

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

Peak Number 2 Adamantane, 1,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.392	17.75 ug/l	254529	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	93
2			1,4-Dimethyladamantane (isomer 1)	164	C12H20	1000460-67-0	87
3			1,4-Dimethyladamantane (isomer 2)	164	C12H20	1000460-67-1	86
4			Pyridine, pentamethyl-	149	C10H15N	003748-83-2	59
5			Pyridinium, 1-(acetylamino)-2,6-...	164	C9H12N2O	031020-35-6	58



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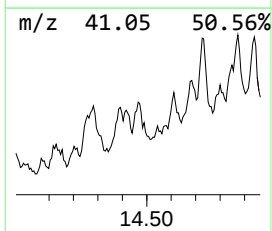
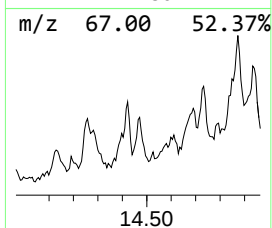
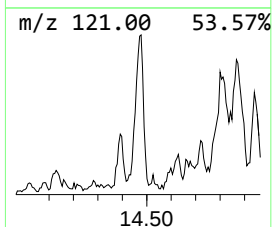
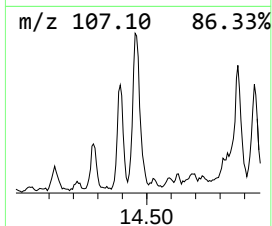
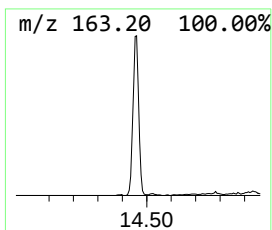
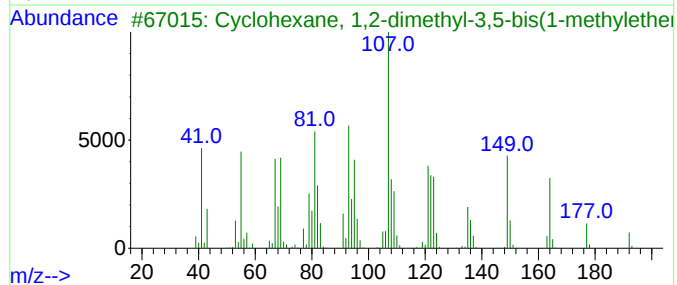
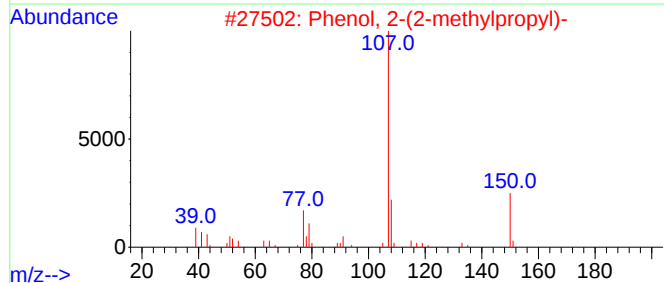
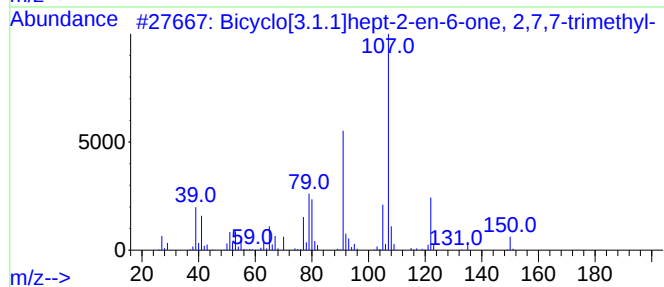
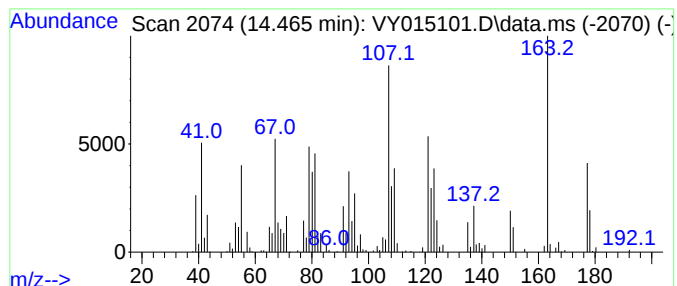
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 unknown14.465 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.465	14.81 ug/l	212482	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[3.1.1]hept-2-en-6-one, 2...	150	C10H14O	000473-06-3	22
2			Phenol, 2-(2-methylpropyl)-	150	C10H14O	004167-75-3	14
3			Cyclohexane, 1,2-dimethyl-3,5-bi...	192	C14H24	074806-55-6	14
4			5,8-Decadien-2-one, 5,9-dimethyl...	180	C12H20O	130876-99-2	11
5			1,6(2H,7H)-Naphthalenedione, 3,4...	178	C11H14O2	020007-72-1	11



