

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW050922\
 Data File : VW022938.D
 Acq On : 09 May 2022 18:28
 Operator : SY/VA
 Sample : N2714-05RE
 Misc : 4.48g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 EW2X6RE

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\SFAMWLM050222SMA.M
 Title : SFAM01.0

Signal : TIC: VW022938.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.843	153	154	157	rVB3	936	859	1.34%	0.186%
2	3.007	180	181	183	rVB2	1201	794	1.24%	0.172%
3	3.044	183	187	188	rBV4	1244	1783	2.78%	0.387%
4	3.178	208	209	212	rBV3	942	1008	1.57%	0.219%
5	3.276	223	225	227	rVB2	1265	953	1.48%	0.207%
6	3.300	227	229	230	rBV	1175	1070	1.67%	0.232%
7	3.355	236	238	240	rBV3	888	984	1.53%	0.213%
8	3.410	244	247	248	rBV2	1139	1193	1.86%	0.259%
9	3.489	256	260	265	rBV5	840	1815	2.82%	0.394%
10	3.611	277	280	281	rBV3	1319	1326	2.06%	0.288%
11	3.702	293	295	301	rVV6	1131	1899	2.96%	0.412%
12	3.782	304	308	311	rVB4	1123	1789	2.78%	0.388%
13	4.032	343	349	358	rVB4	7874	20565	32.01%	4.460%
14	4.093	358	359	362	rBV2	901	804	1.25%	0.174%
15	4.135	362	366	371	rBV5	1367	3121	4.86%	0.677%
16	4.343	399	400	401	rBV5	1257	774	1.20%	0.168%
17	4.434	413	415	420	rVB5	985	1431	2.23%	0.310%
18	4.489	422	424	427	rBV3	646	812	1.26%	0.176%
19	4.885	487	489	490	rBV2	1126	792	1.23%	0.172%
20	5.013	505	510	511	rBV5	2626	4029	6.27%	0.874%
21	5.263	549	551	552	rBV2	865	738	1.15%	0.160%
22	5.330	559	562	563	rBV4	1000	1038	1.62%	0.225%
23	5.403	569	574	576	rBV3	904	1312	2.04%	0.285%
24	5.824	641	643	645	rVB2	1065	850	1.32%	0.184%
25	5.946	660	663	664	rBV3	1460	1826	2.84%	0.396%
26	6.068	682	683	685	rBV2	1029	787	1.22%	0.171%
27	6.220	705	708	710	rBV3	891	982	1.53%	0.213%
28	6.269	714	716	719	rBV4	1050	1217	1.89%	0.264%
29	6.318	722	724	725	rBV2	1137	754	1.17%	0.164%
30	6.415	736	740	744	rBV6	1755	2885	4.49%	0.626%
31	6.513	754	756	759	rVB4	1357	1302	2.03%	0.282%
32	7.025	837	840	841	rBV3	965	812	1.26%	0.176%
33	7.043	841	843	846	rVV3	1108	1194	1.86%	0.259%
34	7.494	916	917	921	rBV4	778	753	1.17%	0.163%
35	7.543	921	925	927	rBV4	860	1214	1.89%	0.263%
36	7.641	935	941	942	rBV6	11174	15039	23.41%	3.261%

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37	7.787	963	965	969	rBV5	1949	2665	4.15%	0.578%
38	7.854	974	976	979	rVB3	844	820	1.28%	0.178%
39	7.976	993	996	999	rBV5	916	1290	2.01%	0.280%
40	8.080	1011	1013	1015	rVB3	1085	911	1.42%	0.198%
41	8.196	1028	1032	1034	rBV4	882	1327	2.07%	0.288%
42	8.275	1038	1045	1057	rVV4	19238	64252	100.00%	13.934%
43	8.781	1123	1128	1129	rBV4	1021	1400	2.18%	0.304%
44	8.842	1133	1138	1146	rVB	20454	40812	63.52%	8.851%
45	9.281	1201	1210	1218	rBV2	15034	31794	49.48%	6.895%
46	9.342	1218	1220	1224	rVB5	1117	1055	1.64%	0.229%
47	9.409	1228	1231	1234	rBV3	1404	1318	2.05%	0.286%
48	9.500	1244	1246	1248	rBV3	651	748	1.16%	0.162%
49	9.598	1260	1262	1266	rVB5	846	905	1.41%	0.196%
50	9.781	1291	1292	1294	rVB2	1041	739	1.15%	0.160%
51	9.860	1303	1305	1306	rBV2	1072	792	1.23%	0.172%
52	9.970	1320	1323	1326	rBV5	1081	1586	2.47%	0.344%
53	10.037	1328	1334	1340	rVV2	5811	11940	18.58%	2.589%
54	10.152	1351	1353	1355	rBV3	1365	846	1.32%	0.183%
55	10.177	1355	1357	1360	rBV2	856	877	1.36%	0.190%
56	10.220	1362	1364	1367	rBV	896	1097	1.71%	0.238%
57	10.250	1367	1369	1372	rVB4	1302	963	1.50%	0.209%
58	10.323	1372	1381	1386	rBV2	24260	46116	71.77%	10.001%
59	10.585	1418	1424	1430	rBV3	4042	7698	11.98%	1.669%
60	10.683	1438	1440	1444	rBV4	954	996	1.55%	0.216%
61	10.890	1473	1474	1478	rVB3	1305	1167	1.82%	0.253%
62	10.933	1478	1481	1484	rBV5	1184	2110	3.28%	0.458%
63	10.969	1484	1487	1492	rVB4	941	1465	2.28%	0.318%
64	11.158	1514	1518	1519	rBV3	730	994	1.55%	0.216%
65	11.256	1531	1534	1540	rBV7	805	1346	2.09%	0.292%
66	11.360	1549	1551	1552	rBV2	1235	830	1.29%	0.180%
67	11.475	1566	1570	1572	rBV4	814	1153	1.79%	0.250%
68	11.579	1583	1587	1589	rBV5	1014	1152	1.79%	0.250%
69	11.634	1589	1596	1605	rBV	24853	47632	74.13%	10.330%
70	11.768	1617	1618	1623	rVB4	1078	1049	1.63%	0.227%
71	11.829	1626	1628	1631	rVV3	1634	1960	3.05%	0.425%
72	12.097	1669	1672	1674	rBV4	1142	1549	2.41%	0.336%
73	12.317	1707	1708	1712	rBV3	793	1055	1.64%	0.229%
74	12.597	1749	1754	1755	rBV3	1099	1555	2.42%	0.337%
75	12.658	1762	1764	1765	rVV2	1263	877	1.36%	0.190%
76	12.689	1765	1769	1778	rVB2	9868	18255	28.41%	3.959%

