

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY060325\
 Data File : VY022520.D
 Acq On : 03 Jun 2025 14:14
 Operator : SY/MD
 Sample : Q2168-03
 Misc : 5.50g/5.0mL/MSVOA_Y/SOIL/A
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 A3

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: VY022520.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.818	15	16	21	rVB3	1000	1003	1.10%	0.149%
2	2.086	51	60	61	rBV4	7619	16611	18.28%	2.460%
3	2.239	83	85	86	rBV2	2202	1271	1.40%	0.188%
4	2.604	142	145	146	rBV2	1379	1140	1.25%	0.169%
5	3.220	243	246	249	rBV4	671	1045	1.15%	0.155%
6	3.324	260	263	267	rBV3	763	1084	1.19%	0.161%
7	3.537	294	298	301	rBV3	638	1079	1.19%	0.160%
8	4.635	475	478	480	rVB2	868	999	1.10%	0.148%
9	5.647	634	644	656	rVB6	3522	10360	11.40%	1.534%
10	6.287	744	749	753	rVB3	663	1423	1.57%	0.211%
11	6.701	810	817	818	rBV3	854	941	1.04%	0.139%
12	7.628	964	969	975	rBV4	5378	13174	14.49%	1.951%
13	7.707	975	982	990	rVV2	18779	42515	46.78%	6.295%
14	8.079	1033	1043	1051	rBV3	23302	64594	71.07%	9.565%
15	8.475	1101	1108	1113	rBV4	1503	2713	2.98%	0.402%
16	8.561	1119	1122	1124	rBV2	812	1004	1.10%	0.149%
17	8.616	1124	1131	1141	rVV	25206	52627	57.90%	7.793%
18	8.695	1143	1144	1149	rVB3	833	1056	1.16%	0.156%
19	8.878	1171	1174	1179	rBV3	526	957	1.05%	0.142%
20	9.109	1205	1212	1218	rBV5	2115	4213	4.64%	0.624%
21	9.743	1310	1316	1318	rVV3	1350	2115	2.33%	0.313%
22	9.780	1321	1322	1327	rVB4	1089	1221	1.34%	0.181%
23	9.884	1333	1339	1341	rBV6	1027	2033	2.24%	0.301%
24	10.103	1367	1375	1381	rBV	35394	63144	69.47%	9.350%
25	10.170	1381	1386	1393	rVV	51804	90890	100.00%	13.459%
26	10.231	1393	1396	1398	rVB2	777	968	1.07%	0.143%
27	10.298	1398	1407	1410	rBV4	3269	5342	5.88%	0.791%
28	10.969	1513	1517	1519	rVB4	1029	1174	1.29%	0.174%
29	11.127	1541	1543	1547	rVB3	772	1088	1.20%	0.161%
30	11.207	1552	1556	1563	rVB5	2269	4438	4.88%	0.657%
31	11.304	1566	1572	1576	rBV5	1521	2948	3.24%	0.437%
32	11.414	1585	1590	1597	rBV	26507	45906	50.51%	6.798%
33	11.518	1602	1607	1614	rBV2	7148	11102	12.21%	1.644%
34	11.627	1617	1625	1633	rVB	30057	58483	64.34%	8.660%
35	11.950	1673	1678	1686	rVB2	16358	28352	31.19%	4.198%
36	12.054	1691	1695	1698	rVV5	711	1203	1.32%	0.178%

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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
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37	12.127	1705	1707	1709	rVB2	1208	962	1.06%	0.142%
38	12.170	1712	1714	1718	rVB2	1298	1480	1.63%	0.219%
39	12.206	1718	1720	1723	rBV3	844	1027	1.13%	0.152%
40	12.408	1748	1753	1758	rBV2	14305	24133	26.55%	3.574%
41	12.499	1763	1768	1769	rBV3	944	1115	1.23%	0.165%
42	12.560	1775	1778	1782	rBV3	1206	1502	1.65%	0.222%
43	12.591	1782	1783	1787	rVB3	1016	1055	1.16%	0.156%
44	12.658	1789	1794	1797	rBV5	3585	5578	6.14%	0.826%
45	12.688	1797	1799	1802	rVV3	2140	2904	3.20%	0.430%
46	12.737	1802	1807	1813	rVB3	5451	8951	9.85%	1.325%
47	12.895	1830	1833	1834	rVV3	1369	1519	1.67%	0.225%
48	12.908	1834	1835	1838	rVV3	1595	1013	1.11%	0.150%
49	12.968	1842	1845	1849	rVB4	1195	1908	2.10%	0.283%
50	13.042	1853	1857	1862	rVV2	6785	10427	11.47%	1.544%
51	13.084	1862	1864	1869	rVV4	761	1035	1.14%	0.153%
52	13.157	1873	1876	1882	rBV5	789	1743	1.92%	0.258%
53	13.249	1887	1891	1894	rBV4	1456	2689	2.96%	0.398%
54	13.346	1901	1907	1916	rVB4	14203	25494	28.05%	3.775%
55	13.542	1934	1939	1943	rBV6	1498	2511	2.76%	0.372%
56	13.663	1956	1959	1964	rVB6	1353	1923	2.12%	0.285%
57	13.731	1964	1970	1974	rVB7	1960	3061	3.37%	0.453%
58	13.798	1980	1981	1984	rVB2	1093	911	1.00%	0.135%
59	13.834	1984	1987	1990	rBV2	1280	1721	1.89%	0.255%
60	13.889	1993	1996	2002	rVB5	1363	2036	2.24%	0.301%
61	13.993	2010	2013	2020	rBV5	805	1325	1.46%	0.196%
62	14.590	2110	2111	2116	rVB4	1173	1548	1.70%	0.229%
63	14.694	2125	2128	2130	rVB3	861	1028	1.13%	0.152%
64	14.761	2134	2139	2140	rVV4	705	1059	1.17%	0.157%
65	14.797	2140	2145	2147	rVV4	811	1313	1.44%	0.194%
66	14.858	2150	2155	2162	rBV5	995	2764	3.04%	0.409%
67	14.968	2171	2173	2177	rVB4	853	1031	1.13%	0.153%
68	15.011	2177	2180	2185	rBV5	752	919	1.01%	0.136%
69	15.139	2195	2201	2208	rBV6	2044	4784	5.26%	0.708%
70	15.297	2225	2227	2229	rBV3	996	913	1.00%	0.135%
71	15.328	2229	2232	2235	rVV4	1069	1744	1.92%	0.258%
72	15.505	2258	2261	2265	rVB4	1272	1495	1.64%	0.221%
73	15.578	2270	2273	2277	rVB4	1119	1373	1.51%	0.203%
74	15.620	2277	2280	2284	rBV5	871	1696	1.87%	0.251%
75	15.809	2308	2311	2314	rVB4	849	1019	1.12%	0.151%
76	16.090	2353	2357	2359	rBV2	1037	1093	1.20%	0.162%