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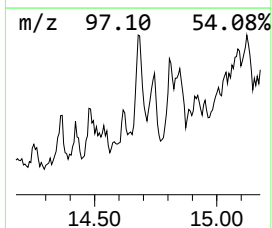
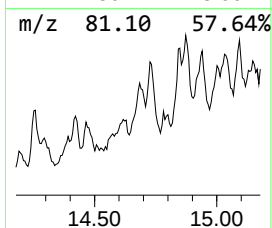
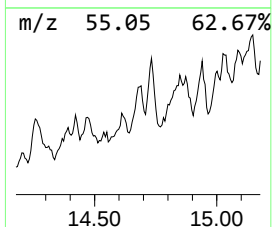
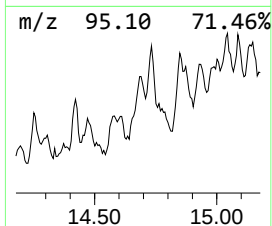
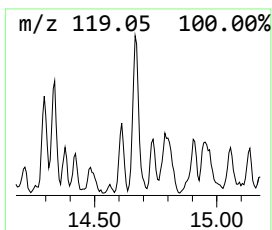
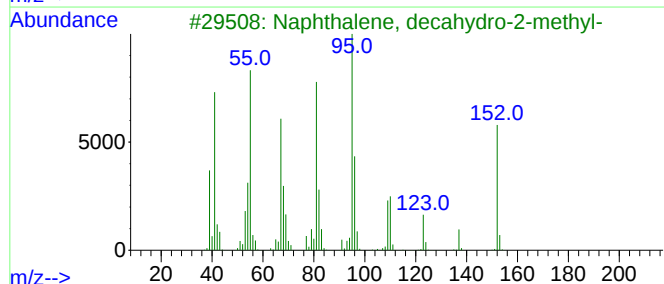
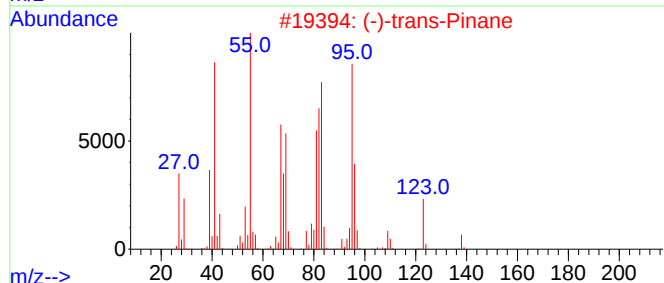
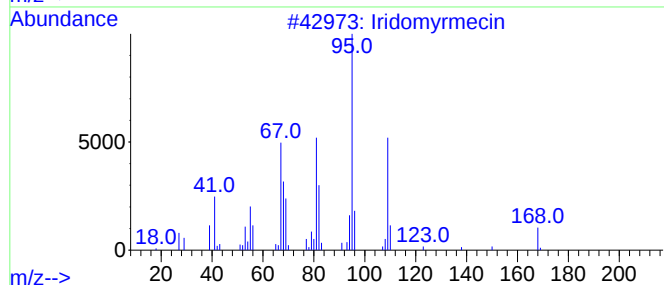
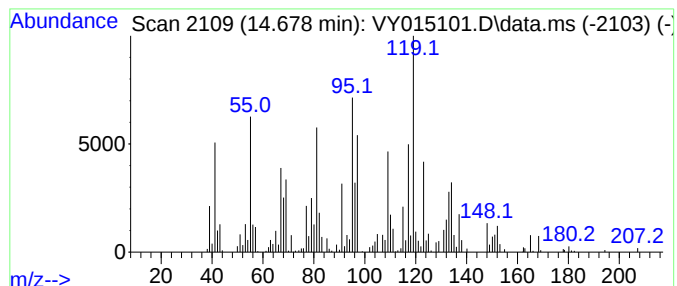
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Peak Number 4 unknown14.678 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.678	21.67 ug/l	310809	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Iridomyrmecin	168	C10H16O2	000485-43-8	38
2			(-)-trans-Pinane	138	C10H18	033626-25-4	35
3			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	35
4			Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	000473-19-8	25
5			trans-1,4-Cyclohexanedimethanol,...	436	C14H14F10O4	1010384-27-9	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY081523\
Data File : VY015101.D
Acq On : 15 Aug 2023 14:20
Operator : SY/MD
Sample : 03961-03
Misc : 5.01g/5.0mL/MSVOA_Y/soil
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
20071

