

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY060925\
 Data File : VY022625.D
 Acq On : 09 Jun 2025 13:13
 Operator : SY/MD
 Sample : Q2223-03
 Misc : 5.25g/5.0mL/MSVOA_Y/SOIL/A
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 HR-04-06042025

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\82Y060225S.M
 Title : SW846 8260

Signal : TIC: VY022625.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.099	51	62	64	rBV5	8247	23884	44.24%	6.357%
2	2.446	117	119	124	rVB4	1074	1040	1.93%	0.277%
3	2.537	130	134	136	rBV5	472	608	1.13%	0.162%
4	2.617	143	147	149	rVB4	522	716	1.33%	0.191%
5	2.714	160	163	165	rVB3	520	612	1.13%	0.163%
6	2.757	168	170	173	rBV3	540	713	1.32%	0.190%
7	2.836	179	183	185	rBV4	801	1028	1.90%	0.274%
8	2.903	191	194	197	rBV	702	704	1.30%	0.187%
9	3.080	220	223	225	rBV3	496	648	1.20%	0.172%
10	3.202	240	243	246	rBV2	752	1110	2.06%	0.295%
11	3.568	299	303	304	rBV3	515	641	1.19%	0.171%
12	3.635	310	314	317	rBV3	652	852	1.58%	0.227%
13	3.757	331	334	337	rVB4	703	841	1.56%	0.224%
14	4.324	424	427	429	rBV2	506	708	1.31%	0.188%
15	4.464	447	450	453	rVB3	557	791	1.47%	0.211%
16	4.507	455	457	460	rVB2	641	649	1.20%	0.173%
17	4.854	510	514	517	rVB3	490	628	1.16%	0.167%
18	5.513	616	622	627	rVB3	452	951	1.76%	0.253%
19	5.775	663	665	670	rBV2	487	672	1.24%	0.179%
20	6.012	702	704	708	rVB3	667	690	1.28%	0.184%
21	6.177	730	731	734	rBV2	536	643	1.19%	0.171%
22	6.238	738	741	744	rVB3	452	699	1.29%	0.186%
23	6.476	778	780	784	rBV2	797	828	1.53%	0.220%
24	6.549	790	792	795	rVB2	833	786	1.46%	0.209%
25	6.628	804	805	808	rBV	501	603	1.12%	0.161%
26	6.976	859	862	865	rBV2	831	879	1.63%	0.234%
27	7.317	917	918	923	rBV2	568	828	1.53%	0.220%
28	7.451	937	940	943	rVB2	530	640	1.19%	0.170%
29	7.640	963	971	976	rBV3	4719	10947	20.28%	2.914%
30	7.713	976	983	993	rVB3	12251	29904	55.39%	7.960%
31	7.884	1008	1011	1014	rVB2	842	940	1.74%	0.250%
32	7.927	1016	1018	1022	rVB3	637	843	1.56%	0.224%
33	8.067	1034	1041	1051	rBV5	8237	19884	36.83%	5.293%
34	8.189	1058	1061	1063	rBV2	839	880	1.63%	0.234%
35	8.256	1069	1072	1076	rBV3	479	687	1.27%	0.183%
36	8.366	1087	1090	1092	rVB3	572	682	1.26%	0.182%

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37	8.408	1092	1097	1100	rVB2	771	1155	2.14%	0.307%
38	8.616	1125	1131	1140	rBV2	18886	39200	72.60%	10.434%
39	8.677	1140	1141	1145	rVB2	859	748	1.39%	0.199%
40	8.823	1163	1165	1170	rBV2	470	647	1.20%	0.172%
41	9.018	1193	1197	1200	rBV2	804	1140	2.11%	0.303%
42	9.225	1230	1231	1233	rBV	614	595	1.10%	0.158%
43	9.817	1326	1328	1333	rBV3	713	1203	2.23%	0.320%
44	9.963	1349	1352	1355	rBV3	824	1275	2.36%	0.339%
45	10.048	1361	1366	1367	rBV3	600	1046	1.94%	0.278%
46	10.109	1369	1376	1384	rBV	30243	53991	100.00%	14.371%
47	10.591	1454	1455	1458	rVB2	691	681	1.26%	0.181%
48	10.652	1458	1465	1466	rBV5	2032	3298	6.11%	0.878%
49	10.695	1470	1472	1477	rVB3	1052	1176	2.18%	0.313%
50	11.115	1538	1541	1542	rVB2	951	947	1.75%	0.252%
51	11.146	1542	1546	1552	rBV5	874	1796	3.33%	0.478%
52	11.201	1552	1555	1560	rVB5	707	1395	2.58%	0.371%
53	11.420	1585	1591	1599	rVB	26962	45828	84.88%	12.199%
54	11.548	1611	1612	1615	rBV2	1264	1135	2.10%	0.302%
55	11.585	1615	1618	1619	rVV2	835	694	1.29%	0.185%
56	11.639	1624	1627	1629	rVV4	1028	1393	2.58%	0.371%
57	11.670	1629	1632	1635	rVB3	1713	2168	4.02%	0.577%
58	11.719	1635	1640	1641	rBV5	946	1219	2.26%	0.324%
59	11.853	1659	1662	1664	rBV4	554	719	1.33%	0.191%
60	11.932	1673	1675	1677	rBV2	737	670	1.24%	0.178%
61	12.085	1698	1700	1702	rBV3	770	784	1.45%	0.209%
62	12.328	1738	1740	1742	rBV2	929	960	1.78%	0.256%
63	12.408	1747	1753	1759	rBV2	18164	29784	55.16%	7.928%
64	12.737	1802	1807	1809	rBV5	2184	2812	5.21%	0.748%
65	12.962	1842	1844	1850	rVB6	1203	1658	3.07%	0.441%
66	13.115	1867	1869	1871	rBV2	1342	1374	2.54%	0.366%
67	13.139	1871	1873	1875	rBV3	800	929	1.72%	0.247%
68	13.292	1894	1898	1901	rBV6	1990	2749	5.09%	0.732%
69	13.347	1901	1907	1914	rVV2	13096	22811	42.25%	6.072%
70	13.499	1930	1932	1933	rBV2	1192	799	1.48%	0.213%
71	13.517	1933	1935	1936	rBV2	1308	965	1.79%	0.257%
72	13.584	1945	1946	1951	rVB5	2682	2839	5.26%	0.756%
73	13.670	1954	1960	1964	rBV6	3485	7407	13.72%	1.972%
74	13.737	1969	1971	1975	rBV4	1110	1820	3.37%	0.484%
75	14.170	2038	2042	2045	rBV5	1862	3607	6.68%	0.960%
76	14.291	2059	2062	2067	rVB7	1566	2649	4.91%	0.705%