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 Title : SFAM01.0

77	13.012	1819	1822	1823	rBV3	1185	1048	1.63%	0.227%
78	13.067	1830	1831	1835	rVB3	858	848	1.32%	0.184%
79	13.371	1877	1881	1884	rBV5	1667	1766	2.75%	0.383%
80	13.402	1884	1886	1889	rVB3	859	734	1.14%	0.159%
81	13.554	1906	1911	1921	rVV2	15320	27443	42.71%	5.951%
82	13.652	1925	1927	1929	rVV	1067	860	1.34%	0.187%
83	13.695	1933	1934	1938	rVB4	832	945	1.47%	0.205%
84	13.853	1954	1960	1965	rBV2	12120	20354	31.68%	4.414%
85	13.999	1982	1984	1987	rVB3	1238	972	1.51%	0.211%
86	14.201	2016	2017	2019	rVB2	1142	754	1.17%	0.164%
87	14.341	2038	2040	2041	rBV2	1190	740	1.15%	0.160%
88	14.438	2051	2056	2057	rBV4	1070	1209	1.88%	0.262%
89	14.579	2077	2079	2080	rBV	822	804	1.25%	0.174%
90	14.804	2114	2116	2118	rBV2	1371	1519	2.36%	0.329%
91	14.871	2125	2127	2128	rBV2	1237	751	1.17%	0.163%
92	14.920	2134	2135	2138	rBV3	872	1003	1.56%	0.218%
93	14.993	2145	2147	2149	rVB3	1204	947	1.47%	0.205%
94	15.152	2171	2173	2175	rBV3	632	738	1.15%	0.160%
95	15.213	2181	2183	2186	rBV3	808	875	1.36%	0.190%
96	15.322	2200	2201	2204	rBV3	966	1054	1.64%	0.229%
97	15.920	2297	2299	2302	rVB2	1480	929	1.45%	0.201%
98	16.164	2336	2339	2342	rBV5	1677	2329	3.62%	0.505%
99	16.206	2342	2346	2352	rBV8	1602	4140	6.44%	0.898%
100	16.481	2389	2391	2393	rBV3	781	756	1.18%	0.164%

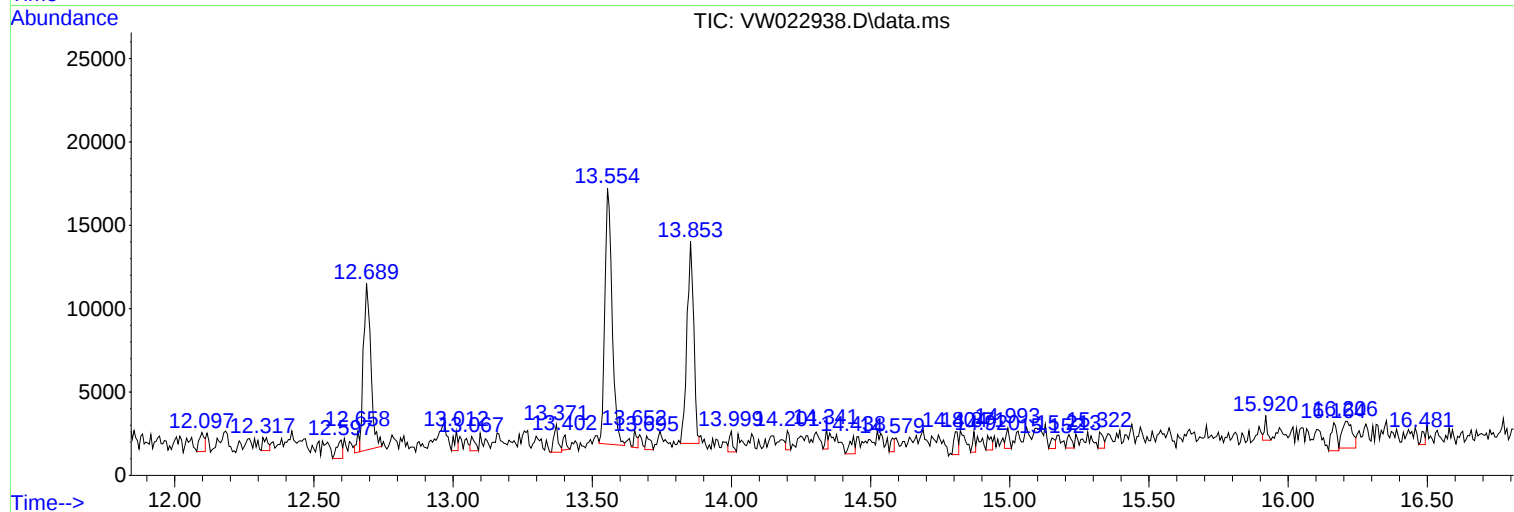
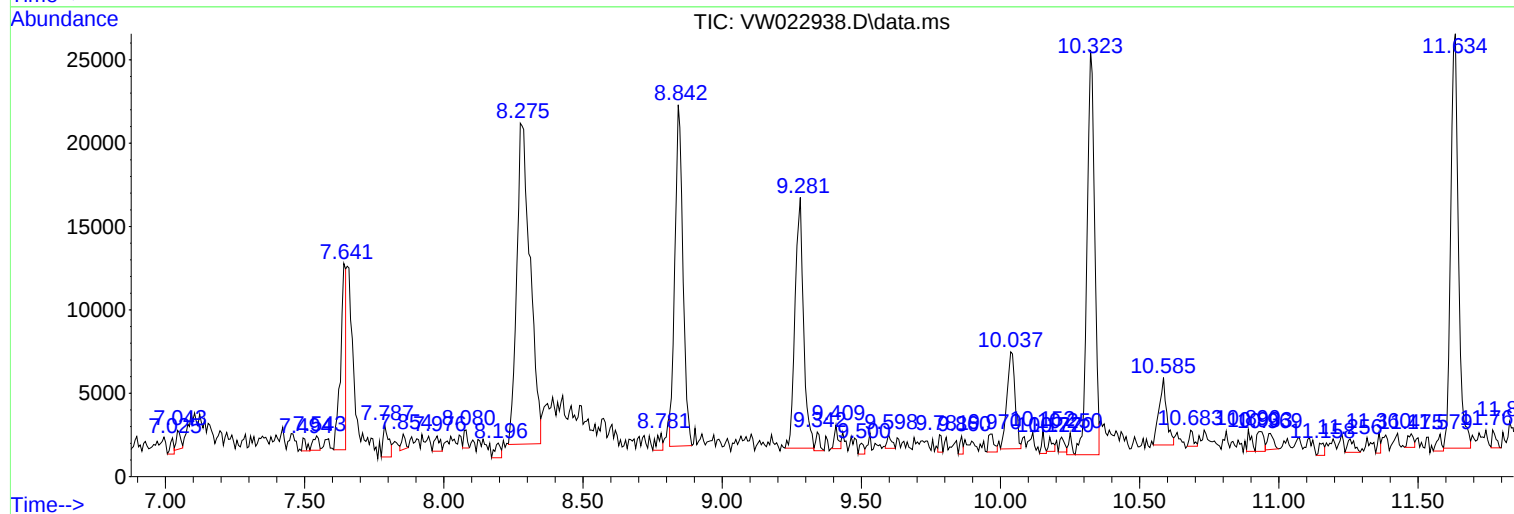
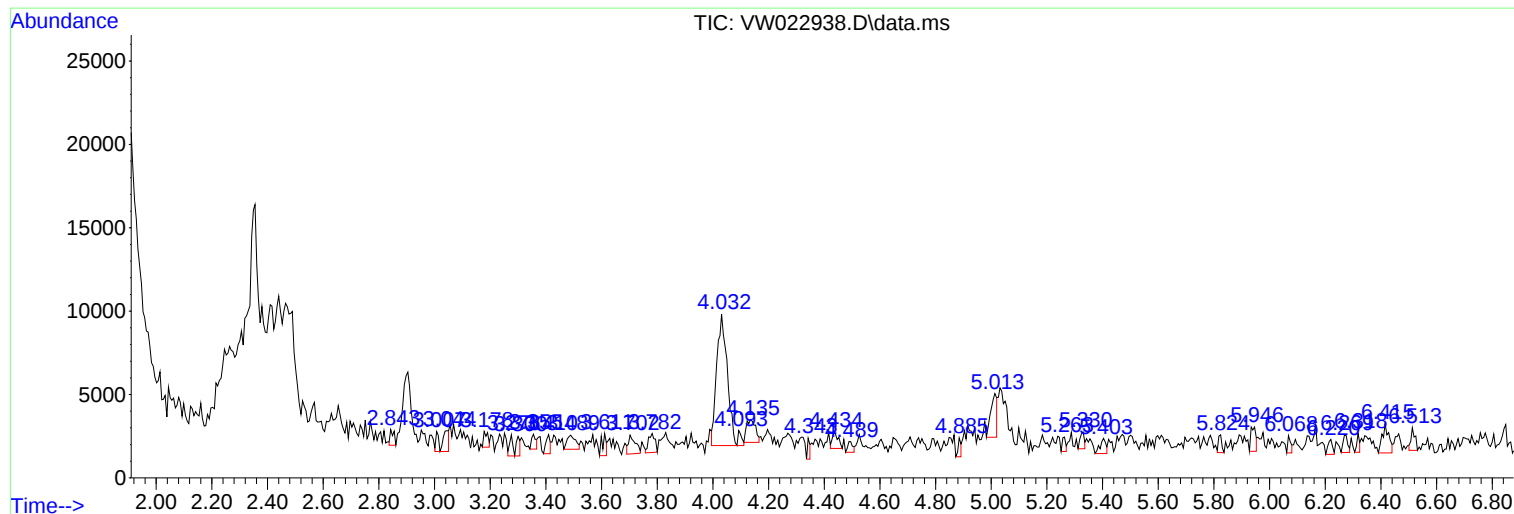
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM050222SMA.M
Quant Title : SFAM01.0