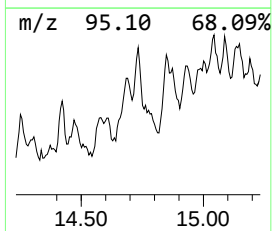
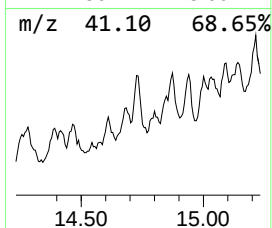
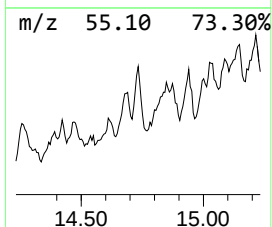
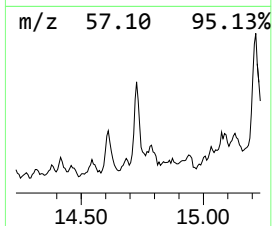
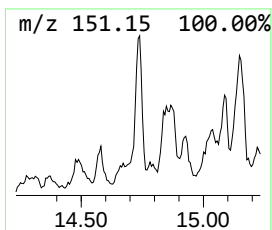
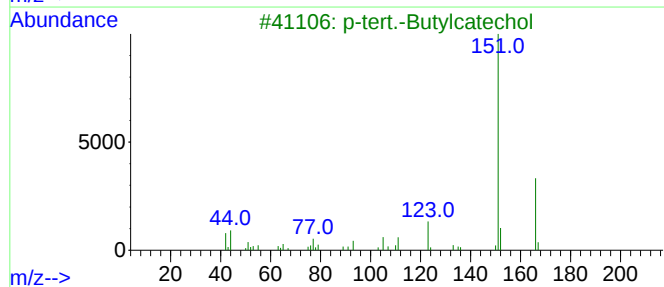
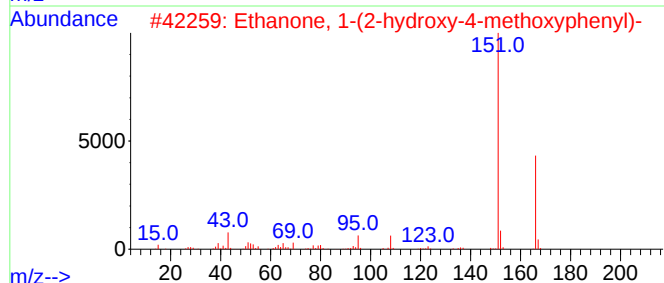
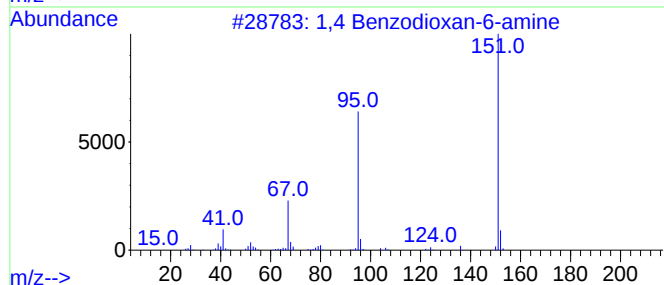
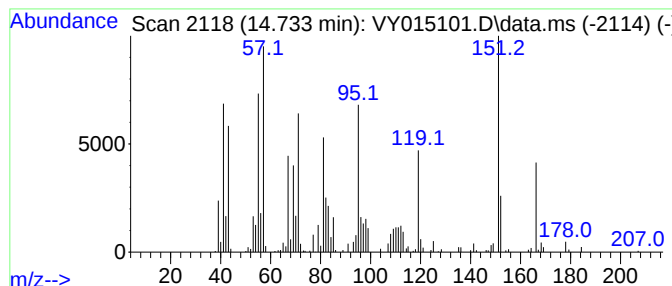
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Quant Title : SW846 8260

