

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW071422\
 Data File : VW023707.D
 Acq On : 14 Jul 2022 18:03
 Operator : SY/VA
 Sample : N3698-04RE
 Misc : 5.86g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 F5B69RE

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % 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_W\Method\SFAMWLM071322SMA.M
 Title : SFAM01.0

Signal : TIC: VW023707.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.001	339	344	353	rVB	16222	39181	26.59%	2.842%
2	4.062	353	354	358	rVB4	1348	1062	0.72%	0.077%
3	4.672	452	454	455	rBV2	1483	1093	0.74%	0.079%
4	4.873	484	487	488	rBV3	1718	1795	1.22%	0.130%
5	5.135	527	530	531	rBV3	1331	958	0.65%	0.069%
6	5.409	570	575	576	rBV5	2751	4150	2.82%	0.301%
7	5.696	620	622	624	rBV3	878	847	0.57%	0.061%
8	6.013	670	674	675	rBV4	954	1019	0.69%	0.074%
9	6.080	682	685	686	rBV3	1547	1648	1.12%	0.120%
10	6.147	694	696	698	rBV3	950	748	0.51%	0.054%
11	6.196	701	704	705	rBV2	965	980	0.67%	0.071%
12	6.257	711	714	716	rVB3	1018	1412	0.96%	0.102%
13	6.281	716	718	719	rBV2	1457	1153	0.78%	0.084%
14	6.354	728	730	733	rBV3	1320	1651	1.12%	0.120%
15	6.531	758	759	761	rBV2	950	722	0.49%	0.052%
16	6.556	761	763	766	rVB4	1311	919	0.62%	0.067%
17	6.879	808	816	819	rBV9	3942	10480	7.11%	0.760%
18	6.970	828	831	833	rBV4	1973	2605	1.77%	0.189%
19	7.092	844	851	855	rBV2	5567	15145	10.28%	1.099%
20	7.293	882	884	887	rBV4	1042	1225	0.83%	0.089%
21	7.403	900	902	903	rBV2	1380	882	0.60%	0.064%
22	7.647	935	942	949	rBV2	26677	64735	43.94%	4.696%
23	7.757	958	960	963	rBV4	1239	1358	0.92%	0.099%
24	7.842	972	974	975	rBV2	1154	947	0.64%	0.069%
25	8.031	997	1005	1012	rVB4	21020	52825	35.85%	3.832%
26	8.110	1016	1018	1019	rBV2	1892	1511	1.03%	0.110%
27	8.275	1037	1045	1058	rVB2	46482	147341	100.00%	10.687%
28	8.476	1073	1078	1090	rVB	33225	84570	57.40%	6.134%
29	8.689	1110	1113	1119	rBV7	1754	3060	2.08%	0.222%
30	8.842	1130	1138	1149	rVB	50037	102000	69.23%	7.399%
31	9.037	1166	1170	1172	rBV5	1309	1443	0.98%	0.105%
32	9.195	1192	1196	1200	rBV7	1372	2819	1.91%	0.204%
33	9.275	1202	1209	1214	rBV	36252	75566	51.29%	5.481%
34	9.567	1255	1257	1258	rBV2	1078	576	0.39%	0.042%
35	9.756	1282	1288	1296	rVB	22084	47204	32.04%	3.424%
36	9.896	1305	1311	1318	rBV3	14869	29551	20.06%	2.143%

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Integrator: RTE

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Sampling : 1

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Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM071322SMA.M
 Title : SFAM01.0

37	10.037	1329	1334	1341	rBV	14956	25256	17.14%	1.832%
38	10.183	1357	1358	1359	rBV	1262	689	0.47%	0.050%
39	10.244	1366	1368	1373	rVB6	4152	4271	2.90%	0.310%
40	10.323	1375	1381	1389	rVB	61936	106498	72.28%	7.725%
41	10.579	1418	1423	1433	rVB	10455	19671	13.35%	1.427%
42	10.927	1475	1480	1487	rBV	16385	27499	18.66%	1.995%
43	11.067	1498	1503	1510	rVB5	7252	15422	10.47%	1.119%
44	11.128	1510	1513	1515	rBV4	971	1473	1.00%	0.107%
45	11.390	1554	1556	1557	rVB2	1058	750	0.51%	0.054%
46	11.469	1568	1569	1572	rBV3	991	1139	0.77%	0.083%
47	11.518	1575	1577	1578	rBV2	1132	926	0.63%	0.067%
48	11.628	1589	1595	1603	rBV	72382	124592	84.56%	9.037%
49	11.811	1622	1625	1628	rBV5	1652	2183	1.48%	0.158%
50	11.878	1632	1636	1640	rVB5	1542	2643	1.79%	0.192%
51	11.914	1640	1642	1644	rBV3	1132	1065	0.72%	0.077%
52	12.048	1660	1664	1666	rBV5	1716	2367	1.61%	0.172%
53	12.189	1685	1687	1689	rBV3	1541	1535	1.04%	0.111%
54	12.298	1704	1705	1708	rBV3	1301	1215	0.82%	0.088%
55	12.524	1740	1742	1747	rVB5	1341	1877	1.27%	0.136%
56	12.603	1747	1755	1760	rBV5	6332	12826	8.70%	0.930%
57	12.689	1763	1769	1776	rVB	33094	57177	38.81%	4.147%
58	12.847	1793	1795	1797	rBV2	1116	876	0.59%	0.064%
59	12.884	1799	1801	1805	rVB4	1466	1902	1.29%	0.138%
60	12.920	1805	1807	1812	rBV6	2506	4874	3.31%	0.354%
61	13.073	1830	1832	1834	rBV3	694	785	0.53%	0.057%
62	13.109	1834	1838	1840	rBV4	1531	1607	1.09%	0.117%
63	13.188	1847	1851	1855	rVB6	2266	3483	2.36%	0.253%
64	13.292	1864	1868	1871	rBV6	1539	2378	1.61%	0.172%
65	13.396	1878	1885	1891	rBV6	4315	11784	8.00%	0.855%
66	13.469	1896	1897	1901	rBV4	1273	1363	0.93%	0.099%
67	13.554	1905	1911	1916	rBV	59180	98012	66.52%	7.109%
68	13.725	1937	1939	1941	rBV3	791	957	0.65%	0.069%
69	13.755	1941	1944	1947	rVV5	2369	3009	2.04%	0.218%
70	13.804	1951	1952	1953	rBV	1416	693	0.47%	0.050%
71	13.853	1953	1960	1967	rVV2	51216	87017	59.06%	6.312%
72	14.024	1986	1988	1989	rBV2	1318	882	0.60%	0.064%
73	14.207	2014	2018	2021	rBV6	3386	5350	3.63%	0.388%
74	14.304	2032	2034	2036	rBV3	1565	1412	0.96%	0.102%
75	14.542	2072	2073	2077	rBV4	956	1190	0.81%	0.086%
76	14.639	2086	2089	2092	rVV5	1636	2170	1.47%	0.157%