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



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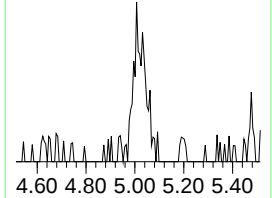
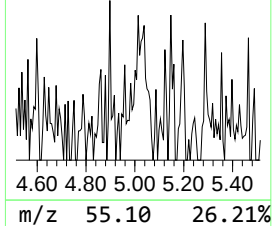
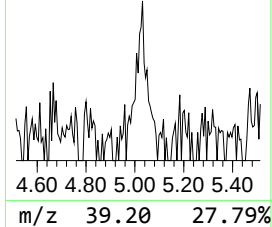
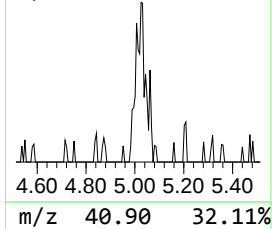
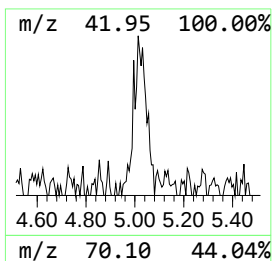
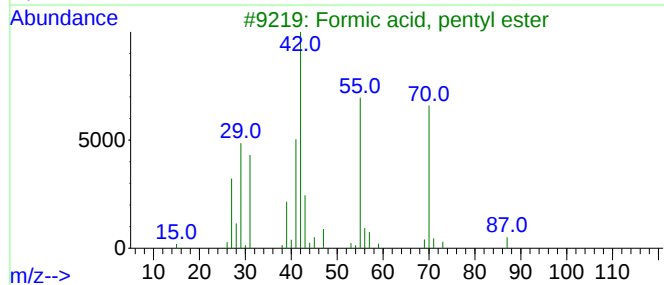
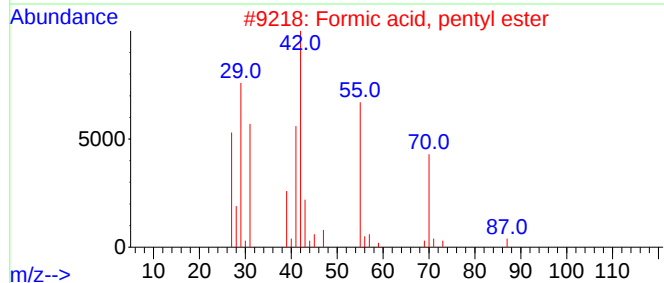
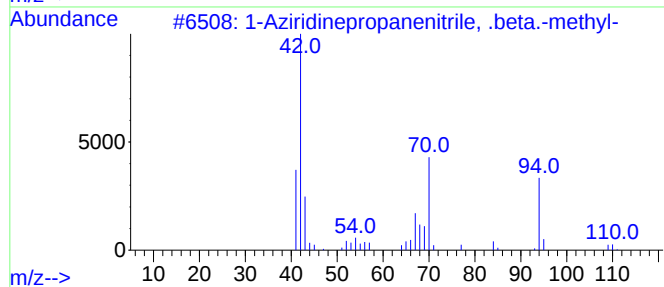
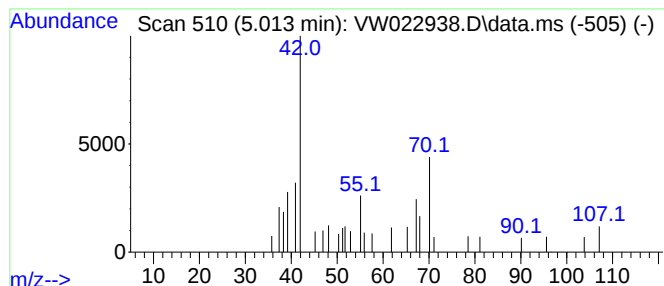
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM050222SMA.M
Quant Title : SFAM01.0