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

Peak Number 5 unknown14.733 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.733	14.77 ug/l	211797	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4 Benzodioxan-6-amine	151	C8H9NO2	022013-33-8	35
2			Ethanone, 1-(2-hydroxy-4-methoxy...	166	C9H10O3	000552-41-0	27
3			p-tert.-Butylcatechol	166	C10H14O2	000098-29-3	27
4			Naphthalene, decahydro-1,6-dimet...	166	C12H22	001750-51-2	25
5			Apocynin	166	C9H10O3	000498-02-2	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY081523\
Data File : VY015101.D
Acq On : 15 Aug 2023 14:20
Operator : SY/MD
Sample : 03961-03
Misc : 5.01g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
20071

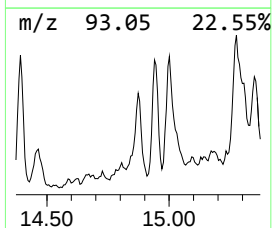
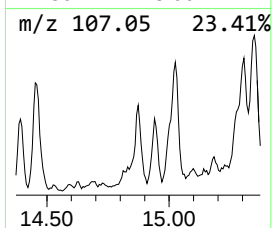
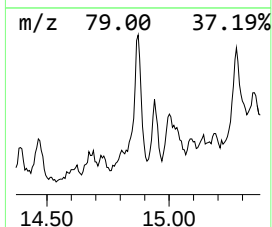
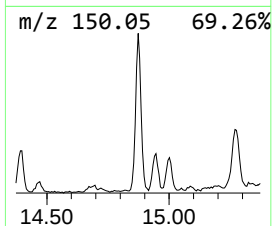
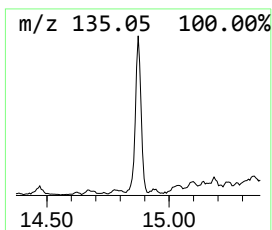
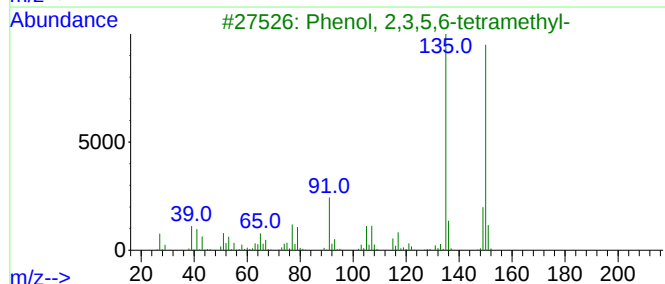
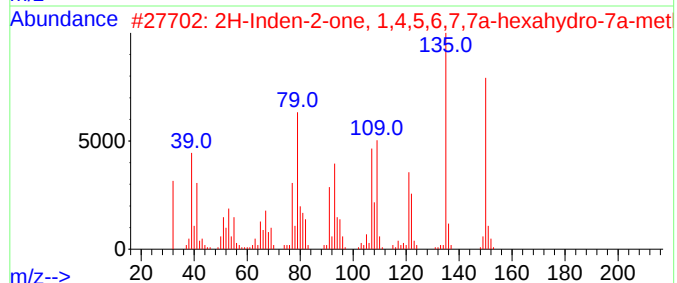
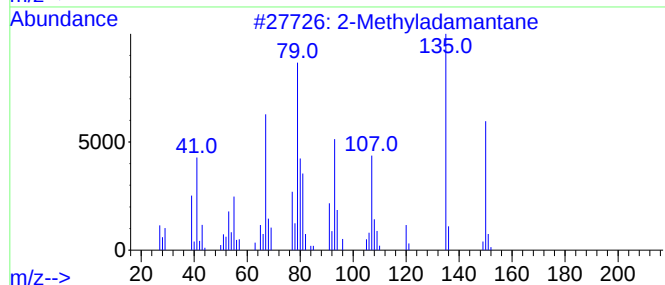
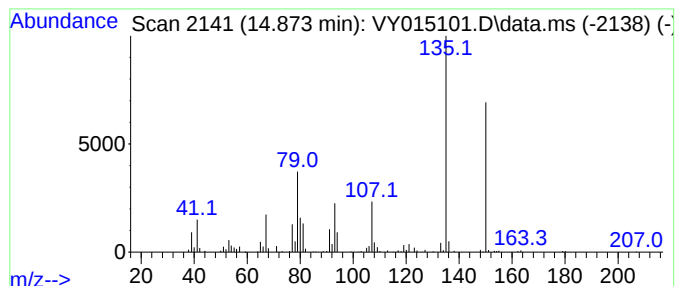
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Quant Title : SW846 8260