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Stop Thrs : 0

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM071322SMA.M
 Title : SFAM01.0

77	14.792	2112	2114	2116	rBV3	1070	774	0.53%	0.056%
78	14.835	2119	2121	2122	rBV2	939	694	0.47%	0.050%
79	14.853	2122	2124	2125	rBV2	1072	753	0.51%	0.055%
80	14.938	2136	2138	2142	rBV5	992	1289	0.87%	0.093%
81	15.024	2149	2152	2155	rVB4	2193	2266	1.54%	0.164%
82	15.084	2155	2162	2164	rBV7	1947	4193	2.85%	0.304%
83	15.158	2172	2174	2175	rBV2	1161	1102	0.75%	0.080%
84	15.401	2212	2214	2215	rBV2	839	657	0.45%	0.048%
85	15.609	2247	2248	2251	rBV3	1155	1095	0.74%	0.079%
86	15.639	2251	2253	2255	rVV2	741	705	0.48%	0.051%
87	15.658	2255	2256	2258	rVV2	962	723	0.49%	0.052%
88	15.804	2278	2280	2284	rVB4	1334	1792	1.22%	0.130%
89	15.840	2284	2286	2288	rVB3	792	718	0.49%	0.052%
90	15.877	2288	2292	2297	rVB7	1754	3732	2.53%	0.271%
91	15.920	2297	2299	2300	rBV2	1400	806	0.55%	0.058%
92	15.981	2307	2309	2312	rBV4	962	1123	0.76%	0.081%
93	16.066	2322	2323	2326	rVB3	1287	1068	0.72%	0.077%
94	16.115	2326	2331	2333	rBV6	1276	2398	1.63%	0.174%
95	16.273	2353	2357	2360	rBV6	1218	1955	1.33%	0.142%
96	16.371	2372	2373	2377	rBV4	1070	1118	0.76%	0.081%
97	16.609	2411	2412	2416	rVB4	1034	1082	0.73%	0.078%
98	16.645	2416	2418	2419	rBV2	1056	896	0.61%	0.065%
99	16.694	2424	2426	2429	rVB4	789	786	0.53%	0.057%
100	16.724	2429	2431	2434	rBV4	812	912	0.62%	0.066%