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77	14.352	2067	2072	2074	rBV5	1820	3809	7.05%	1.014%
78	14.566	2105	2107	2110	rBV4	790	1321	2.45%	0.352%
79	14.779	2140	2142	2144	rVB3	982	746	1.38%	0.199%
80	14.865	2152	2156	2159	rBV6	1602	2966	5.49%	0.789%
81	14.895	2159	2161	2162	rVB2	1601	1010	1.87%	0.269%
82	15.145	2199	2202	2204	rBV3	1043	1133	2.10%	0.302%
83	15.194	2208	2210	2213	rBV4	999	1053	1.95%	0.280%
84	15.395	2239	2243	2244	rBV3	600	755	1.40%	0.201%
85	15.474	2254	2256	2258	rBV3	873	854	1.58%	0.227%
86	15.962	2335	2336	2340	rVV4	682	788	1.46%	0.210%
87	16.005	2340	2343	2344	rVB3	698	598	1.11%	0.159%
88	16.108	2358	2360	2363	rBV4	755	807	1.49%	0.215%
89	16.187	2371	2373	2376	rBV4	528	590	1.09%	0.157%
90	16.364	2399	2402	2404	rBV3	836	787	1.46%	0.209%
91	16.413	2407	2410	2412	rVV2	573	648	1.20%	0.172%
92	16.724	2460	2461	2464	rVB3	786	595	1.10%	0.158%

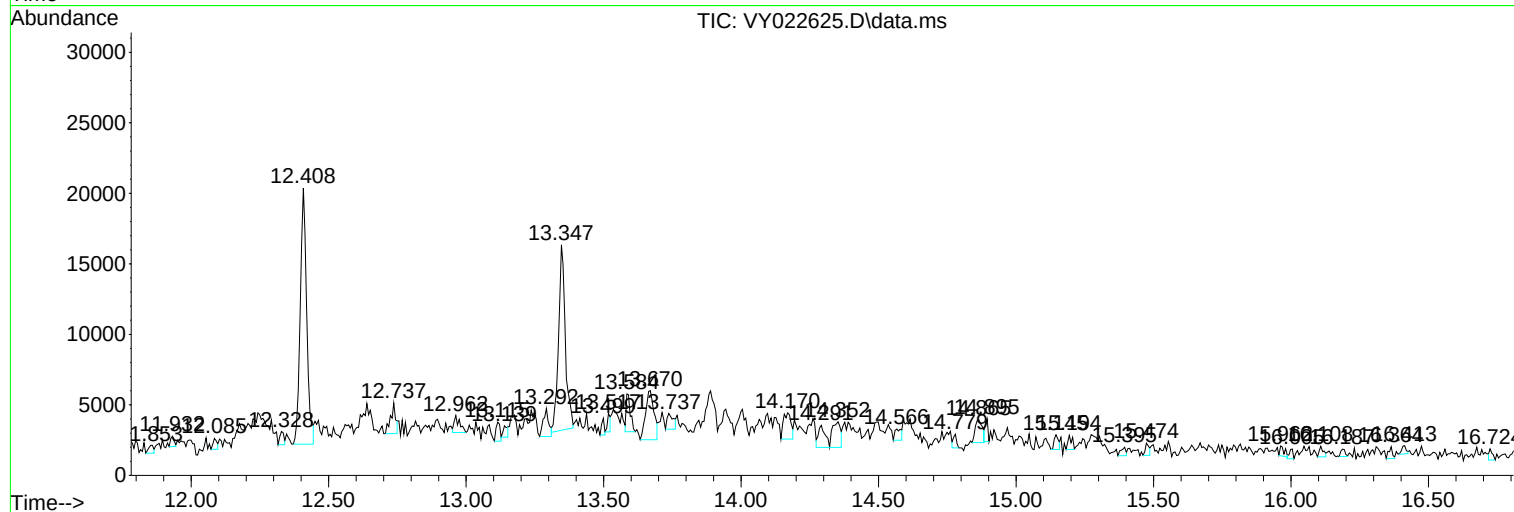
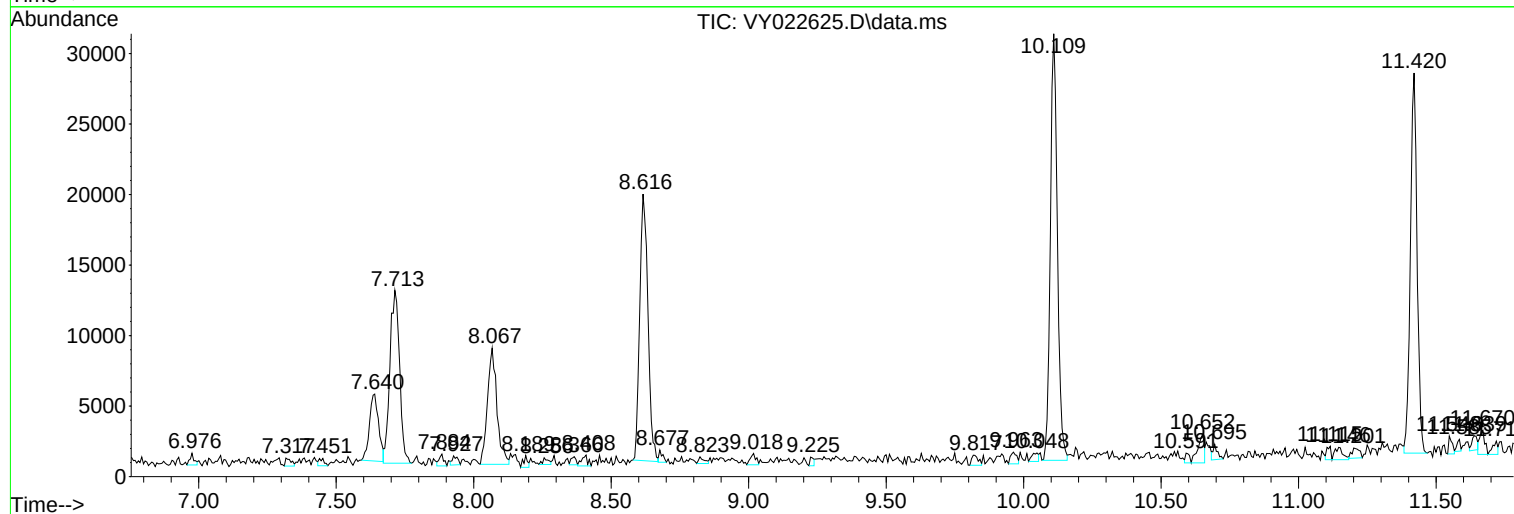
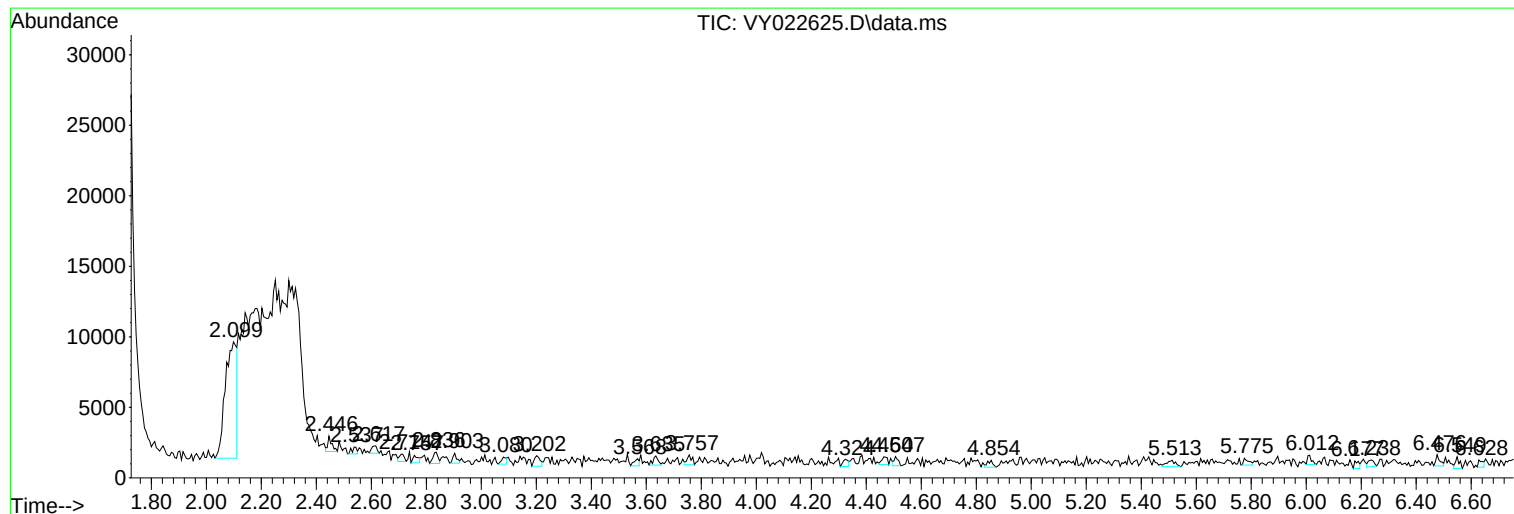
Sum of corrected areas: 375685