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

Peak Number 1 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.013	2.47 ug/L	4029	1,4-Difluorobenzene	8.848

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Aziridinepropanenitrile, .beta...	110	C6H10N2	004078-19-7	28
2			Formic acid, pentyl ester	116	C6H12O2	000638-49-3	27
3			Formic acid, pentyl ester	116	C6H12O2	000638-49-3	27
4			1-Pentene	70	C5H10	000109-67-1	9
5			1-Pentene	70	C5H10	000109-67-1	9



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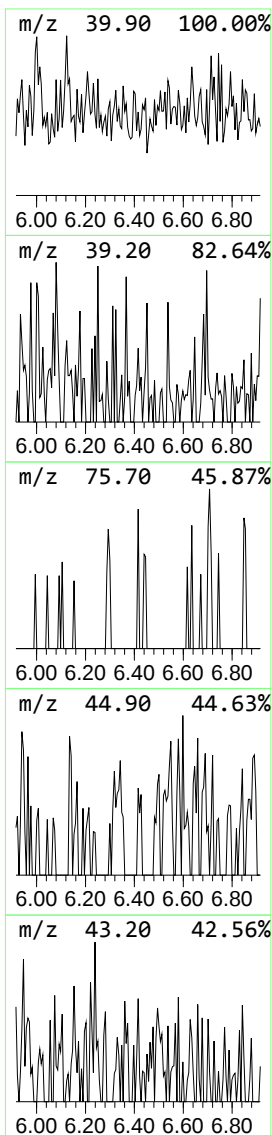
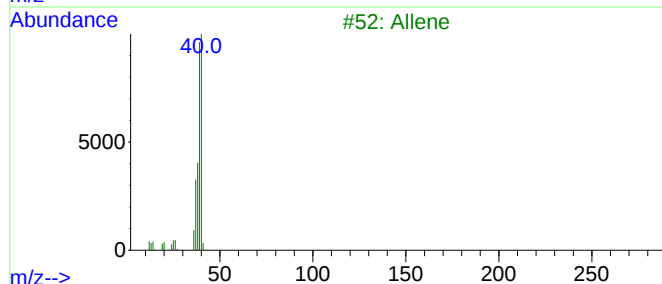
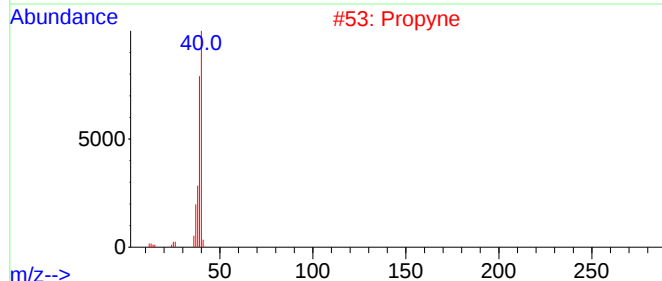
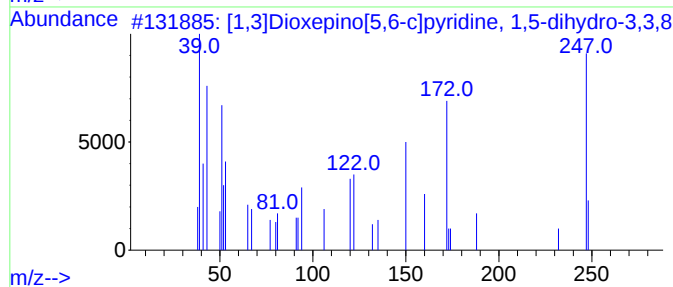
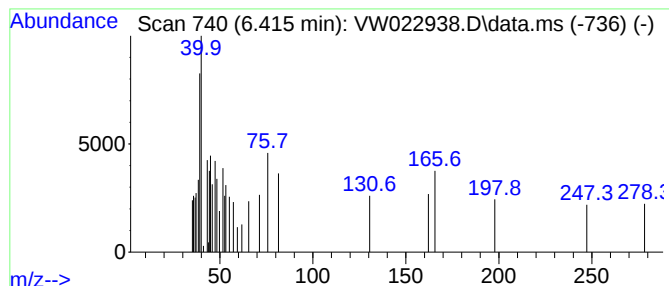
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM050222SMA.M
Quant Title : SFAM01.0

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

Peak Number 2 [1,3]Dioxepino[5,6-c]pyridi... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.415	1.77 ug/L	2885	1,4-Difluorobenzene	8.848

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			[1,3]Dioxepino[5,6-c]pyridine, 1...	247	C14H17N03	069022-74-8	50
2			Propyne	40	C3H4	000074-99-7	43
3			Allene	40	C3H4	000463-49-0	38
4			1-Hexen-4-yne, 3-ethylidene-2-me...	120	C9H12	076003-39-9	25
5			2-Penten-4-yne, 2-methyl-	80	C6H8	001595-53-5	23



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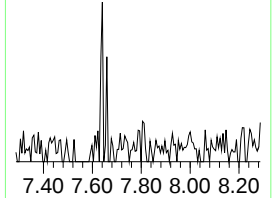
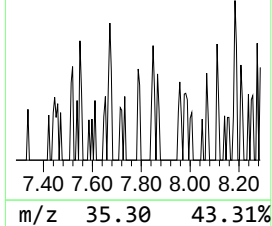
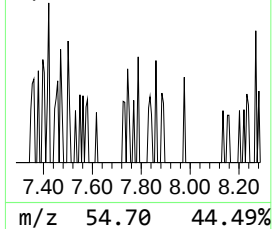
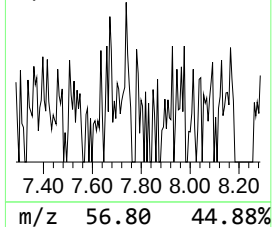
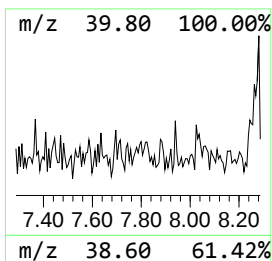
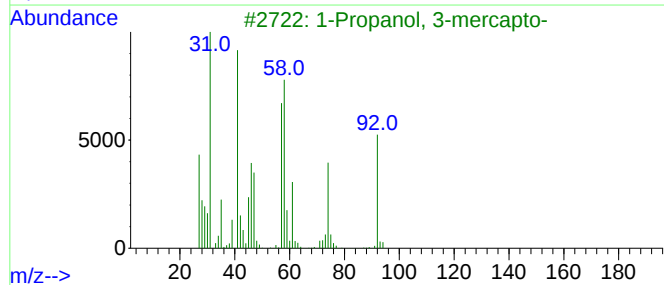
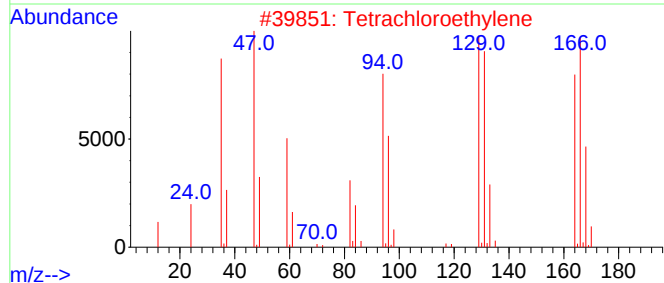
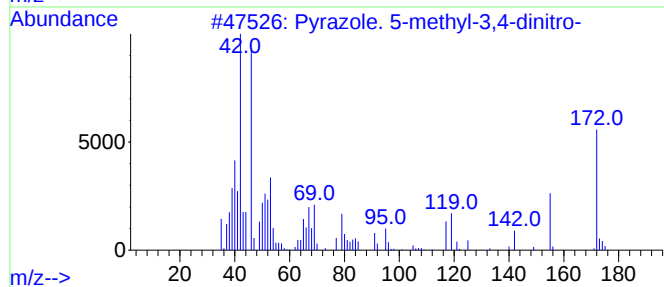
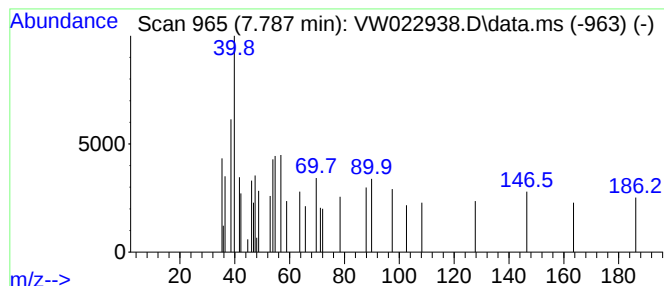
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM050222SMA.M
Quant Title : SFAM01.0