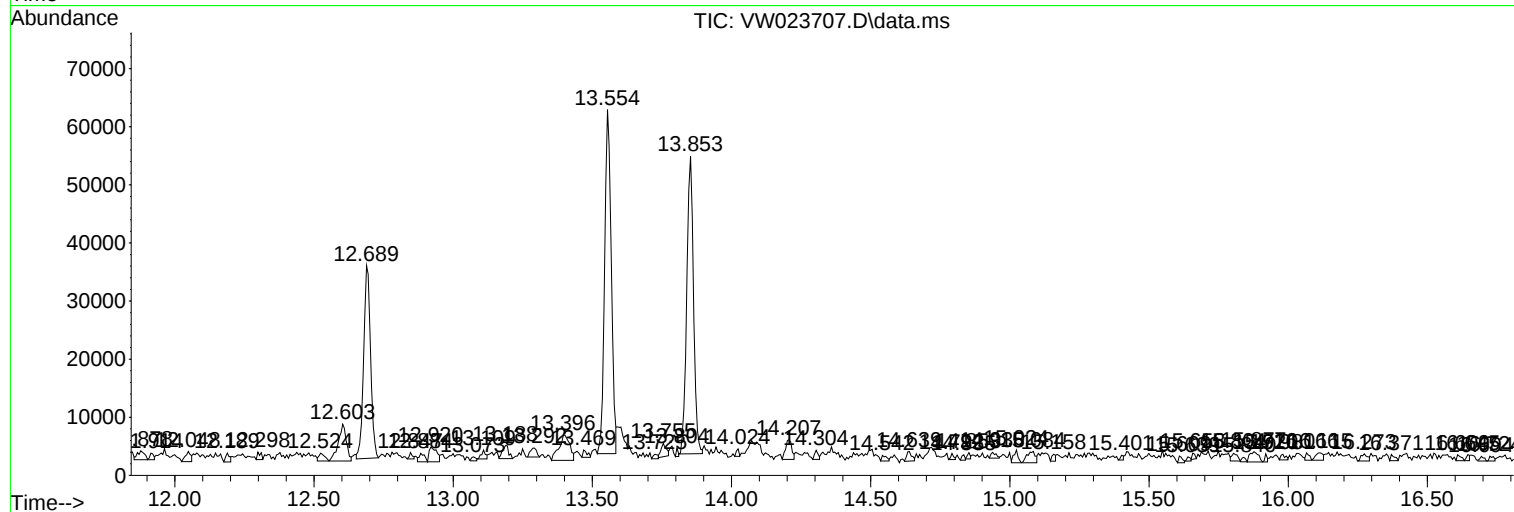
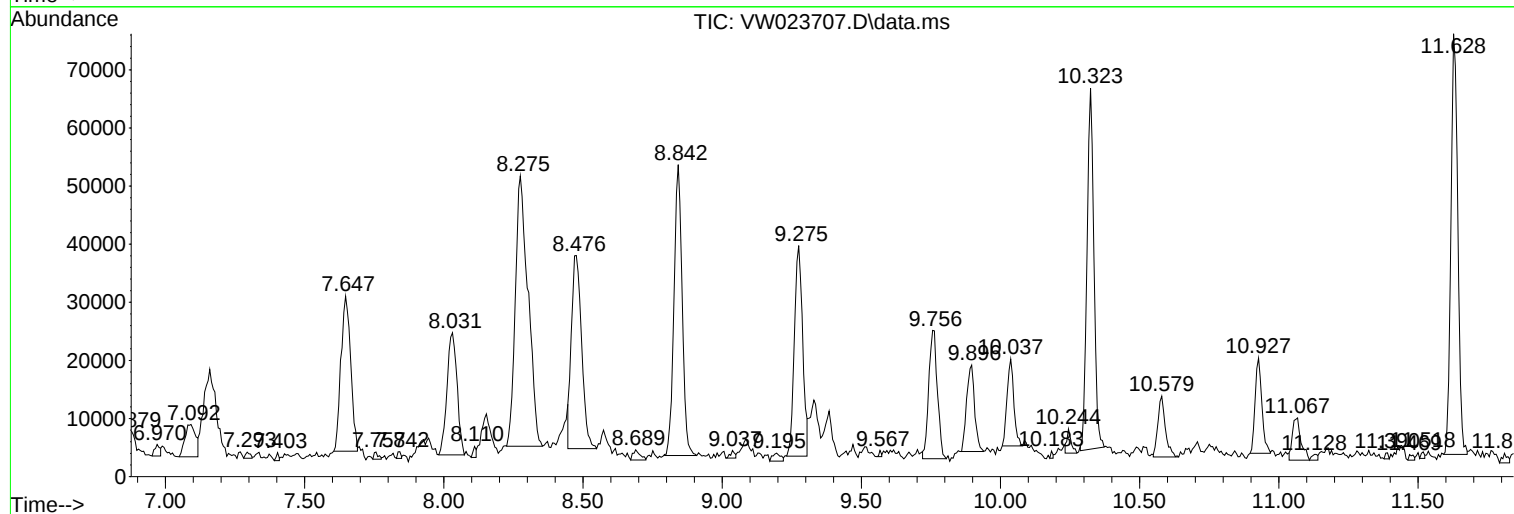
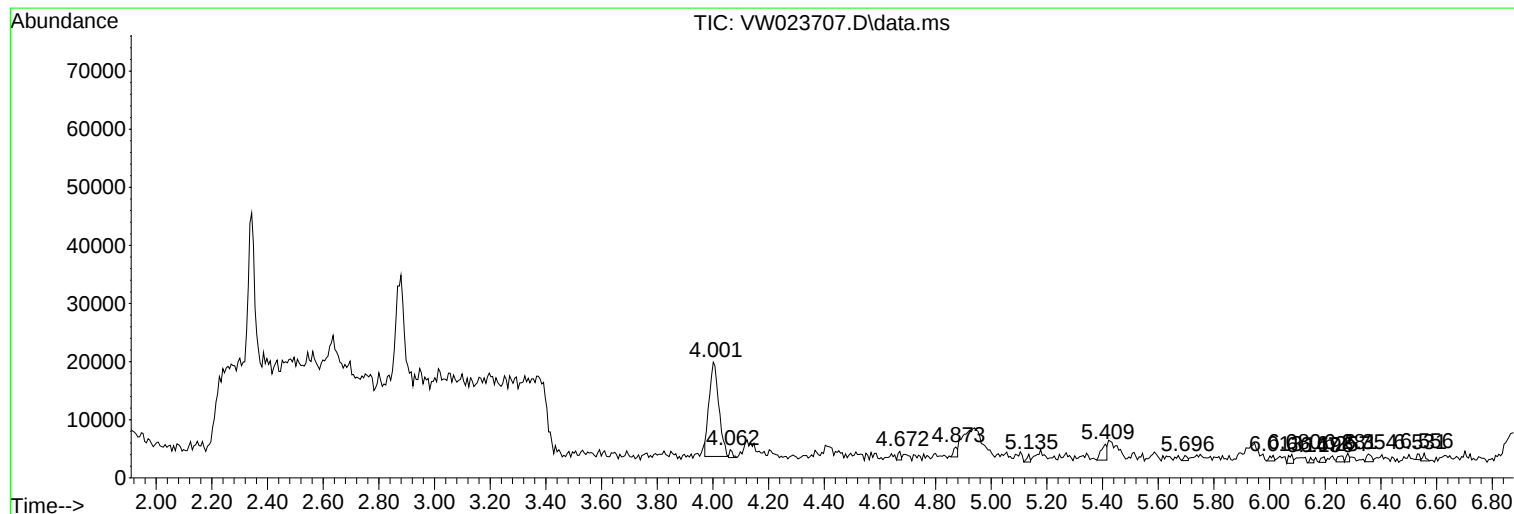
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ALS Vial : 1 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM071322SMA.M
Quant Title : SFAM01.0