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

Peak Number 6 2H-Inden-2-one, 1,4,5,6,7,7... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.873	15.99 ug/l	229291	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methyladamantane	150	C11H18	000700-56-1	87
2			2H-Inden-2-one, 1,4,5,6,7,7a-hex...	150	C10H14O	054725-16-5	78
3			Phenol, 2,3,5,6-tetramethyl-	150	C10H14O	000527-35-5	50
4			3-Adamantanecarboxylic acid, phe...	256	C17H20O2	035856-79-2	50
5			Ethanone, 1-(2-hydroxy-5-methylp...	150	C9H10O2	001450-72-2	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY081523\
Data File : VY015101.D
Acq On : 15 Aug 2023 14:20
Operator : SY/MD
Sample : 03961-03
Misc : 5.01g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
20071

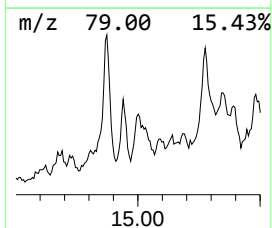
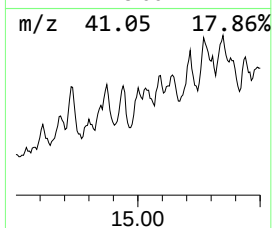
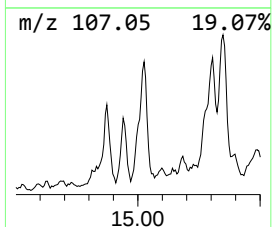
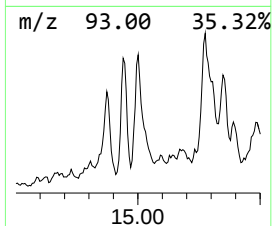
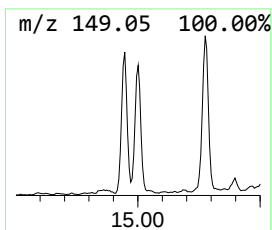
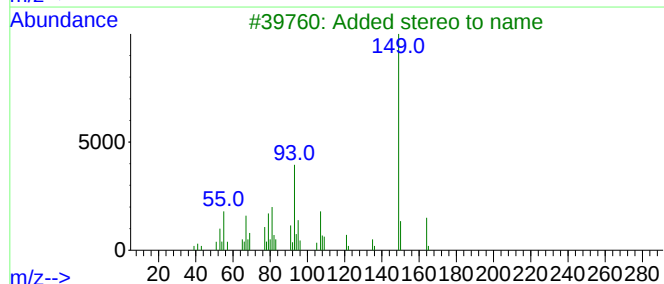
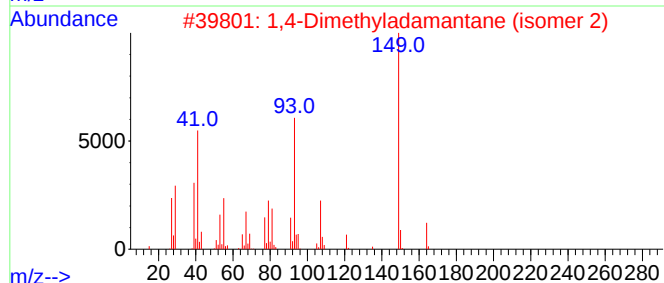
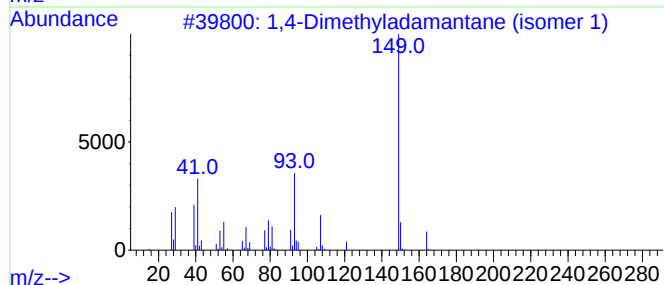
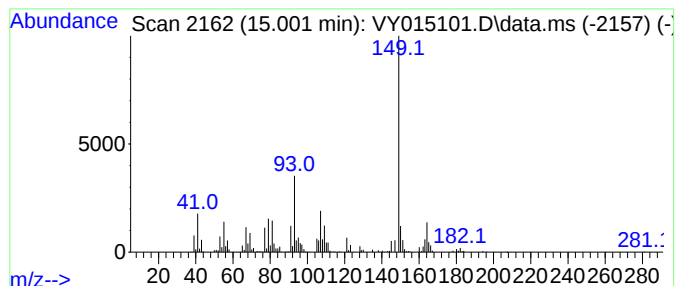
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Quant Title : SW846 8260