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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

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Title : SW846 8260

77	16.437	2412	2414	2417	rVB4	962	1037	1.14%	0.154%
78	16.486	2420	2422	2425	rVV4	871	1062	1.17%	0.157%
79	16.578	2434	2437	2441	rBV5	707	1209	1.33%	0.179%

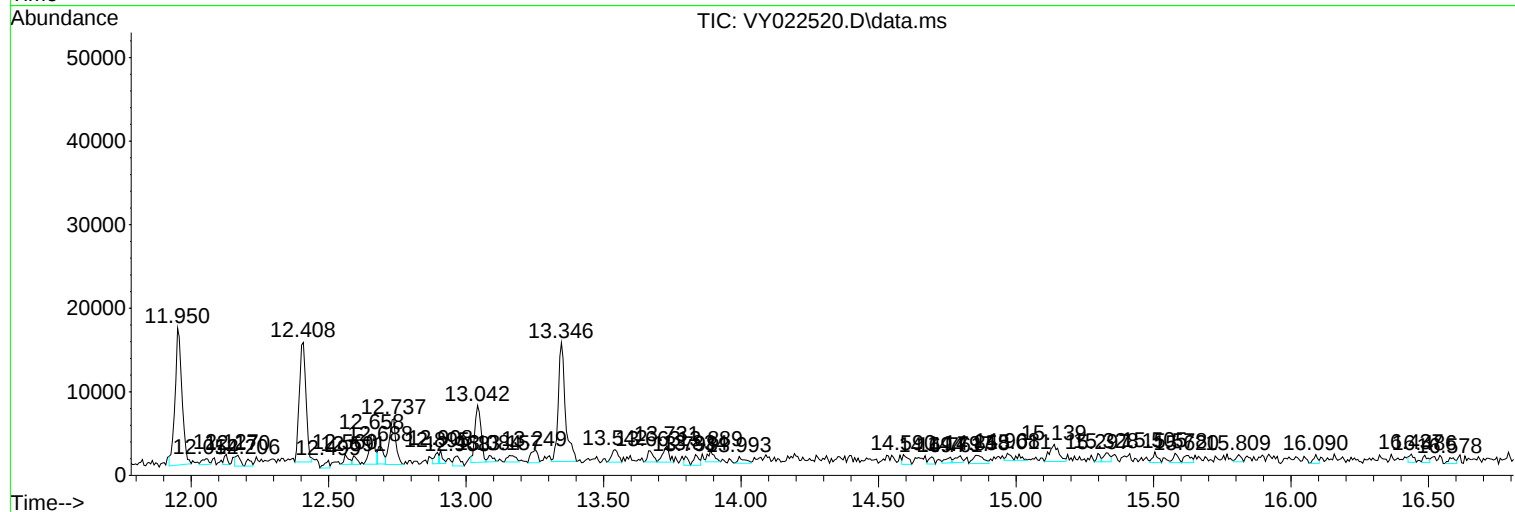
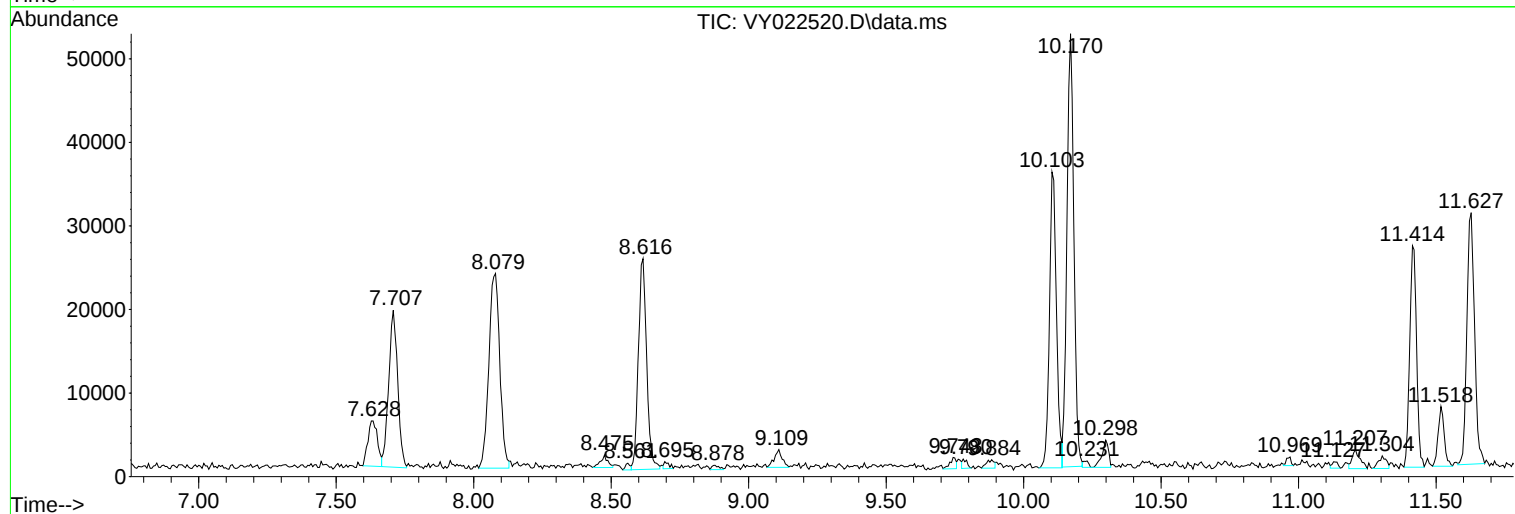
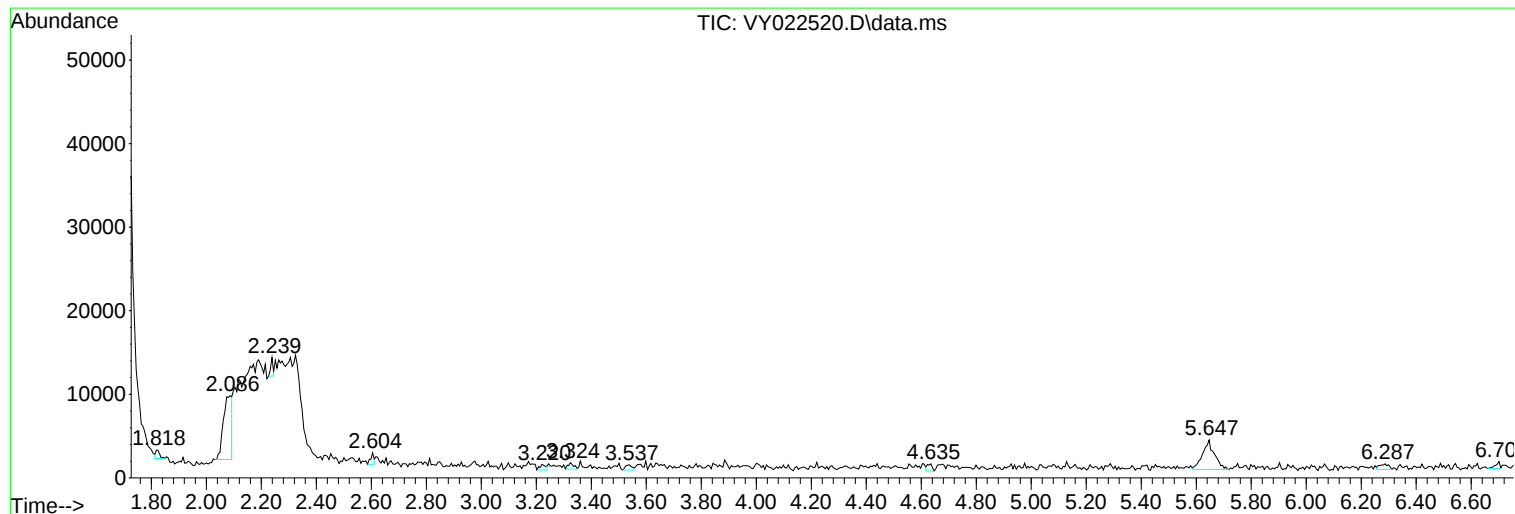
Sum of corrected areas: 675326

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Quant Title : SW846 8260

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



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Operator : SY/MD
Sample : Q2168-03
Misc : 5.50g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
A3