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



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Instrument :
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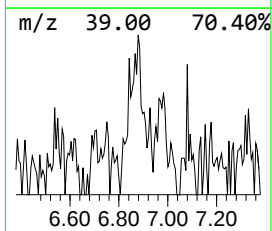
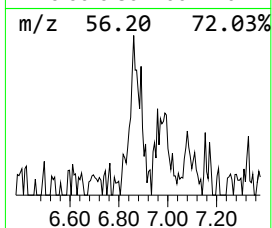
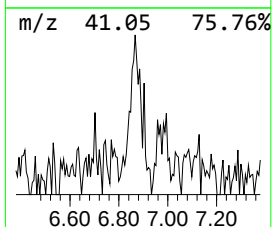
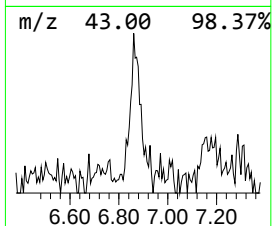
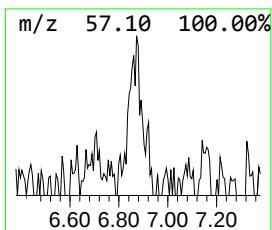
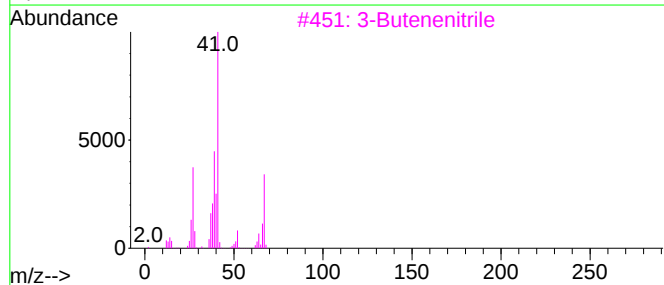
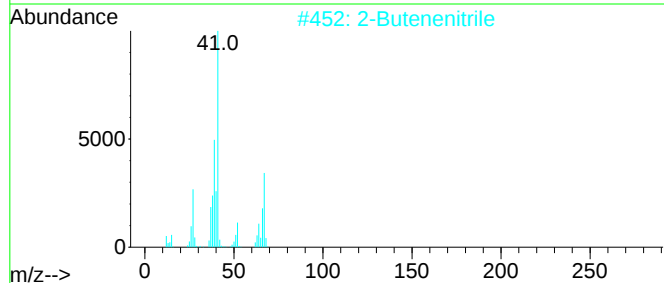
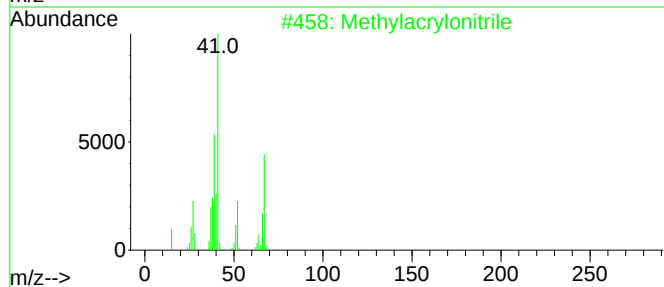
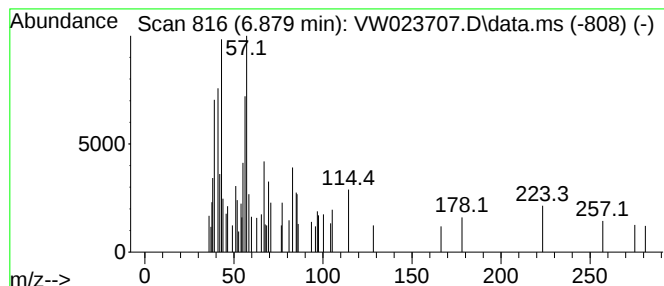
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM071322SMA.M
Quant Title : SFAM01.0

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

Peak Number 1 unknown-01 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.879	2.57 ug/L	10480	1,4-Difluorobenzene	8.842

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methylacrylonitrile	67	C4H5N	000126-98-7	47
2			2-Butenenitrile	67	C4H5N	004786-20-3	47
3			3-Butenenitrile	67	C4H5N	000109-75-1	35
4			Carbamic acid, N-(4-chlorophenyl...	292	C13H9ClN2O4	003848-41-7	27
5			2-Butynoic acid	84	C4H4O2	000590-93-2	17



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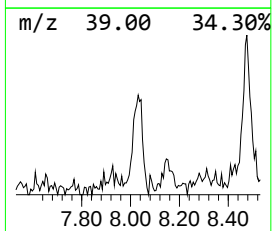
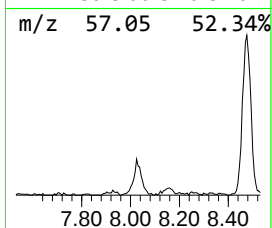
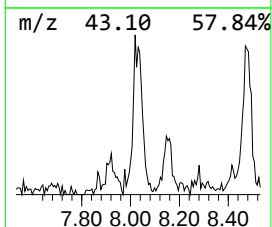
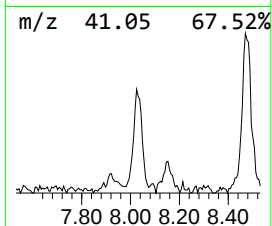
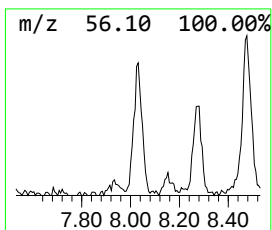
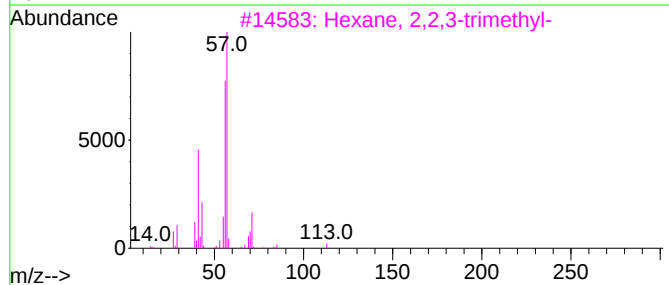
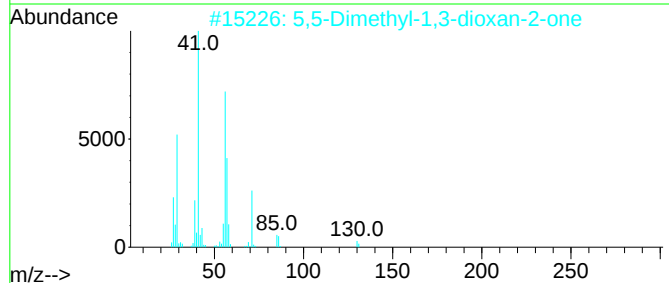
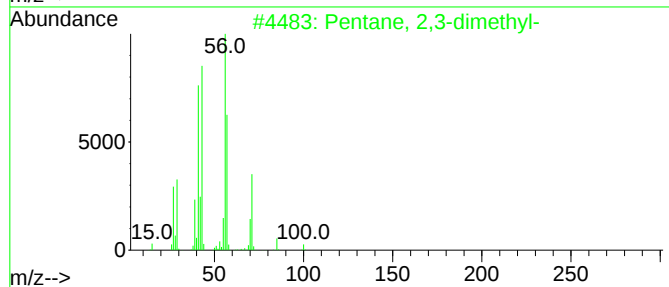
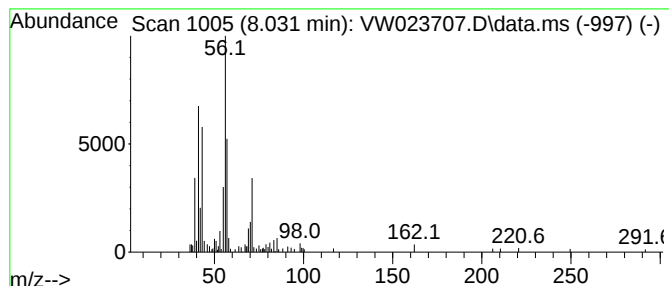
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM071322SMA.M
Quant Title : SFAM01.0