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

Peak Number 8 1,4-Dimethyladamantane (iso... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.001	20.93 ug/l	300234	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	95
2		1,4-Dimethyladamantane (isomer 2)	164	C12H20	1000460-67-1	87
3		Added stereo to name	164	C12H20	024145-88-8	87
4		Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	81
5		1-Methyl-3-ethyladamantane	178	C13H22	001687-34-9	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY081523\
Data File : VY015101.D
Acq On : 15 Aug 2023 14:20
Operator : SY/MD
Sample : 03961-03
Misc : 5.01g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
20071

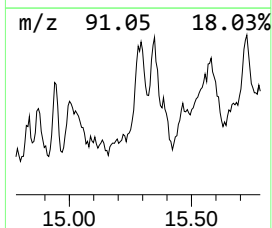
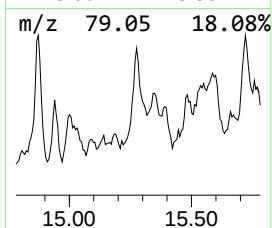
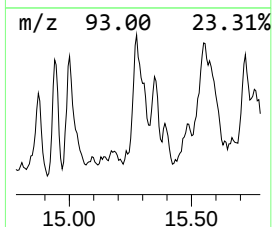
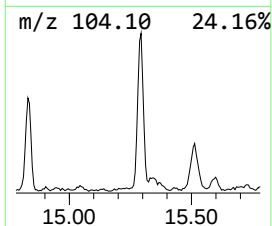
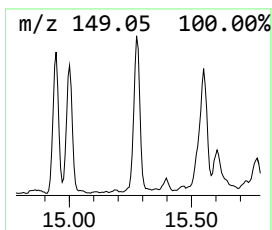
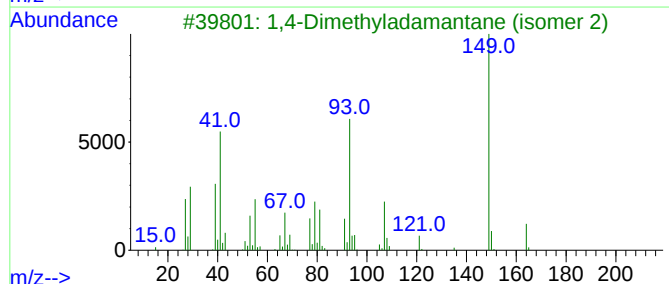
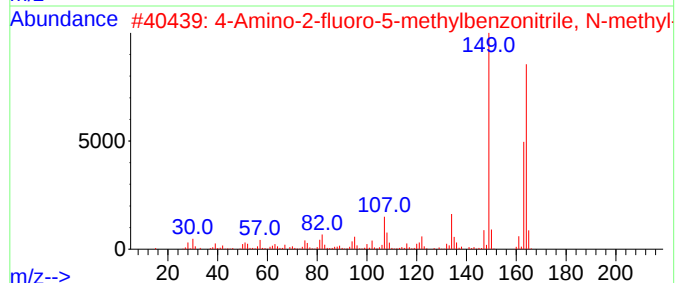
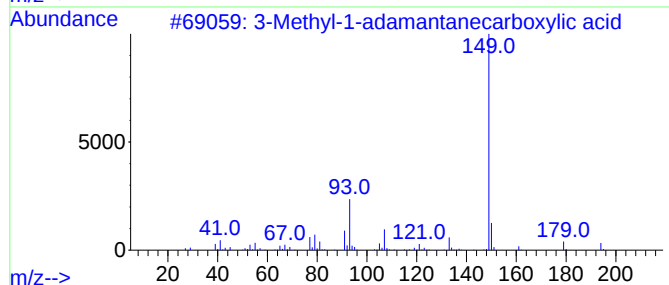
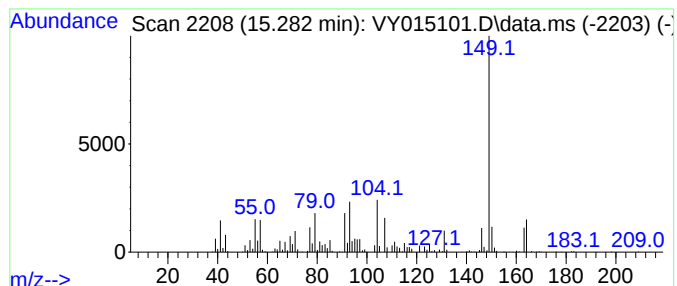
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Quant Title : SW846 8260

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

Peak Number 9 3-Methyl-1-adamantanecarbox... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.281	33.52 ug/l	480808	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Methyl-1-adamantanecarboxylic ...	194	C12H18O2	1000504-38-9	50
2			4-Amino-2-fluoro-5-methylbenzoni...	164	C9H9FN2	1000511-36-9	50
3			1,4-Dimethyladamantane (isomer 2)	164	C12H20	1000460-67-1	49
4			4-(2-Methyl-cyclohex-1-enyl)-but...	164	C11H16O	041437-92-7	47
5			Pyridine, pentamethyl-	149	C10H15N	003748-83-2	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY081523\
Data File : VY015101.D
Acq On : 15 Aug 2023 14:20
Operator : SY/MD
Sample : 03961-03
Misc : 5.01g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
20071