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

Peak Number 3 unknown-02 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.787	1.63 ug/L	2665	1,4-Difluorobenzene	8.848

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrazole. 5-methyl-3,4-dinitro-	172	C4H4N4O4	1000273-82-5	23		
2	Tetrachloroethylene	164	C2Cl4	000127-18-4	9		
3	1-Propanol, 3-mercapto-	92	C3H8OS	019721-22-3	8		
4	3-Aminopropionitrile	70	C3H6N2	000151-18-8	7		
5	Nitrogen fluoride, (E)-	66	F2N2	013776-62-0	7		



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Operator : SY/VA
Sample : N2714-05RE
Misc : 4.48g/10mL/MSVOA_W/SOIL
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
EW2X6RE

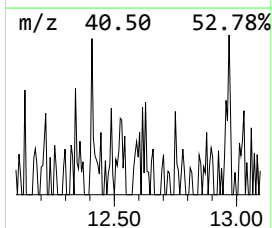
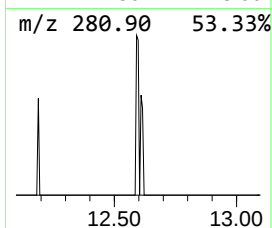
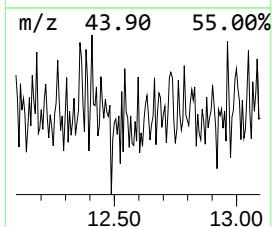
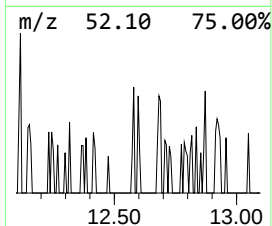
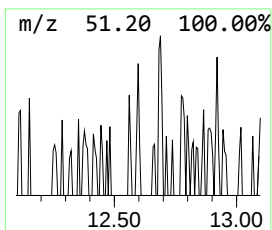
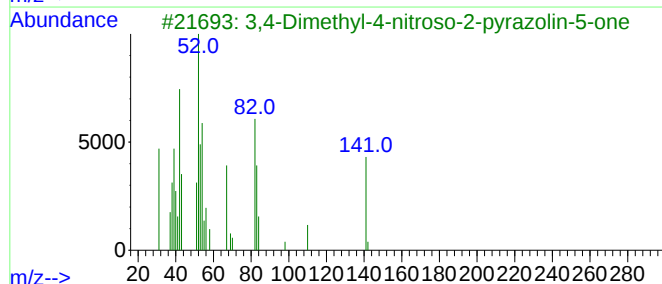
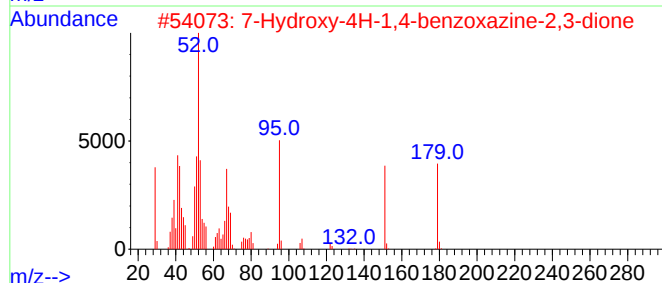
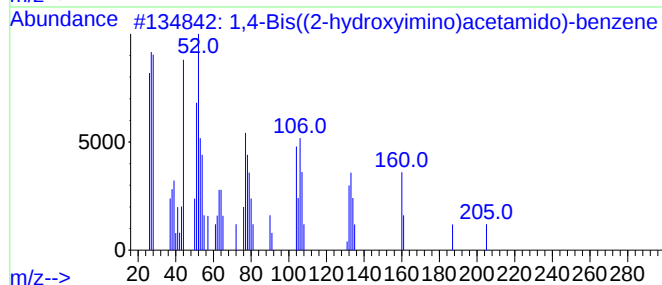
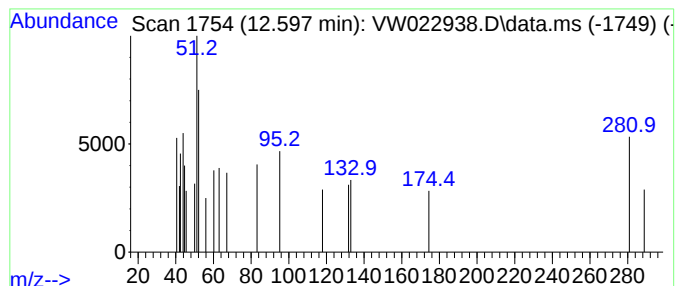
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Quant Title : SFAM01.0