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060225S.M
Quant Title : SW846 8260

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



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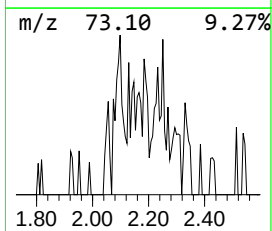
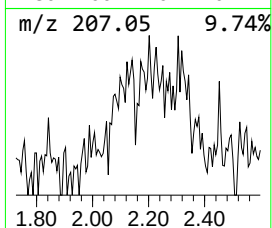
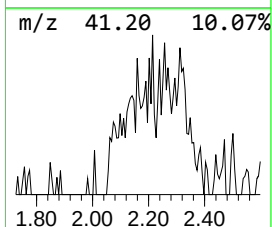
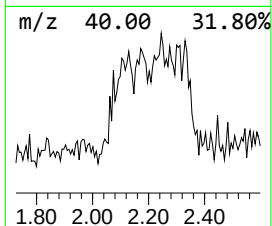
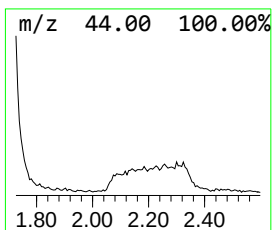
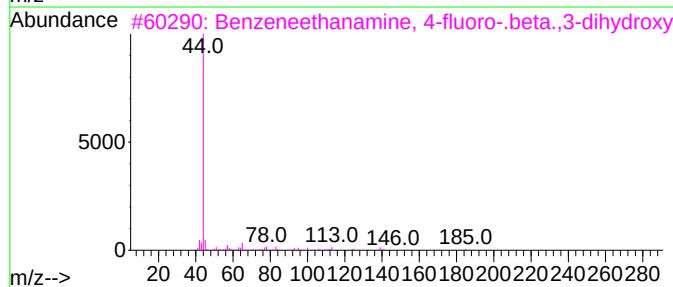
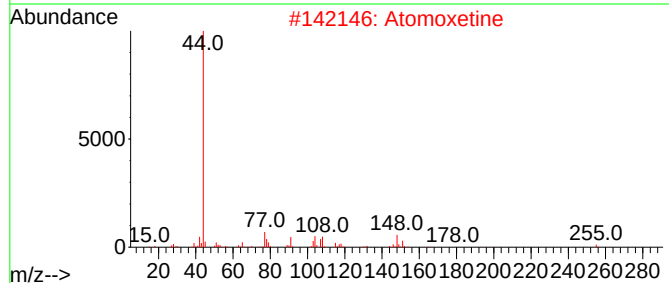
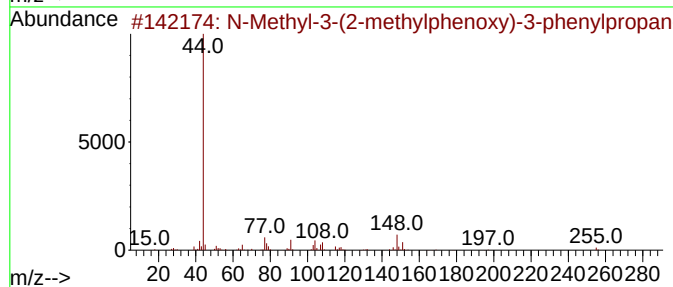
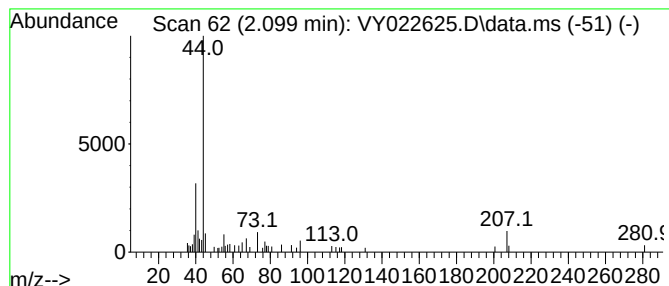
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060225S.M
Quant Title : SW846 8260

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

Peak Number 1 unknown2.099 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.099	39.93 ug/l	23884	Pentafluorobenzene	7.719