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.031	12.95 ug/L	52825	1,4-Difluorobenzene	8.842

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	87
2		5,5-Dimethyl-1,3-dioxan-2-one	130	C6H10O3	003592-12-9	59
3		Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	59
4		Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	56
5		Aziridine, 2-methyl-	57	C3H7N	000075-55-8	53



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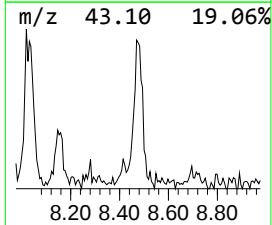
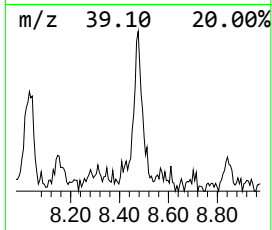
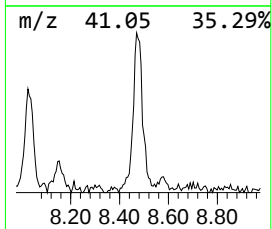
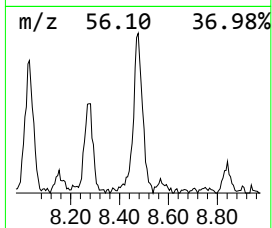
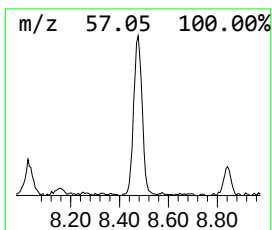
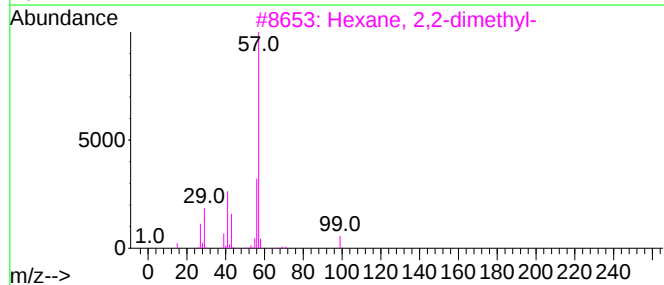
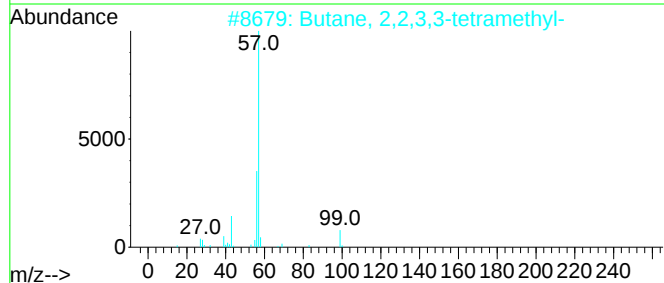
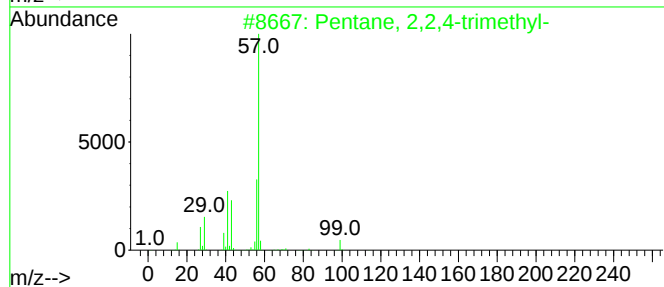
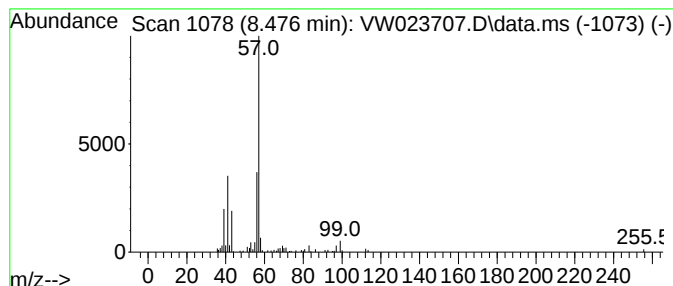
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Quant Title : SFAM01.0

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.476	20.73 ug/L	84570	1,4-Difluorobenzene	8.842

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	64
2		Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	64
3		Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	64
4		Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	53
5		Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW071422\
Data File : VW023707.D
Acq On : 14 Jul 2022 18:03
Operator : SY/VA
Sample : N3698-04RE
Misc : 5.86g/10mL/MSVOA_W/SOIL
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
F5B69RE