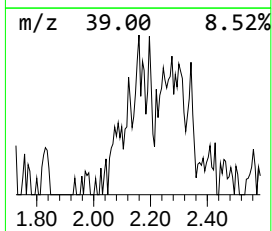
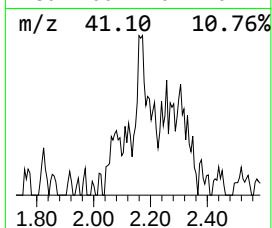
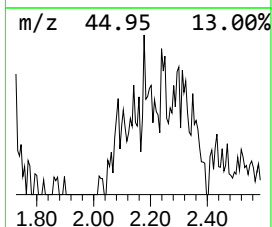
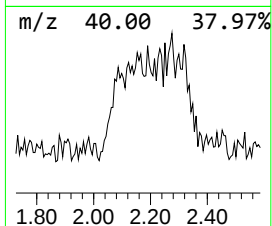
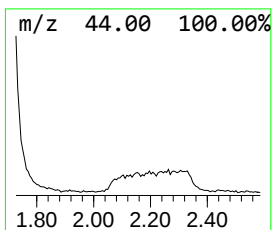
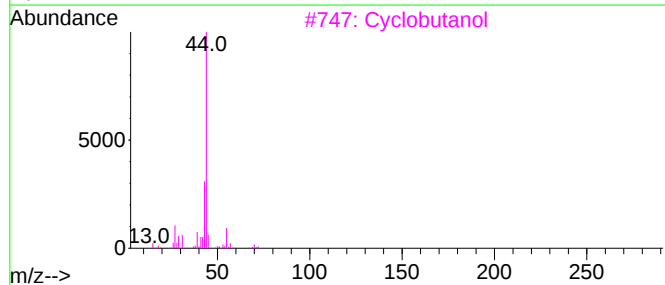
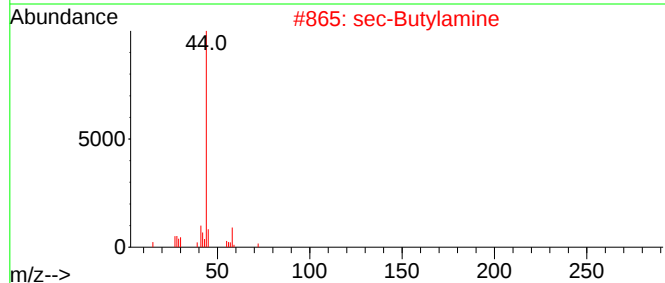
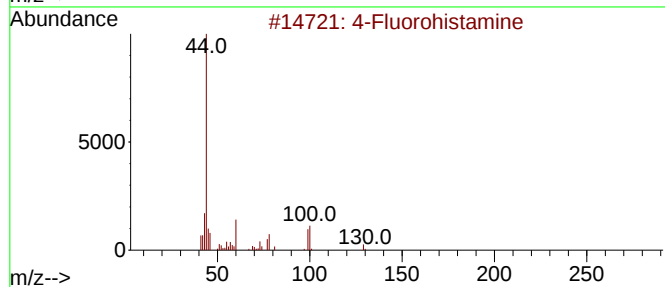
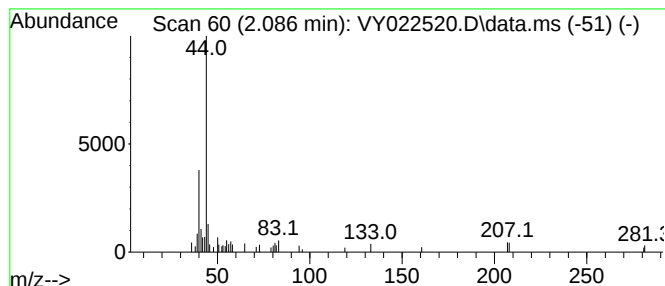
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060225S.M
Quant Title : SW846 8260

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

Peak Number 1 unknown2.086 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.086	19.54 ug/l	16611	Pentafluorobenzene	7.707

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Fluorohistamine	129	C5H8FN3	049872-60-8	38
2			sec-Butylamine	73	C4H11N	013952-84-6	36
3			Cyclobutanol	72	C4H8O	002919-23-5	36
4			2-Hexanamine, 5-methyl-	115	C7H17N	028292-43-5	33
5			3-Cyclohexyl-1-methyl-1-(2-pheny...	260	C16H24N2O	1024470-80-1	28



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Misc : 5.50g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 11 Sample Multiplier: 1