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

Peak Number 5 unknown-03 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.597	1.42 ug/L	1555	1,4-Dichlorobenzene-d4	13.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Bis((2-hydroxyimino)acetamid...	250	C10H10N4O4	006662-54-0	10
2			7-Hydroxy-4H-1,4-benzoxazine-2,3...	179	C8H5N04	081055-25-6	10
3			3,4-Dimethyl-4-nitroso-2-pyrazol...	141	C5H7N3O2	103248-40-4	10
4			2,6,7-Trimethyl-(1,2,4)-triazolo...	163	C7H9N5	061139-77-3	9
5			5-Amino-1-(2-methoxyphenyl)-1H-1...	233	C10H11N5O2	1000387-16-8	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW050922\
Data File : VW022938.D
Acq On : 09 May 2022 18:28
Operator : SY/VA
Sample : N2714-05RE
Misc : 4.48g/10mL/MSVOA_W/SOIL
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
EW2X6RE

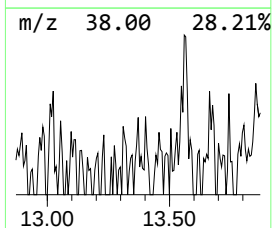
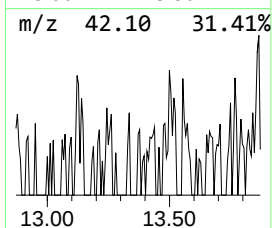
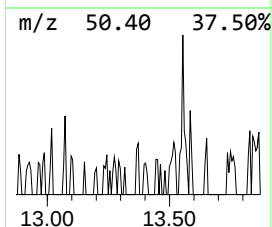
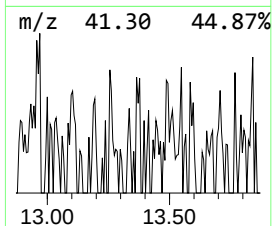
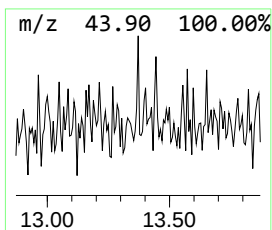
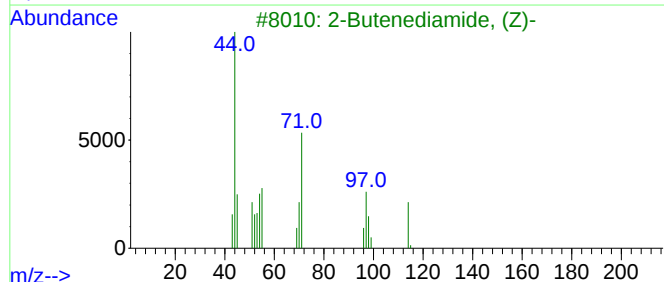
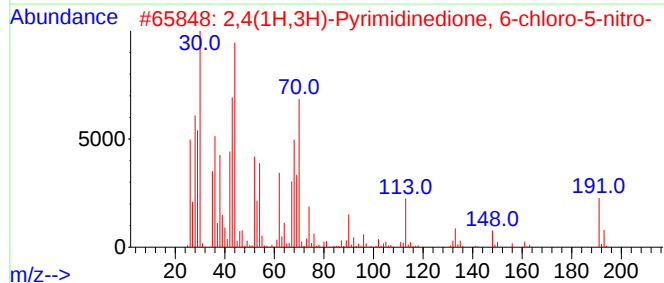
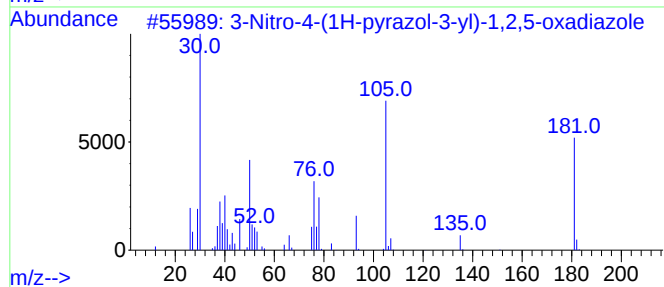
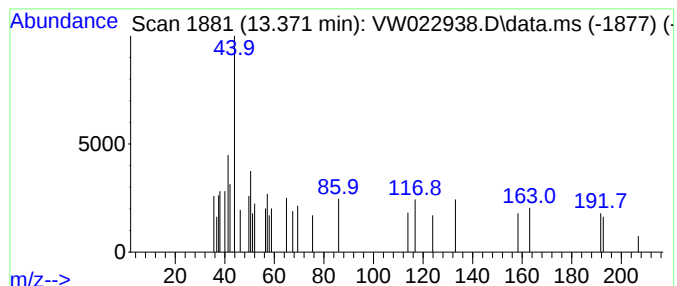
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Quant Title : SFAM01.0

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

Peak Number 6 unknown-04 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.371	1.61 ug/L	1766	1,4-Dichlorobenzene-d4	13.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Nitro-4-(1H-pyrazol-3-yl)-1,2,...	181	C5H3N5O3	1000445-04-8	27		
2	2,4(1H,3H)-Pyrimidinedione, 6-ch...	191	C4H2ClN3O4	006630-30-4	16		
3	2-Butenediamide, (Z)-	114	C4H6N2O2	000928-01-8	9		
4	Pterin-6-carboxylic acid	207	C7H5N5O3	000948-60-7	7		
5	N-Methyl-N-[2-cyanoethyl]-2-merc...	158	C7H14N2S	1000257-11-6	7		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW050922\
Data File : VW022938.D
Acq On : 09 May 2022 18:28
Operator : SY/VA
Sample : N2714-05RE
Misc : 4.48g/10mL/MSVOA_W/SOIL
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
EW2X6RE