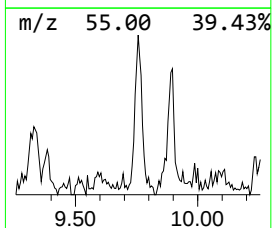
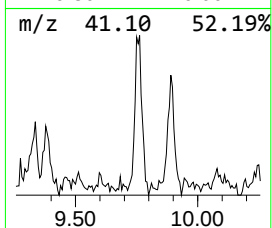
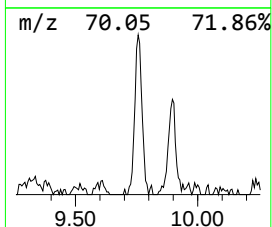
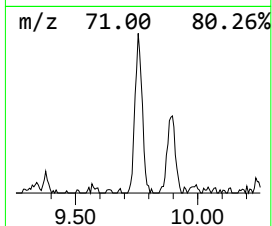
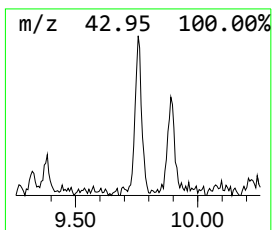
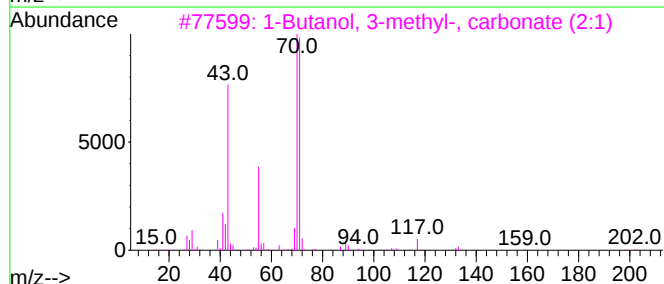
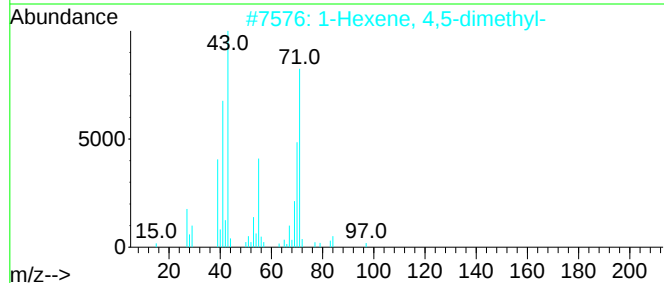
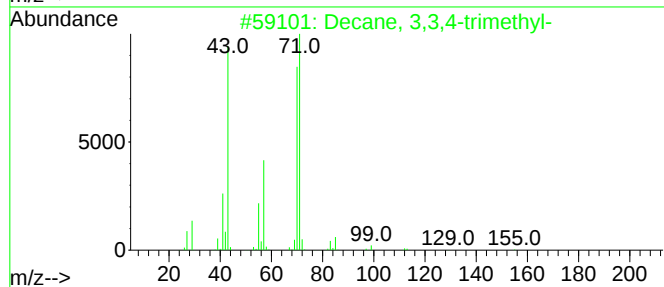
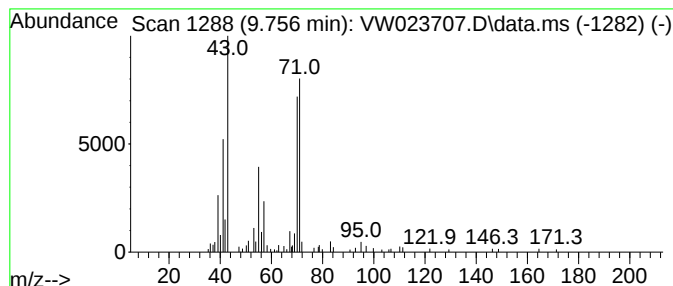
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Quant Title : SFAM01.0

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.756	11.57 ug/L	47204	1,4-Difluorobenzene	8.842

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	64
2		1-Hexene, 4,5-dimethyl-	112	C8H16	016106-59-5	59
3		1-Butanol, 3-methyl-, carbonate ...	202	C11H22O3	002050-95-5	59
4		1-Hexene, 3,4,5-trimethyl-	126	C9H18	056728-10-0	53
5		2-Butene, 1-methoxy-, (Z)-	86	C5H10O	010034-16-9	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW071422\
Data File : VW023707.D
Acq On : 14 Jul 2022 18:03
Operator : SY/VA
Sample : N3698-04RE
Misc : 5.86g/10mL/MSVOA_W/SOIL
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
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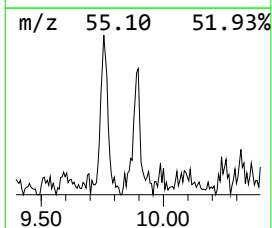
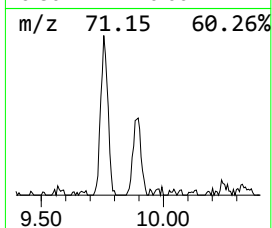
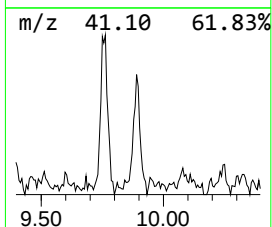
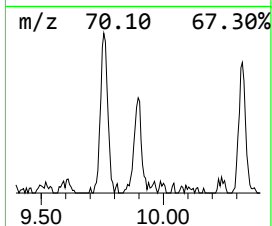
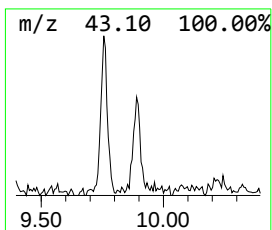
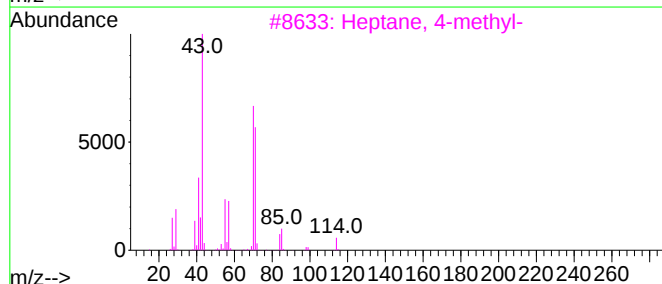
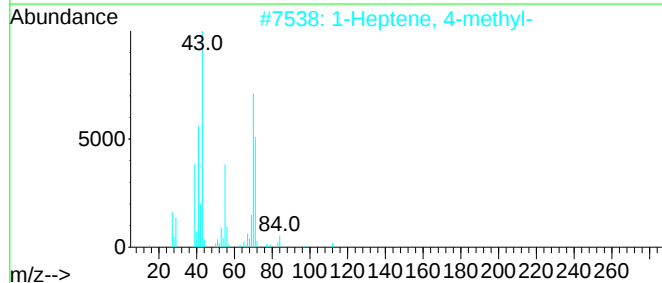
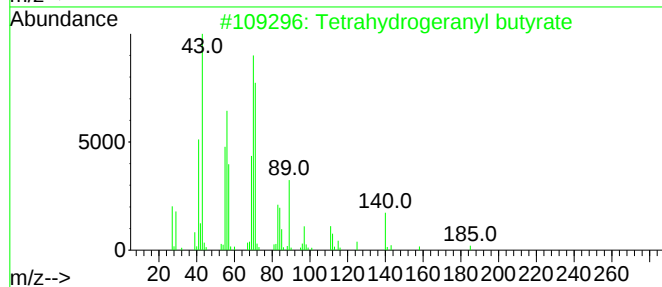
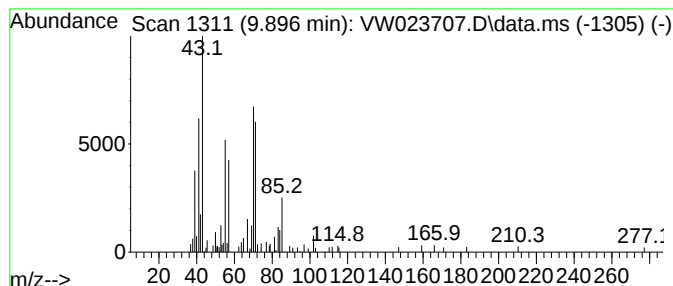
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Quant Title : SFAM01.0