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N-Methyl-3-(2-methylphenoxy)-3-p...	255	C17H21NO	063940-51-2	47
2			Atomoxetine	255	C17H21NO	083015-26-3	38
3			Benzeneethanamine, 4-fluoro-.bet...	185	C9H12FN02	103439-06-1	33
4			Fluoxetine	309	C17H18F3NO	054910-89-3	33
5			2-Pentanamine, 4-methyl-	101	C6H15N	000108-09-8	33



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Instrument :
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ClientSampleId :
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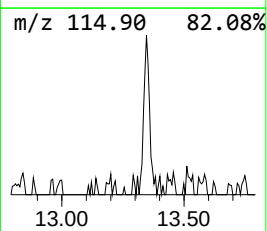
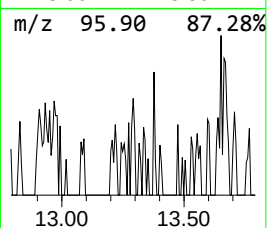
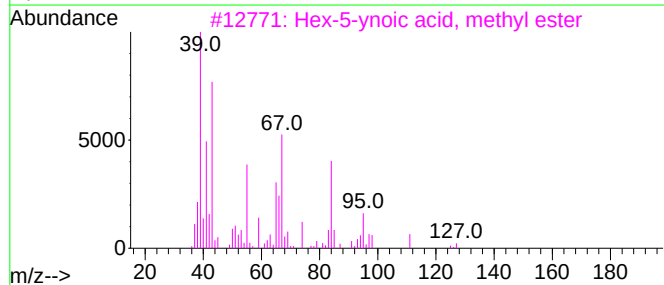
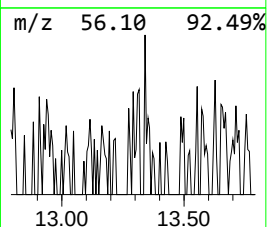
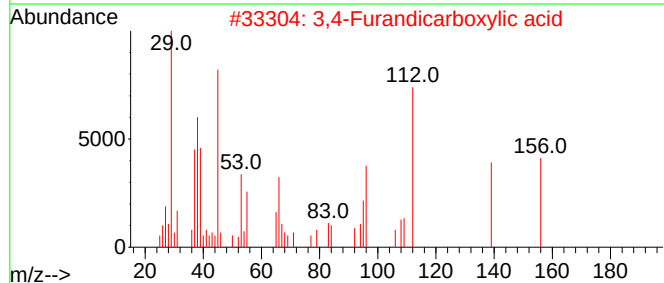
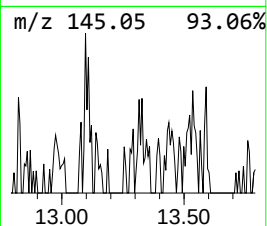
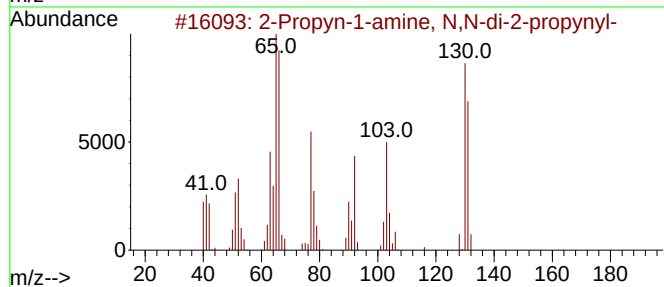
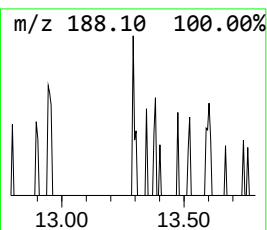
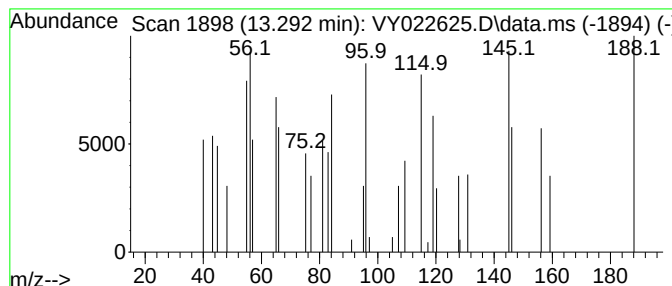
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060225S.M
Quant Title : SW846 8260

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

Peak Number 3 unknown13.292 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	6.03 ug/l	2749	1,4-Dichlorobenzene-d4	13.347

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propyn-1-amine, N,N-di-2-propy...	131	C9H9N	006921-29-5	27
2			3,4-Furandicarboxylic acid	156	C6H4O5	003387-26-6	12
3			Hex-5-ynoic acid, methyl ester	126	C7H10O2	077758-51-1	12
4			1-Methyl-4-sulfonylbenzene	156	C7H8O2S	1000410-47-3	10
5			2-Indolinemalonic acid, 3,3-dime...	305	C17H23NO4	018781-64-1	10