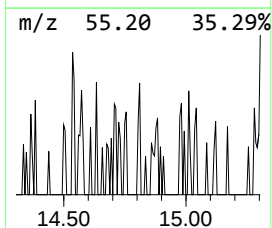
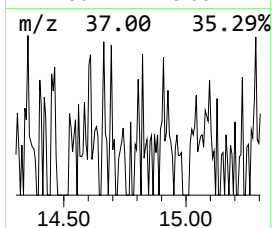
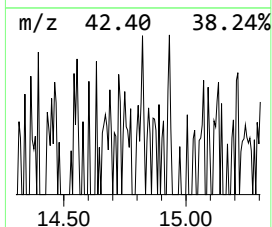
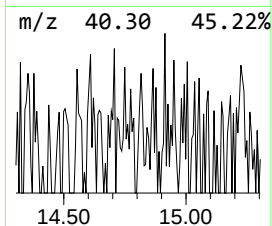
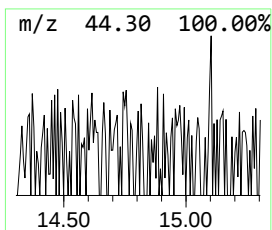
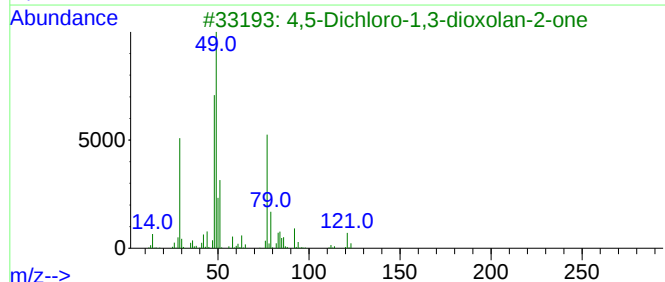
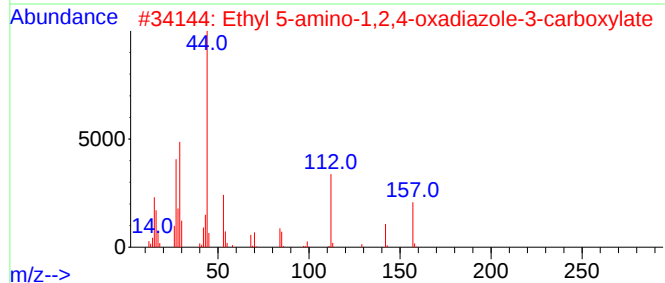
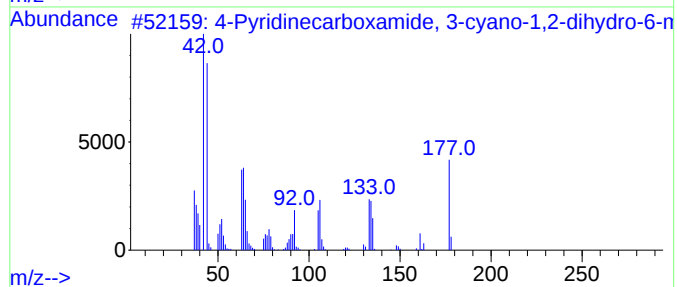
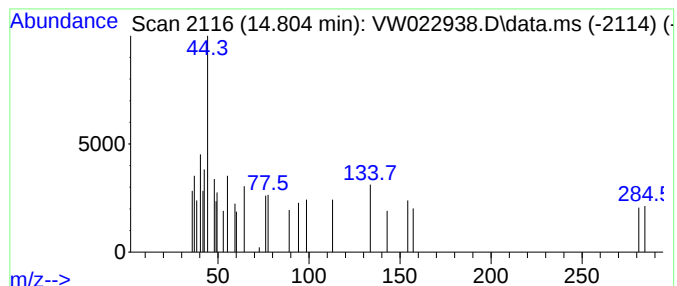
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Quant Title : SFAM01.0

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

Peak Number 7 unknown-05 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.804	1.38 ug/L	1519	1,4-Dichlorobenzene-d4	13.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Pyridinecarboxamide, 3-cyano-1...	177	C8H7N3O2	1000389-14-4	13		
2	Ethyl 5-amino-1,2,4-oxadiazole-3...	157	C5H7N3O3	144167-51-1	9		
3	4,5-Dichloro-1,3-dioxolan-2-one	156	C3H2Cl2O3	003967-55-3	9		
4	4,5-Dichloro-1,3-dioxolan-2-one	156	C3H2Cl2O3	003967-55-3	9		
5	4-Amino-1-butanol	89	C4H11NO	013325-10-5	7		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW050922\
Data File : VW022938.D
Acq On : 09 May 2022 18:28
Operator : SY/VA
Sample : N2714-05RE
Misc : 4.48g/10mL/MSVOA_W/SOIL
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
EW2X6RE

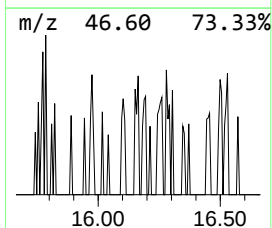
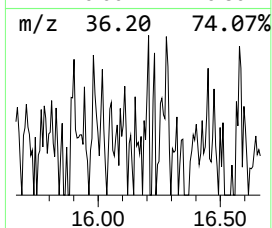
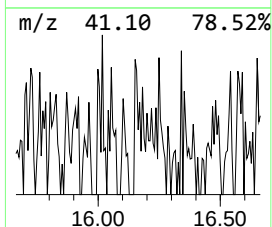
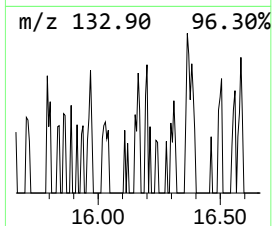
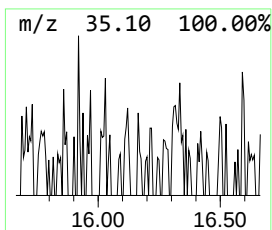
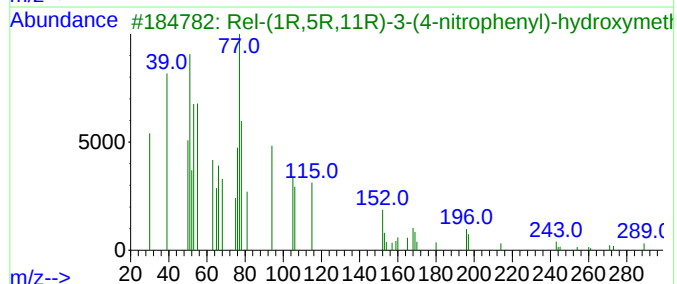
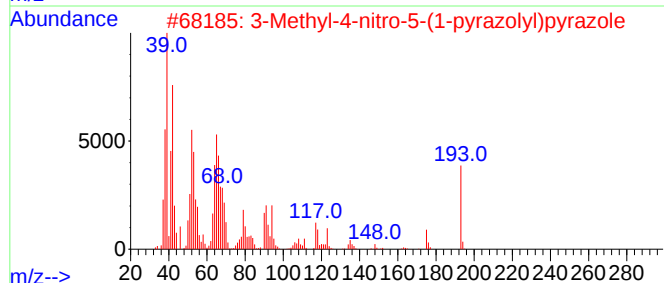
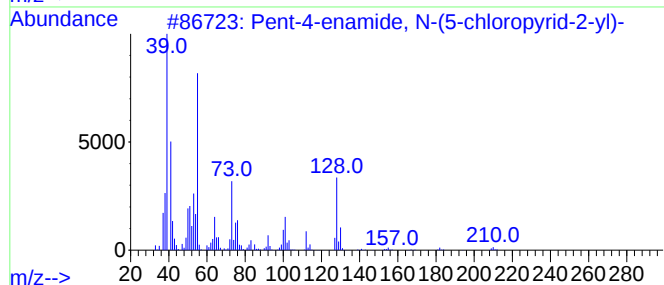
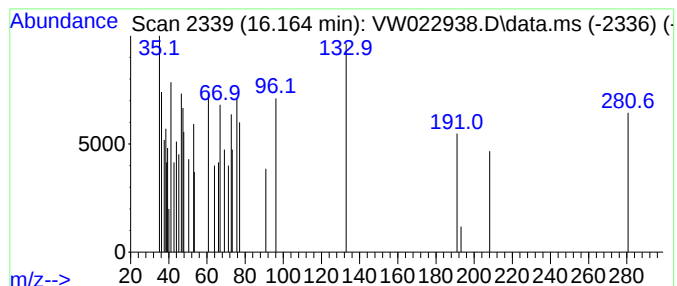
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Quant Title : SFAM01.0