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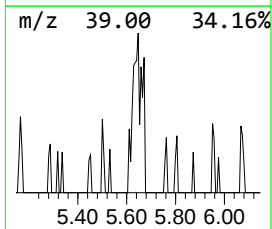
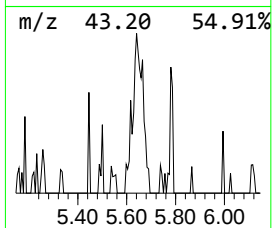
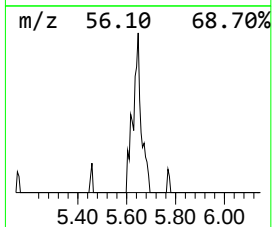
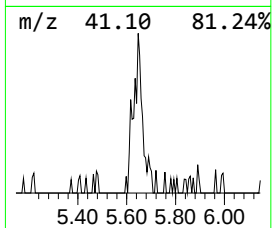
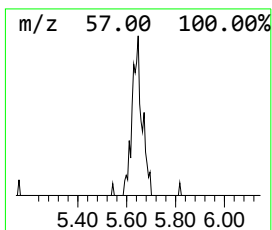
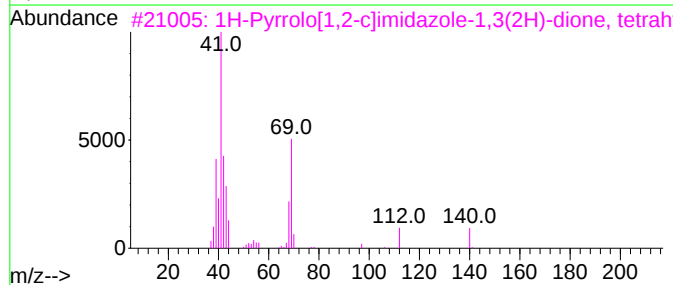
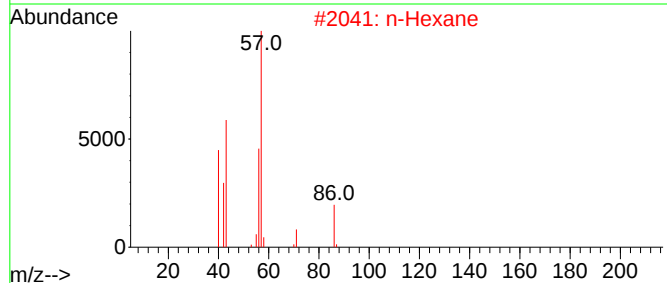
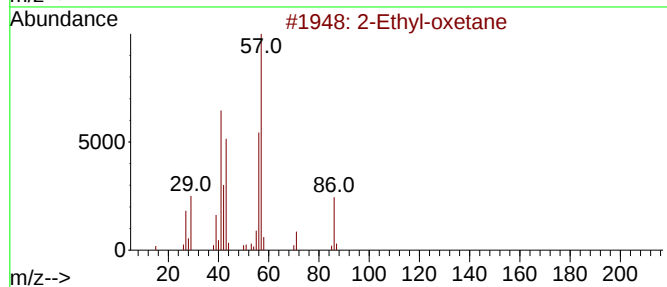
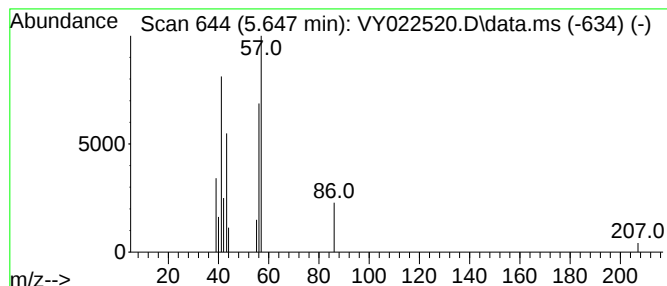
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060225S.M
Quant Title : SW846 8260

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

Peak Number 2 2-Ethyl-oxetane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.647	12.18 ug/l	10360	Pentafluorobenzene	7.707

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Ethyl-oxetane	86	C5H10O	1010386-40-2	64