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

Peak Number 5 Tetrahydrogeranyl butyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.896	7.24 ug/L	29551	1,4-Difluorobenzene	8.842

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetrahydrogeranyl butyrate	228	C14H28O2	1000428-75-4	59
2			1-Heptene, 4-methyl-	112	C8H16	013151-05-8	58
3			Heptane, 4-methyl-	114	C8H18	000589-53-7	53
4			Hexane, 3-methyl-	100	C7H16	000589-34-4	50
5			1-Nonene, 4,6,8-trimethyl-	168	C12H24	054410-98-9	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW071422\
Data File : VW023707.D
Acq On : 14 Jul 2022 18:03
Operator : SY/VA
Sample : N3698-04RE
Misc : 5.86g/10mL/MSVOA_W/SOIL
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
F5B69RE

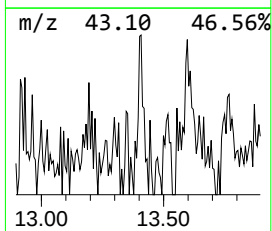
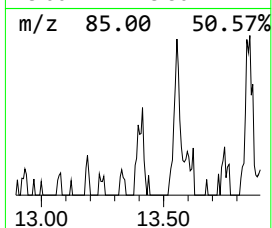
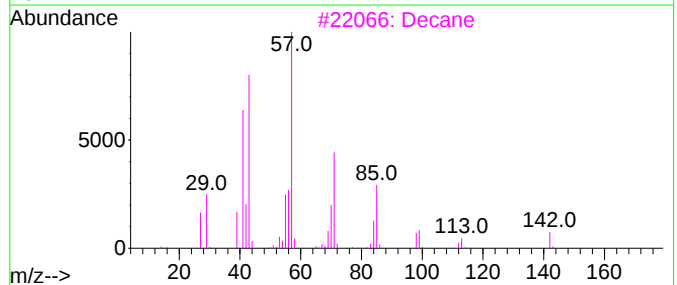
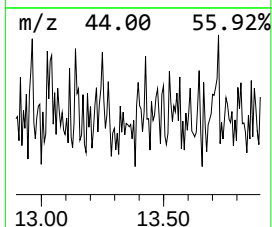
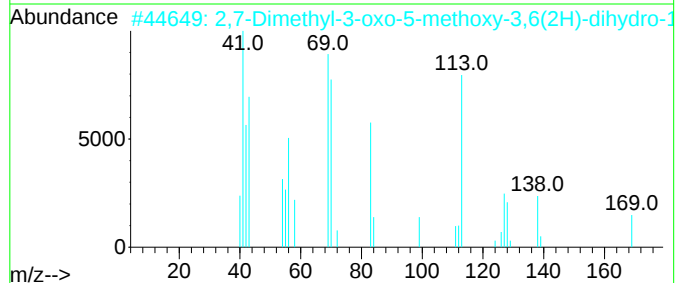
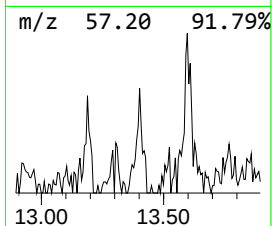
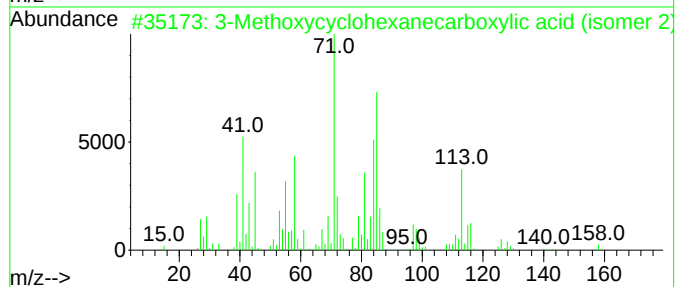
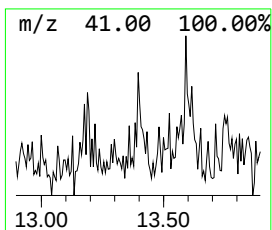
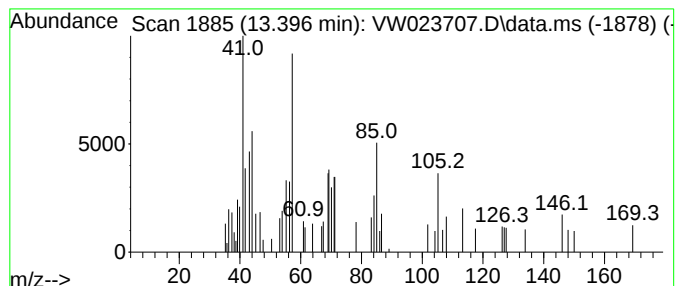
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Quant Title : SFAM01.0