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

Peak Number 8 unknown-06 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.164	2.12 ug/L	2329	1,4-Dichlorobenzene-d4	13.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pent-4-enamide, N-(5-chloropyrid-2-yl)-	210	C10H11ClN2O	306743-90-8	25
2			3-Methyl-4-nitro-5-(1-pyrazolyl)pyrazole	193	C7H7N5O2	292855-42-6	16
3			Rel-(1R,5R,11R)-3-(4-nitrophenyl)-hydroxymethyl-5-nitro-1H-pyrazole	289	C14H11NO6	1000433-34-4	10
4			3-Methyl-4-nitro-5-(1-pyrazolyl)pyrazole	193	C7H7N5O2	292855-42-6	10
5			2-Butenenitrile	67	C4H5N	004786-20-3	10



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW050922\
Data File : VW022938.D
Acq On : 09 May 2022 18:28
Operator : SY/VA
Sample : N2714-05RE
Misc : 4.48g/10mL/MSVOA_W/SOIL
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
EW2X6RE

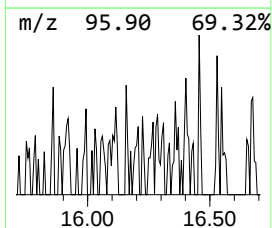
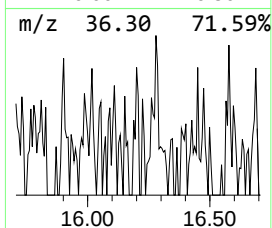
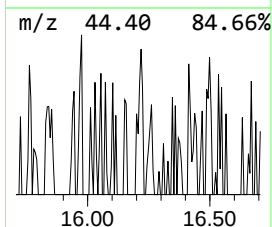
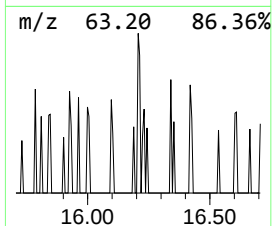
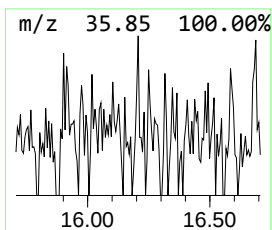
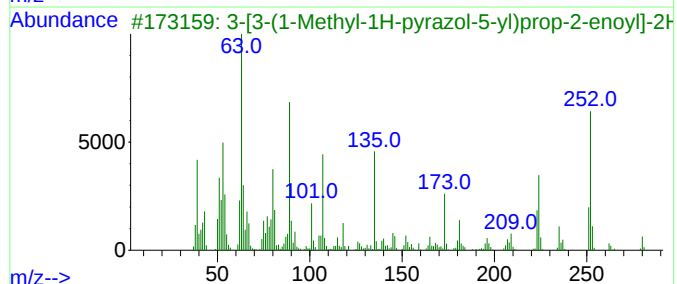
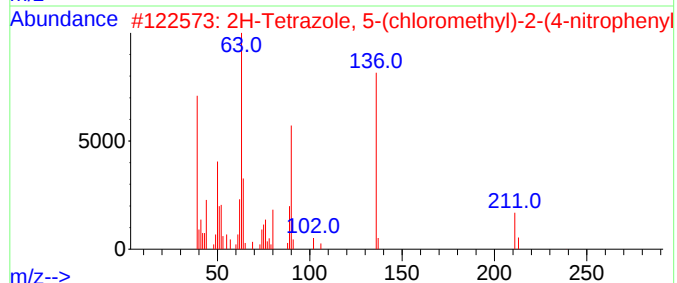
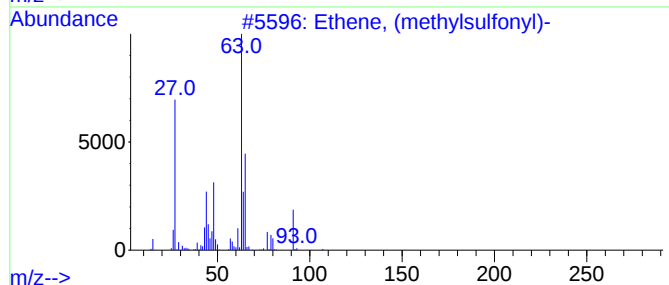
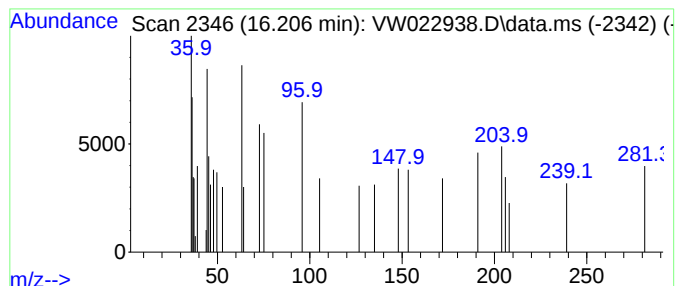
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Quant Title : SFAM01.0

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

Peak Number 9 unknown-07 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.206	3.77 ug/L	4140	1,4-Dichlorobenzene-d4	13.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethene, (methylsulfonyl)-	106	C3H6O2S	003680-02-2	9
2			2H-Tetrazole, 5-(chloromethyl)-2...	239	C8H6ClN5O2	065251-34-5	9
3			3-[3-(1-Methyl-1H-pyrazol-5-yl)p...	280	C16H12N2O3	1000386-87-0	9
4			5-Bromo-2-(2H-tetrazol-5-yl)pyri...	225	C6H4BrN5	380380-60-9	9
5			o,S,S'-Trimethyl phosphorotriethi...	188	C3H9OPS3	1000306-06-4	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW050922\
 Data File : VW022938.D
 Acq On : 09 May 2022 18:28
 Operator : SY/VA
 Sample : N2714-05RE
 Misc : 4.48g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 EW2X6RE

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM050222SMA.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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[1,3]Dioxepino[...]	6.415	1.8	ug/L	2885	1	8.848	40812	25.0
unknown-02	7.787	1.6	ug/L	2665	1	8.848	40812	25.0
unknown-03	12.597	1.4	ug/L	1555	3	13.554	27443	25.0
unknown-04	13.371	1.6	ug/L	1766	3	13.554	27443	25.0
unknown-05	14.804	1.4	ug/L	1519	3	13.554	27443	25.0
unknown-06	16.164	2.1	ug/L	2329	3	13.554	27443	25.0
unknown-07	16.206	3.8	ug/L	4140	3	13.554	27443	25.0