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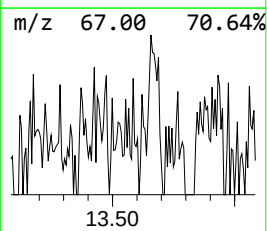
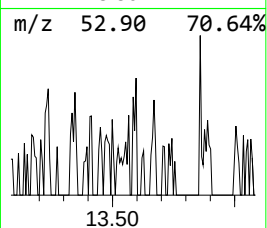
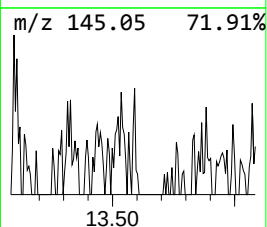
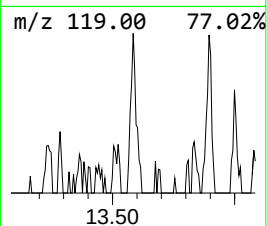
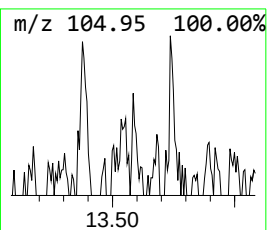
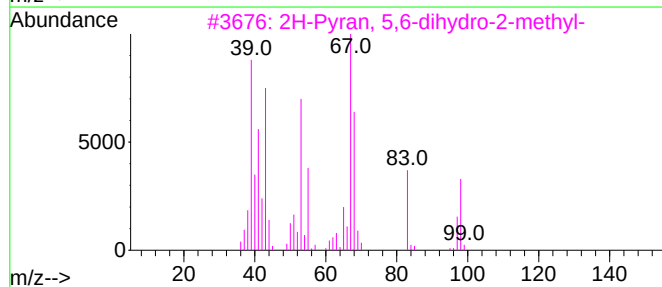
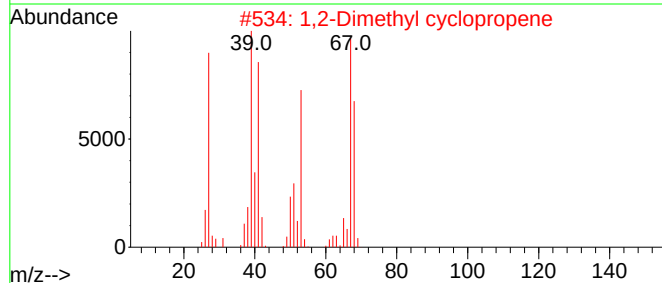
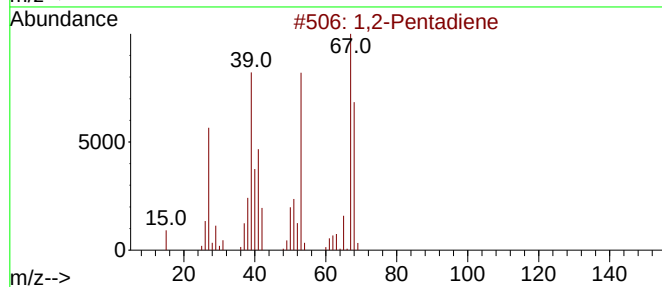
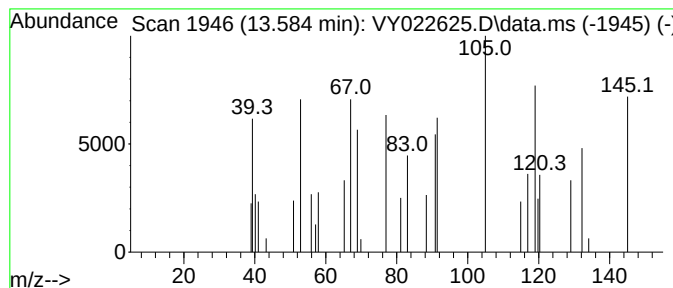
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060225S.M
Quant Title : SW846 8260

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

Peak Number 4 unknown13.584 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.584	6.22 ug/l	2839	1,4-Dichlorobenzene-d4	13.347

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Pentadiene	68	C5H8	000591-95-7	47
2			1,2-Dimethyl cyclopropene	68	C5H8	014309-32-1	38
3			2H-Pyran, 5,6-dihydro-2-methyl-	98	C6H10O	055230-25-6	28
4			2,8-Decadiyne	134	C10H14	004116-93-2	25
5			1,3-Butadiene, 2-chloro-	88	C4H5Cl	000126-99-8	9



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Operator : SY/MD
Sample : Q2223-03
Misc : 5.25g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
HR-04-06042025

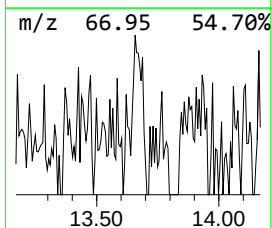
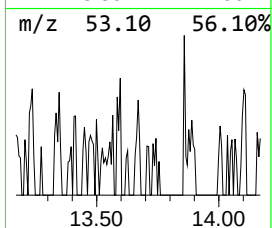
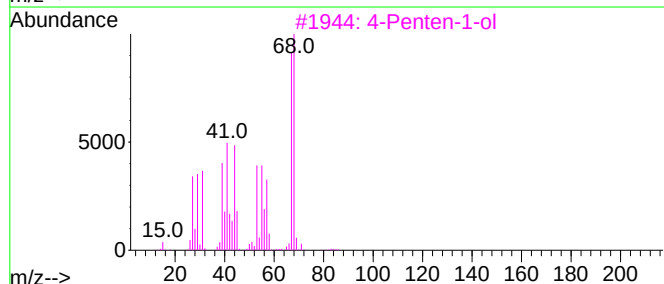
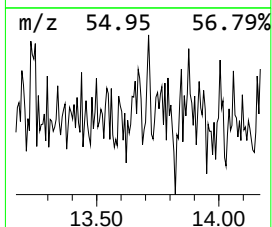
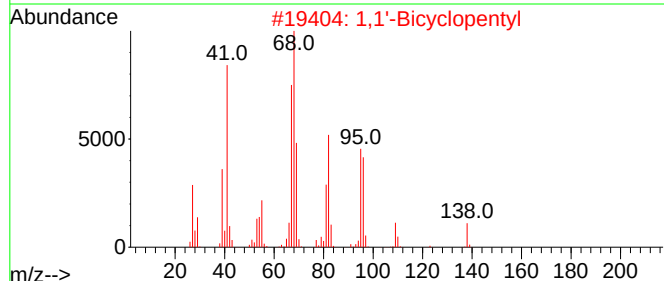
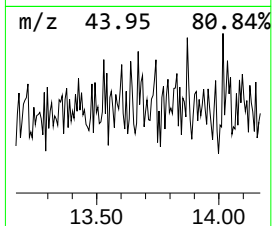
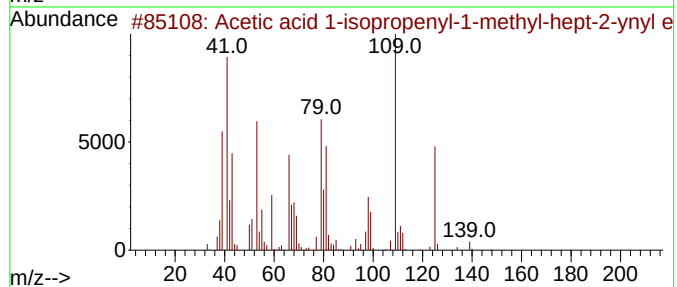
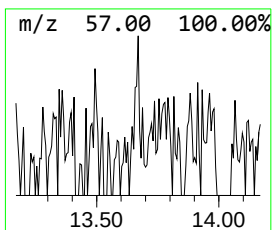
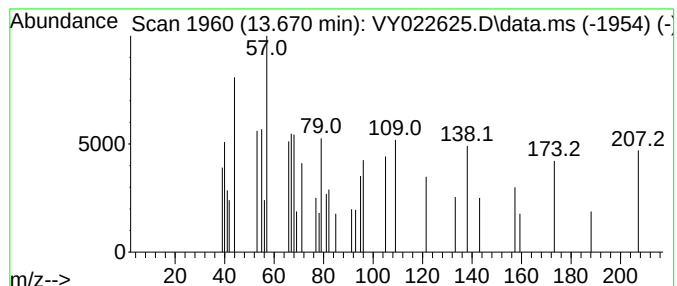
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Quant Title : SW846 8260

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

Peak Number 5 unknown13.670 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.670	16.24 ug/l	7407	1,4-Dichlorobenzene-d4	13.347