2			n-Hexane	86	C6H14	000110-54-3	47
3			1H-Pyrrolo[1,2-c]imidazole-1,3(2...)	140	C6H8N2O2	1000351-31-8	10
4			Azetidine, 1-nitroso-	86	C3H6N2O	015216-10-1	9
5			3-Buten-1-ol, 3-methyl-	86	C5H10O	000763-32-6	9



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ALS Vial : 11 Sample Multiplier: 1

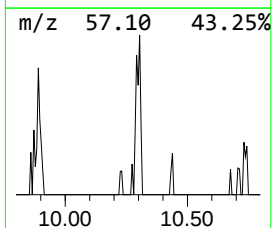
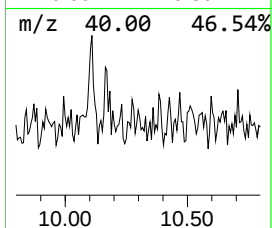
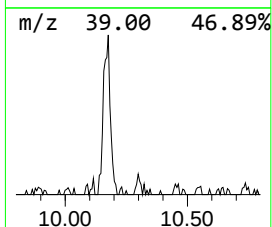
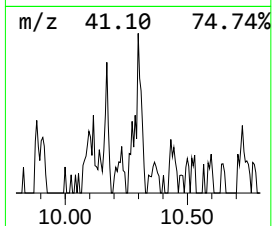
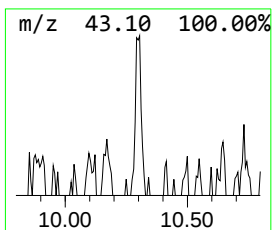
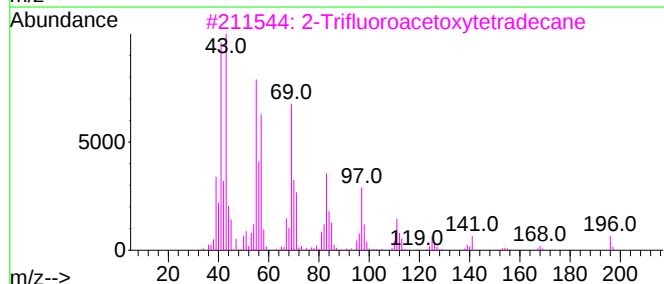
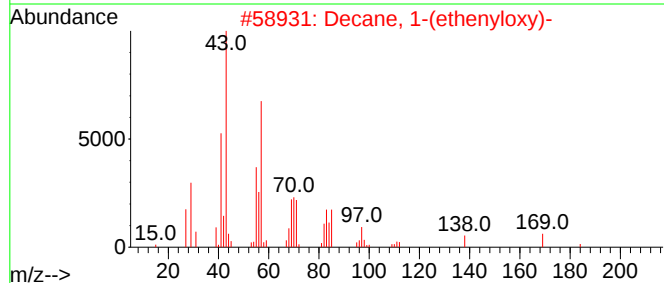
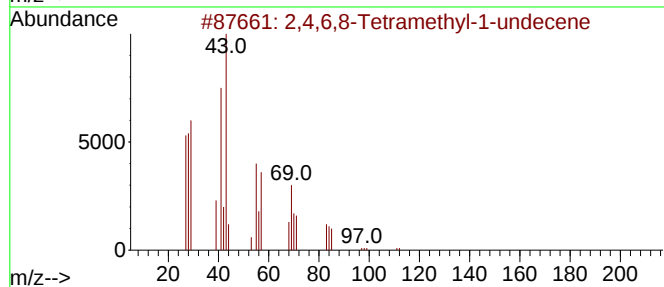
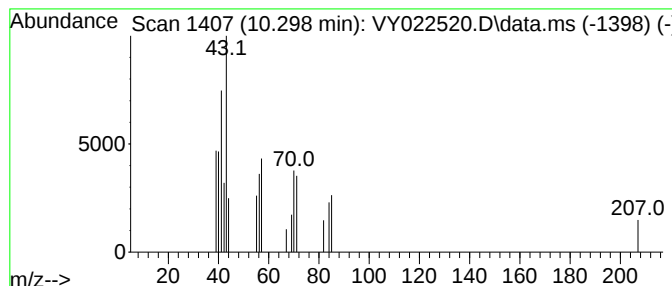
Instrument :
MSVOA_Y
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060225S.M
Quant Title : SW846 8260