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

Peak Number 9 unknown-02 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.396	3.01 ug/L	11784	1,4-Dichlorobenzene-d4	13.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Methoxycyclohexanecarboxylic a...	158	C8H14O3	1000453-57-3	16
2			2,7-Dimethyl-3-oxo-5-methoxy-3,6...	169	C7H11N3O2	1000143-29-0	16
3			Decane	142	C10H22	000124-18-5	14
4			3-Ethyl-3-methylheptane	142	C10H22	017302-01-1	12
5			Oxalic acid, butyl 6-ethyloct-3-...	286	C16H30O4	1000309-34-2	12



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW071422\
Data File : VW023707.D
Acq On : 14 Jul 2022 18:03
Operator : SY/VA
Sample : N3698-04RE
Misc : 5.86g/10mL/MSVOA_W/SOIL
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
F5B69RE

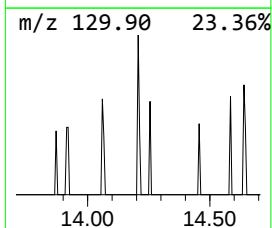
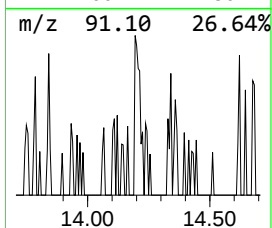
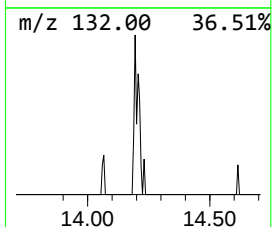
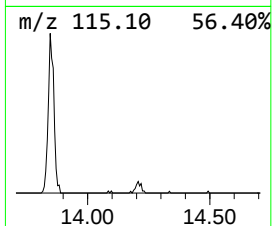
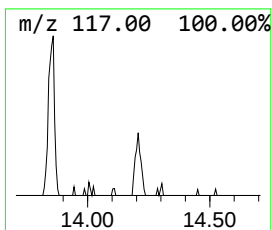
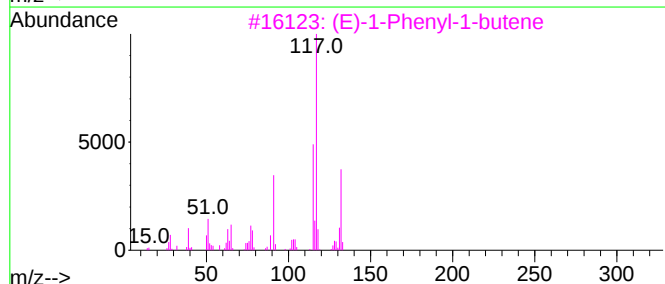
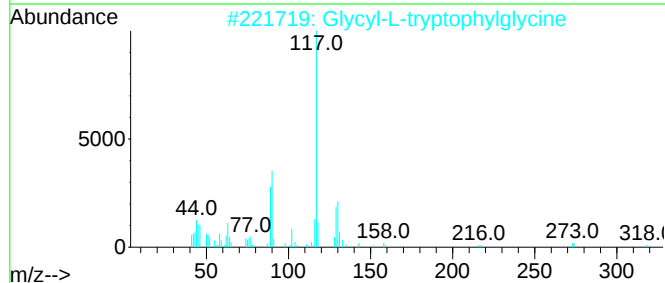
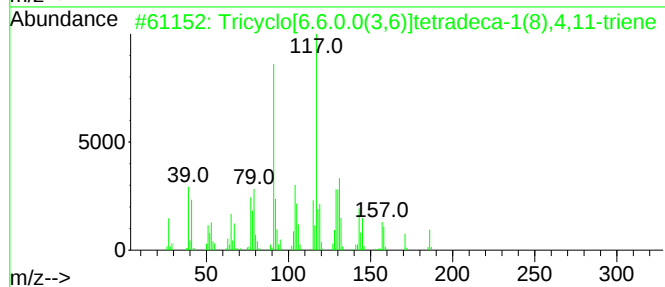
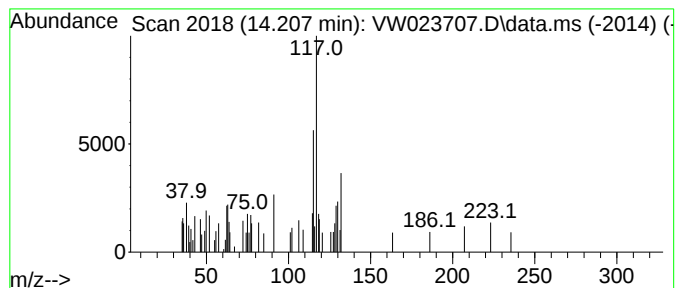
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Quant Title : SFAM01.0

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

Peak Number 10 unknown-03 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.207	1.36 ug/L	5350	1,4-Dichlorobenzene-d4	13.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tricyclo[6.6.0.0(3,6)]tetradeca-	186	C14H18	1000151-40-9	38
2			Glycyl-L-tryptophylglycine	318	C15H18N4O4	023067-32-5	35
3			(E)-1-Phenyl-1-butene	132	C10H12	001005-64-7	18
4			1H-Indole-1-carboxaldehyde, 2,3-	163	C9H9NO2	013303-68-9	16
5			3-Phenylbut-1-ene	132	C10H12	000934-10-1	14



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW071422\
Data File : VW023707.D
Acq On : 14 Jul 2022 18:03
Operator : SY/VA
Sample : N3698-04RE
Misc : 5.86g/10mL/MSVOA_W/SOIL
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
F5B69RE

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM071322SMA.M
Quant Title : SFAM01.0

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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(DEL) Alkane: S...	8.031	12.9	ug/L	52825	1	8.842	102000	25.0
(DEL) Alkane: S...	8.476	20.7	ug/L	84570	1	8.842	102000	25.0
(DEL) Alkane: S...	9.756	11.6	ug/L	47204	1	8.842	102000	25.0
Tetrahydrogeran...	9.896	7.2	ug/L	29551	1	8.842	102000	25.0
unknown-02	13.396	3.0	ug/L	11784	3	13.554	98012	25.0
unknown-03	14.207	1.4	ug/L	5350	3	13.554	98012	25.0