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid 1-isopropenyl-1-meth...	208	C13H20O2	1010296-08-1	43
2			1,1'-Bicyclopentyl	138	C10H18	001636-39-1	28
3			4-Penten-1-ol	86	C5H10O	000821-09-0	22
4			4,5,6,7-Tetrahydro-3H-cyclopenta...	138	C8H10O2	005587-71-3	12
5			Bicyclo[2.2.1]heptan-2-one, 3-et...	138	C9H14O	054345-87-8	12



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY060925\
Data File : VY022625.D
Acq On : 09 Jun 2025 13:13
Operator : SY/MD
Sample : Q2223-03
Misc : 5.25g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
HR-04-06042025

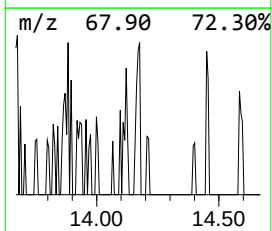
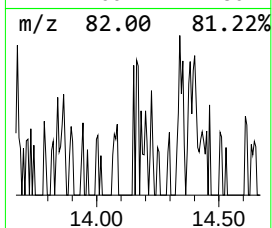
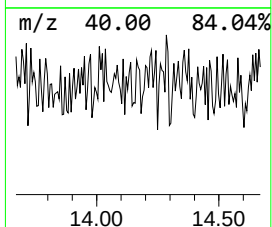
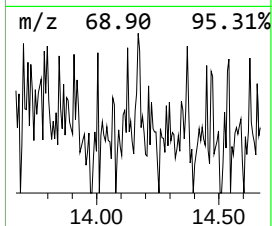
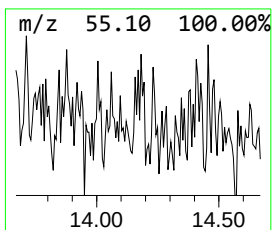
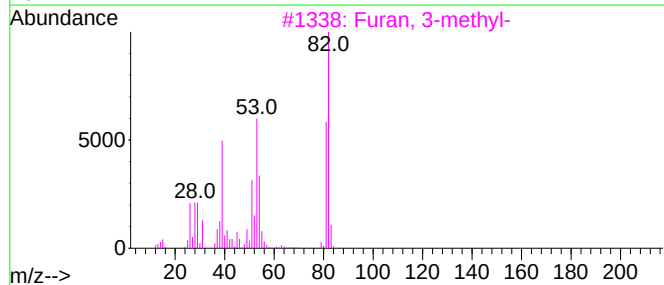
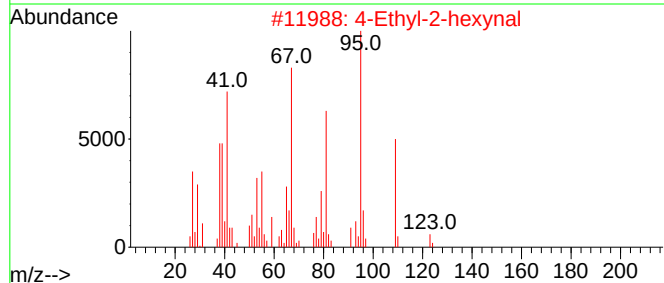
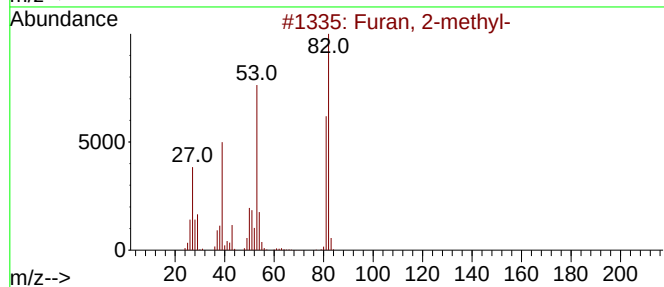
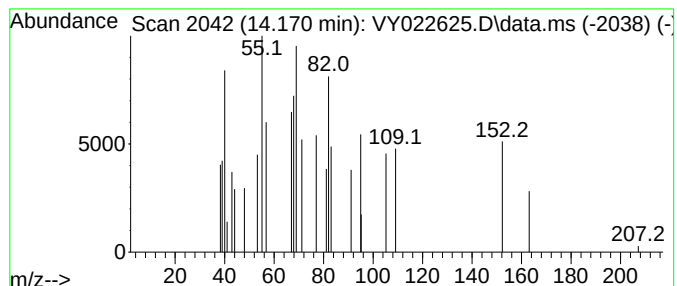
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Quant Title : SW846 8260

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

Peak Number 6 unknown14.169 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.169	7.91 ug/l	3607	1,4-Dichlorobenzene-d4	13.347

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, 2-methyl-	82	C5H6O	000534-22-5	22
2			4-Ethyl-2-hexynal	124	C8H12O	071932-97-3	22
3			Furan, 3-methyl-	82	C5H6O	000930-27-8	22
4			2-Hexyne	82	C6H10	000764-35-2	22
5			Bicyclo(3.3.1)nonane-2,6-dione	152	C9H12O2	016473-11-3	18



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY060925\
Data File : VY022625.D
Acq On : 09 Jun 2025 13:13
Operator : SY/MD
Sample : Q2223-03
Misc : 5.25g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
HR-04-06042025