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

Peak Number 3 2,4,6,8-Tetramethyl-1-undecene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.298	5.82 ug/l	5342	Chlorobenzene-d5	11.420	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,6,8-Tetramethyl-1-undecene	210	C15H30	059920-26-2	72
2	Decane, 1-(ethenyl)-	184	C12H24O	000765-05-9	40
3	2-Trifluoroacetoxytetradecane	310	C16H29F3O2	1000245-47-4	40
4	Trichloroacetic acid, 2-tetradec...	358	C16H29Cl3O2	1000282-06-6	38
5	Pentadecafluorooctanoic acid, no...	540	C17H19F15O2	1000406-03-9	37



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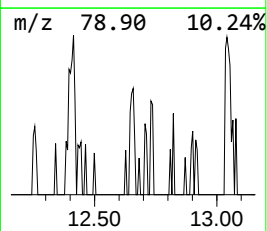
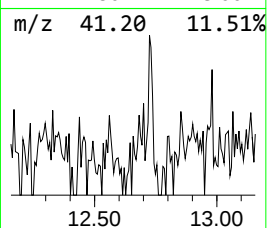
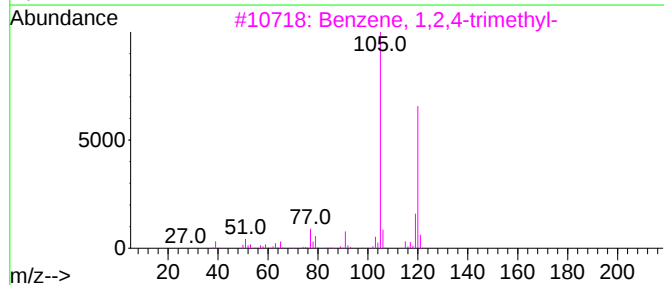
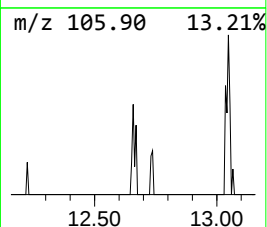
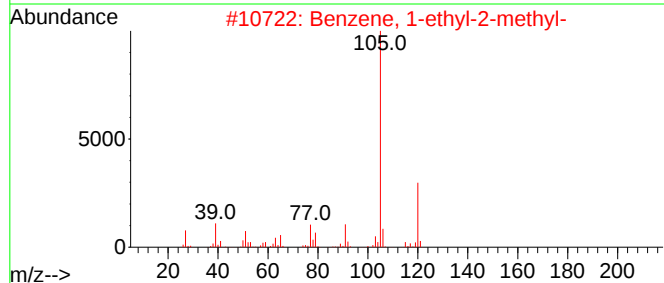
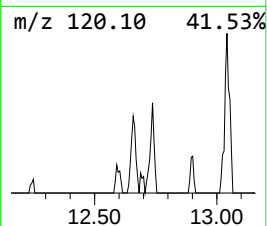
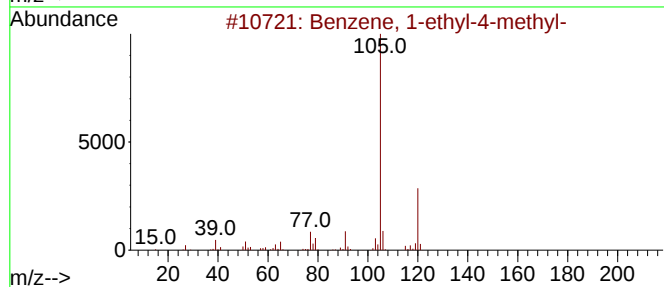
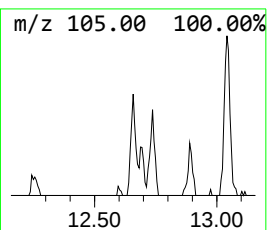
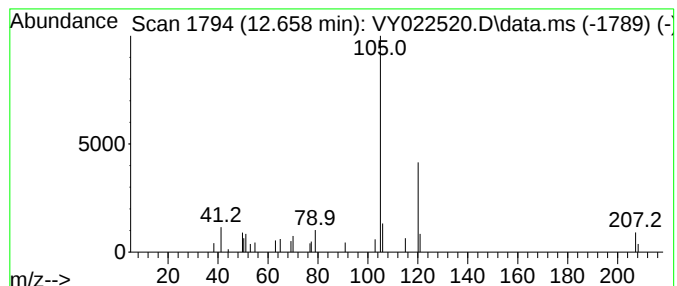
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Quant Title : SW846 8260