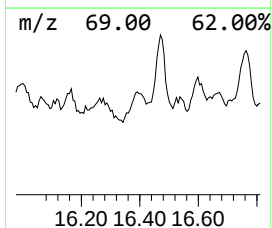
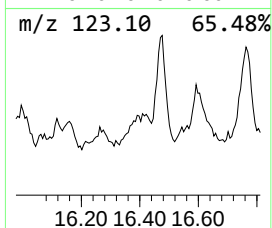
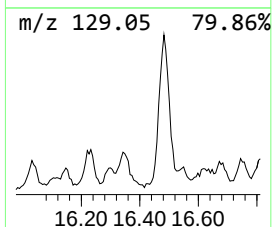
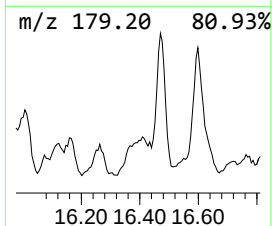
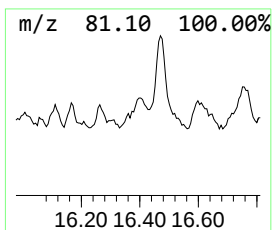
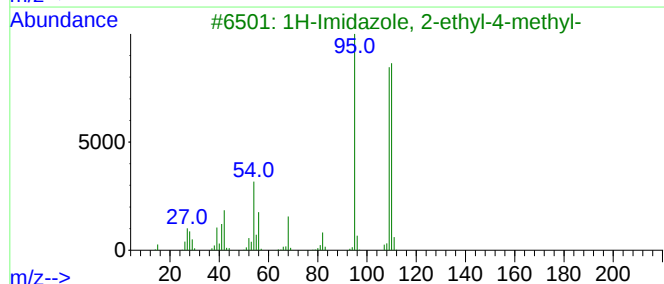
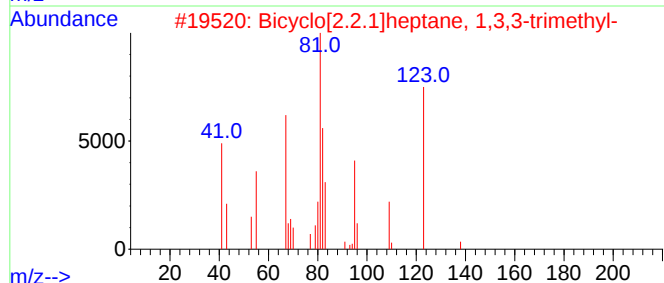
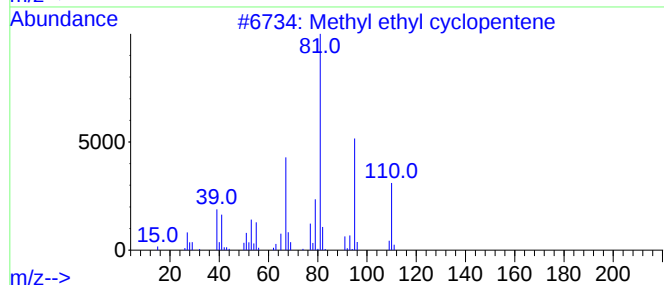
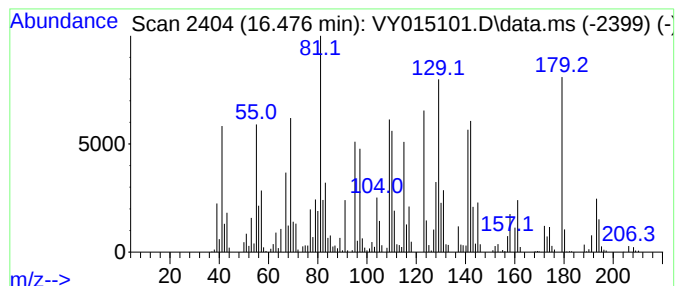
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Quant Title : SW846 8260

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

Peak Number 10 unknown16.476 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.476	43.99 ug/l	631027	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl ethyl cyclopentene	110	C8H14	019780-56-4	18
2			Bicyclo[2.2.1]heptane, 1,3,3-tri...	138	C10H18	006248-88-0	18
3			1H-Imidazole, 2-ethyl-4-methyl-	110	C6H10N2	000931-36-2	15
4			3-Heptyne, 5-methyl-	110	C8H14	061228-09-9	14
5			2-Propenyl-3-vinylloxirane	110	C7H10O	070597-49-8	14



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY081523\
Data File : VY015101.D
Acq On : 15 Aug 2023 14:20
Operator : SY/MD
Sample : 03961-03
Misc : 5.01g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
20071

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y081423S.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, 1,3...	14.392	17.8	ug/l	254529	4	13.422	717164	50.0
unknown14.465	14.465	14.8	ug/l	212482	4	13.422	717164	50.0
unknown14.678	14.678	21.7	ug/l	310809	4	13.422	717164	50.0
unknown14.733	14.733	14.8	ug/l	211797	4	13.422	717164	50.0
2H-Inden-2-one,...	14.873	16.0	ug/l	229291	4	13.422	717164	50.0
1,4-Dimethylada...	15.001	20.9	ug/l	300234	4	13.422	717164	50.0
3-Methyl-1-adam...	15.281	33.5	ug/l	480808	4	13.422	717164	50.0
unknown16.476	16.476	44.0	ug/l	631027	4	13.422	717164	50.0