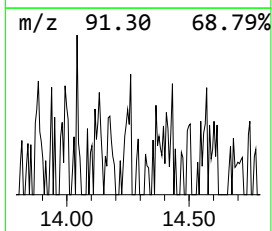
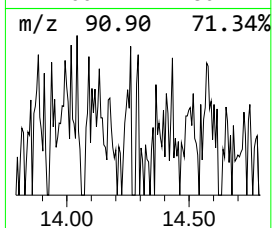
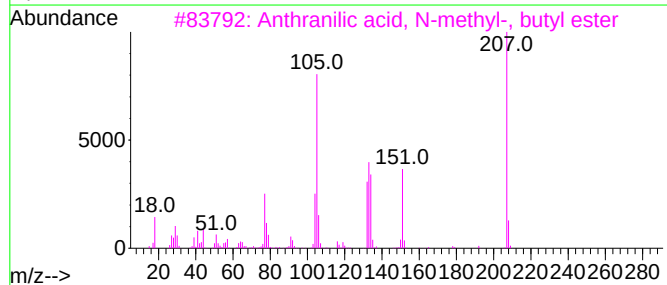
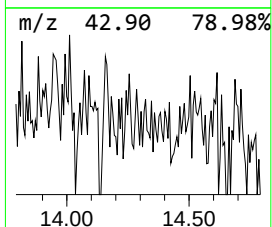
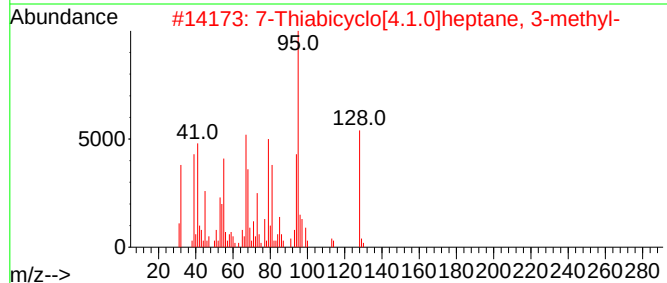
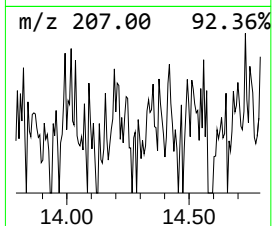
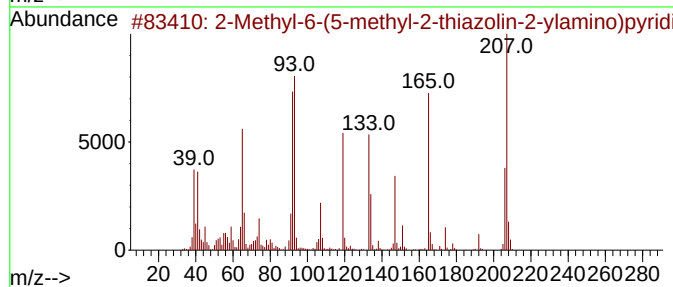
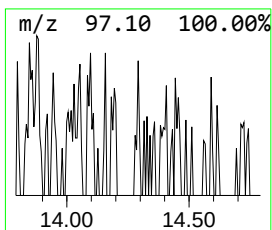
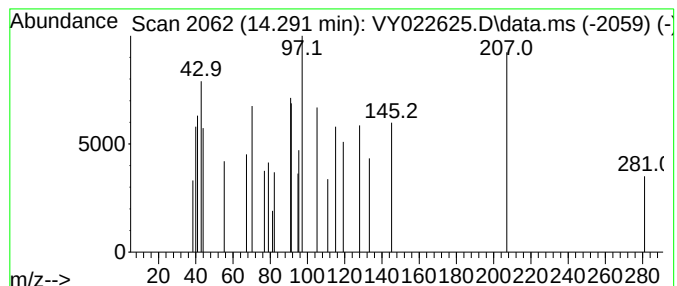
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Quant Title : SW846 8260

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

Peak Number 7 unknown14.291 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.291	5.81 ug/l	2649	1,4-Dichlorobenzene-d4	13.347

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methyl-6-(5-methyl-2-thiazolin...	207	C10H13N3S	339352-50-0	10
2			7-Thiabicyclo[4.1.0]heptane, 3-m...	128	C7H12S	054725-38-1	10
3			Anthranilic acid, N-methyl-, but...	207	C12H17NO2	015236-34-7	9
4			1,2-Ethanediol, 1-(2-furanyl)-	128	C6H8O3	019377-75-4	9
5			2,3-Dihydroxy-6-nitroquinoxaline	207	C8H5N3O4	002379-56-8	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY060925\
Data File : VY022625.D
Acq On : 09 Jun 2025 13:13
Operator : SY/MD
Sample : Q2223-03
Misc : 5.25g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
HR-04-06042025

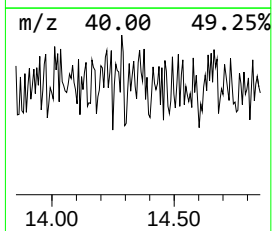
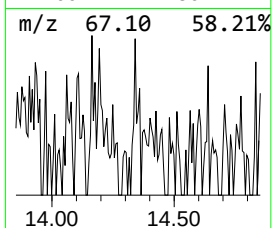
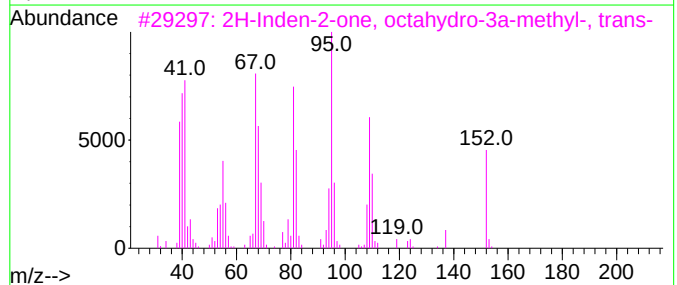
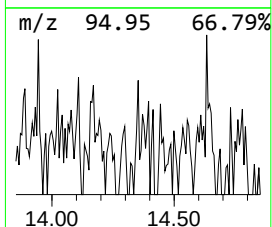
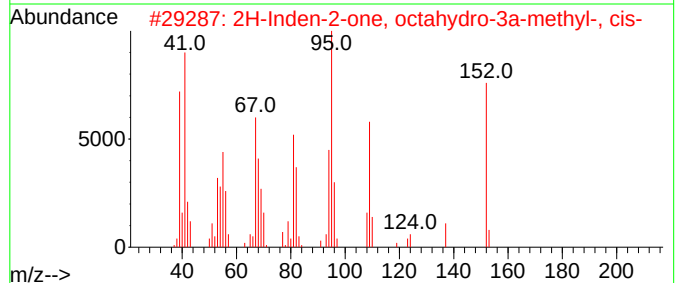
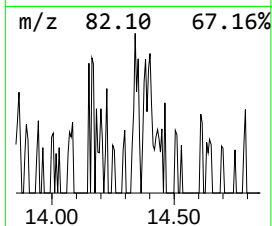
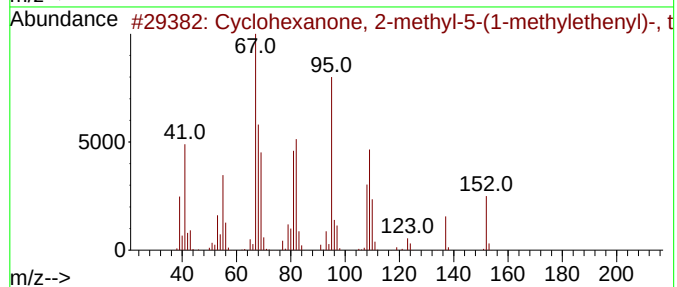
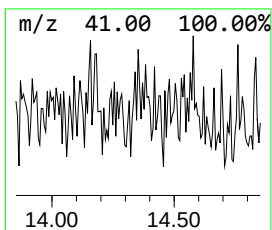
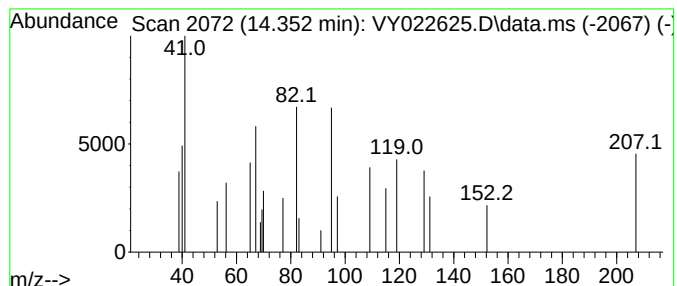
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060225S.M
Quant Title : SW846 8260