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

Peak Number 4 Benzene, 1-ethyl-4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.658	10.94 ug/l	5578	1,4-Dichlorobenzene-d4	13.347

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	64
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	59
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	59
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	59
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY060325\
Data File : VY022520.D
Acq On : 03 Jun 2025 14:14
Operator : SY/MD
Sample : Q2168-03
Misc : 5.50g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
A3

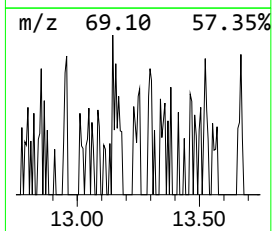
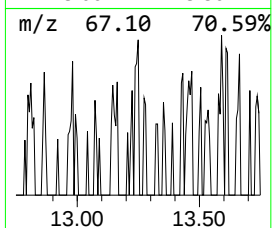
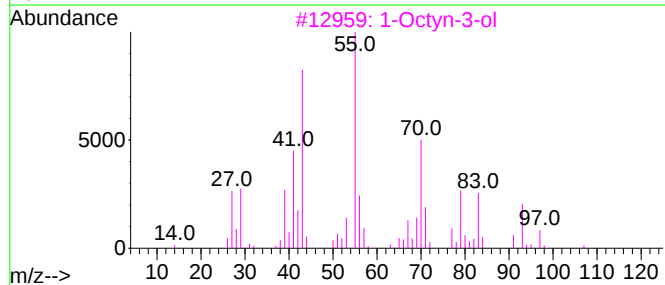
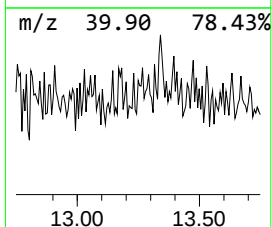
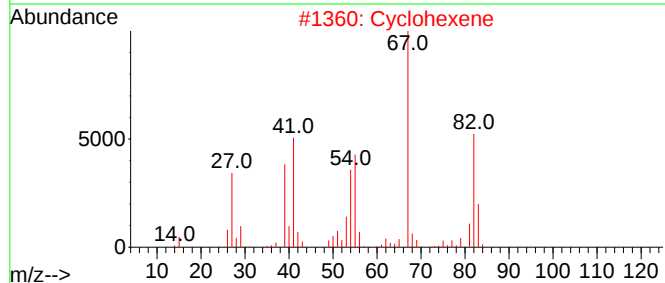
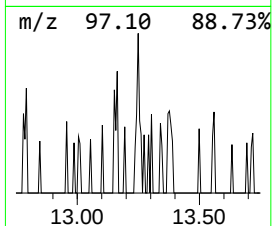
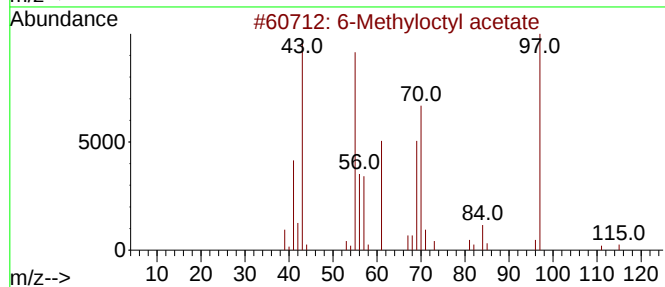
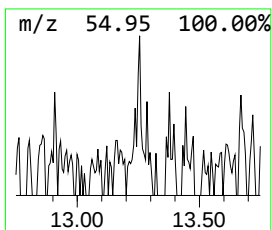
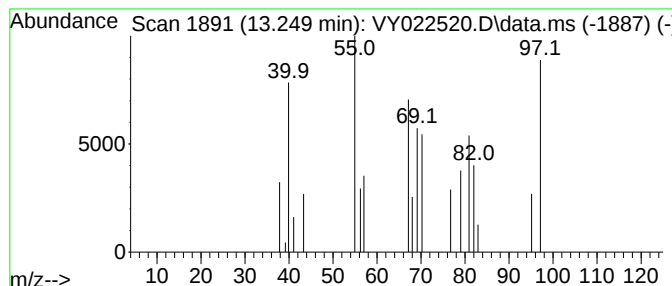
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060225S.M
Quant Title : SW846 8260

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

Peak Number 5 unknown13.249 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.249	5.27 ug/l	2689	1,4-Dichlorobenzene-d4	13.347

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			6-Methyloctyl acetate	186	C11H22O2	1000439-66-5	32
2			Cyclohexene	82	C6H10	000110-83-8	9
3			1-Octyn-3-ol	126	C8H14O	000818-72-4	9
4			1-Heptyn-3-ol	112	C7H12O	007383-19-9	9
5			trans-2-Methylcyclohexanol, trif...	210	C9H13F3O2	1000364-13-3	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY060325\
Data File : VY022520.D
Acq On : 03 Jun 2025 14:14
Operator : SY/MD
Sample : Q2168-03
Misc : 5.50g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
A3

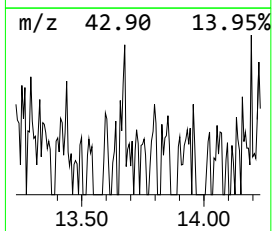
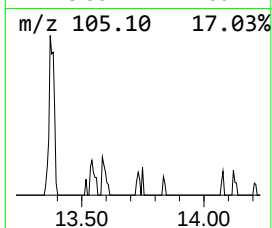
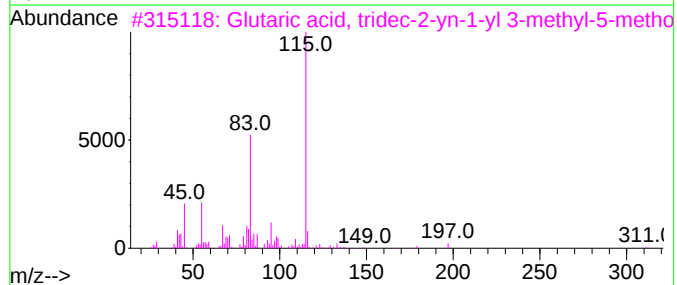
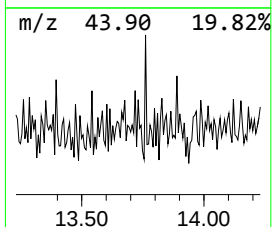
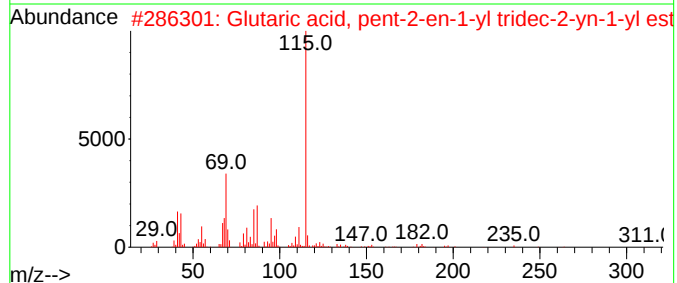
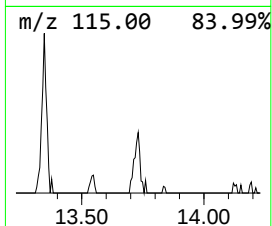
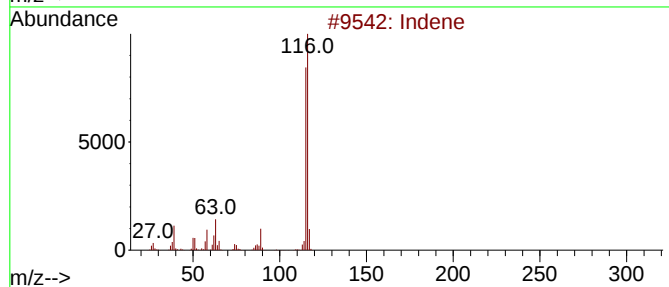
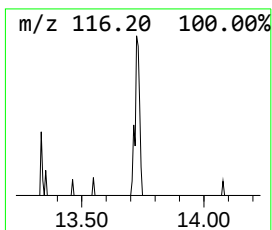
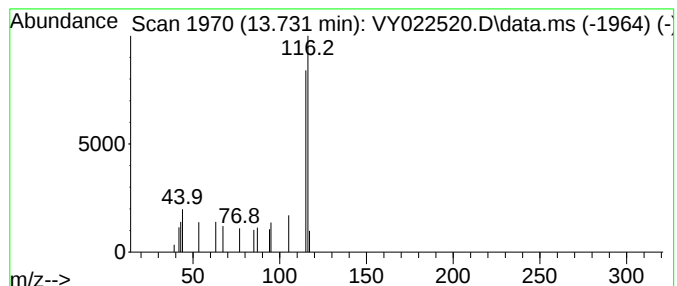
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060225S.M
Quant Title : SW846 8260

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

Peak Number 6 Indene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.730	6.00 ug/l	3061	1,4-Dichlorobenzene-d4	13.347

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indene	116	C9H8	000095-13-6	53
2			Glutaric acid, pent-2-en-1-yl tr...	378	C23H38O4	1000405-26-7	17
3			Glutaric acid, tridec-2-yn-1-yl ...	424	C25H44O5	1000393-53-3	17
4			4-Amino-3-mercapto-1,2,4-triazole	116	C2H4N4S	004343-75-3	9
5			Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY060325\
Data File : VY022520.D
Acq On : 03 Jun 2025 14:14
Operator : SY/MD
Sample : Q2168-03
Misc : 5.50g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
A3

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown2.086	2.086	19.5	ug/l	16611	1	7.707	42515	50.0
2-Ethyl-oxetane	5.647	12.2	ug/l	10360	1	7.707	42515	50.0
2,4,6,8-Tetrame...	10.298	5.8	ug/l	5342	3	11.420	45906	50.0
Benzene, 1-ethy...	12.658	10.9	ug/l	5578	4	13.347	25494	50.0
unknown13.249	13.249	5.3	ug/l	2689	4	13.347	25494	50.0
Indene	13.730	6.0	ug/l	3061	4	13.347	25494	50.0