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

Peak Number 8 unknown14.352 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.352	8.35 ug/l	3809	1,4-Dichlorobenzene-d4	13.347

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanone, 2-methyl-5-(1-met...	152	C10H16O	005948-04-9	18
2			2H-Inden-2-one, octahydro-3a-met...	152	C10H16O	013351-29-6	11
3			2H-Inden-2-one, octahydro-3a-met...	152	C10H16O	020379-99-1	10
4			trans-1,4-Cyclohexanedimethanol,...	436	C14H14F10O4	1010384-27-9	10
5			Cyclohexanone, 2-methyl-5-(1-met...	152	C10H16O	007764-50-3	10



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY060925\
Data File : VY022625.D
Acq On : 09 Jun 2025 13:13
Operator : SY/MD
Sample : Q2223-03
Misc : 5.25g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 13 Sample Multiplier: 1

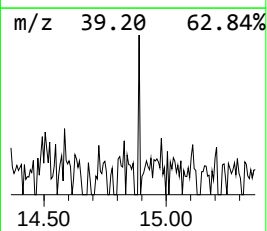
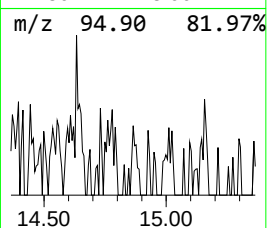
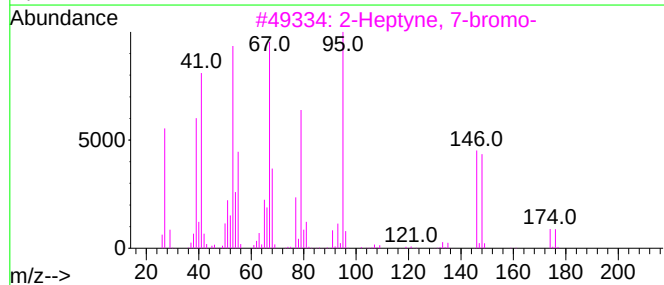
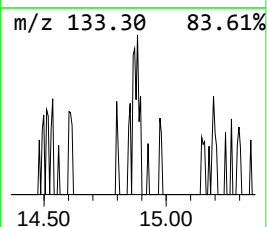
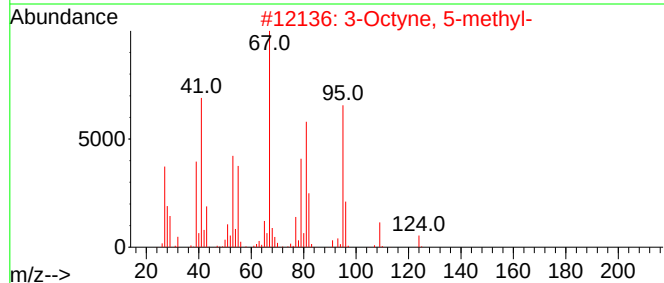
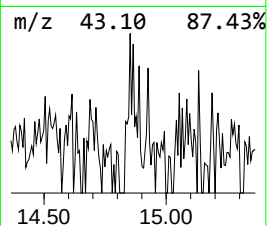
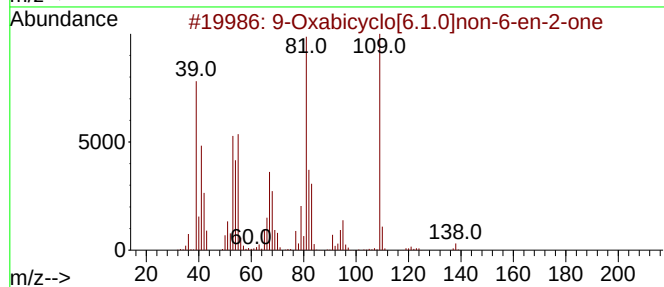
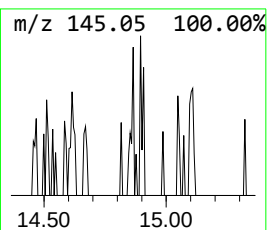
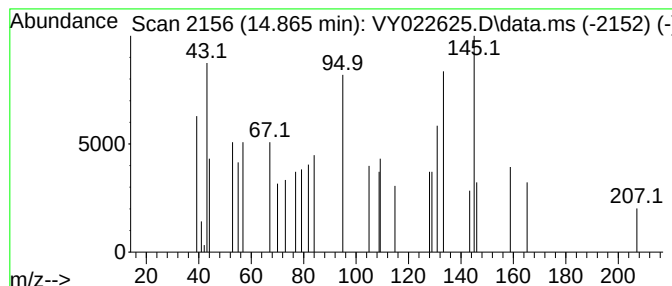
Instrument :
MSVOA_Y
ClientSampleId :
HR-04-06042025

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060225S.M
Quant Title : SW846 8260

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

Peak Number 9 unknown14.865 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.865	6.50 ug/l	2966	1,4-Dichlorobenzene-d4	13.347	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Oxabicyclo[6.1.0]non-6-en-2-one	138	C8H10O2	1000211-01-6	16
2	3-Octyne, 5-methyl-	124	C9H16	062108-33-2	12
3	2-Heptyne, 7-bromo-	174	C7H11Br	231620-79-4	12
4	1,4-Undecadiene, (Z)-	152	C11H20	055976-14-2	12
5	Cyclopentanemethanol, 2-nitro-.a...	247	C14H17NO3	103130-01-4	10



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY060925\
Data File : VY022625.D
Acq On : 09 Jun 2025 13:13
Operator : SY/MD
Sample : Q2223-03
Misc : 5.25g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
HR-04-06042025

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060225S.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--			
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unknown13.584	13.584	6.2	ug/l	2839	4	13.347	22811	50.0
unknown13.670	13.670	16.2	ug/l	7407	4	13.347	22811	50.0
unknown14.169	14.169	7.9	ug/l	3607	4	13.347	22811	50.0
unknown14.291	14.291	5.8	ug/l	2649	4	13.347	22811	50.0
unknown14.352	14.352	8.3	ug/l	3809	4	13.347	22811	50.0
unknown14.865	14.865	6.5	ug/l	2966	4	13.347	22811	50.0