

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW041924\
 Data File : VW028495.D
 Acq On : 19 Apr 2024 14:44
 Operator : SY/MD
 Sample : P2203-03
 Misc : 5.02g/10mL/MSVOA_W/SOIL/A
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 E1CX3

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\SFAMWLM040824SMA.M
 Title : SFAM01.0

Signal : TIC: VW028495.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.229	51	56	57	rBV4	3178	4820	9.24%	1.020%
2	2.899	161	166	173	rVB3	4225	9440	18.09%	1.998%
3	3.033	186	188	190	rBV3	1444	1188	2.28%	0.252%
4	3.375	240	244	247	rBV6	1753	2876	5.51%	0.609%
5	3.491	261	263	265	rBV2	1219	895	1.72%	0.189%
6	3.539	268	271	273	rBV4	1535	1486	2.85%	0.315%
7	3.619	282	284	285	rBV2	966	736	1.41%	0.156%
8	3.716	298	300	301	rVB2	1415	863	1.65%	0.183%
9	4.027	346	351	363	rVB3	7275	23629	45.29%	5.002%
10	4.112	363	365	367	rBV3	1315	1418	2.72%	0.300%
11	4.344	398	403	404	rBV5	933	1236	2.37%	0.262%
12	4.557	434	438	440	rBV5	1180	1093	2.09%	0.231%
13	4.673	453	457	458	rBV4	1279	1680	3.22%	0.356%
14	4.917	496	497	501	rBV4	1255	1375	2.64%	0.291%
15	5.021	513	514	516	rVB2	1355	743	1.42%	0.157%
16	5.088	520	525	527	rBV6	848	1502	2.88%	0.318%
17	5.618	609	612	615	rBV5	1157	1731	3.32%	0.366%
18	5.886	654	656	660	rBV5	1090	1649	3.16%	0.349%
19	6.008	672	676	677	rBV3	1321	1368	2.62%	0.290%
20	6.222	708	711	714	rBV4	1538	2091	4.01%	0.443%
21	6.417	741	743	746	rVB4	1400	1366	2.62%	0.289%
22	6.466	749	751	752	rVB2	1367	785	1.50%	0.166%
23	6.594	770	772	774	rBV3	904	693	1.33%	0.147%
24	6.789	802	804	806	rVB3	937	746	1.43%	0.158%
25	6.886	817	820	822	rVB4	1103	1437	2.75%	0.304%
26	6.966	831	833	837	rVV5	909	1043	2.00%	0.221%
27	7.033	842	844	846	rBV3	1116	878	1.68%	0.186%
28	7.088	851	853	854	rBV2	1877	1230	2.36%	0.260%
29	7.411	904	906	909	rBV4	1471	1326	2.54%	0.281%
30	7.807	968	971	974	rBV5	1263	1375	2.64%	0.291%
31	7.831	974	975	980	rBV5	1202	1867	3.58%	0.395%
32	7.953	993	995	997	rVB3	1691	1128	2.16%	0.239%
33	8.081	1013	1016	1017	rBV3	1017	873	1.67%	0.185%
34	8.282	1042	1049	1061	rVB3	17383	52177	100.00%	11.046%
35	8.417	1068	1071	1077	rBV8	1444	2825	5.41%	0.598%
36	8.465	1077	1079	1082	rVB4	1521	1235	2.37%	0.261%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM040824SMA.M
 Title : SFAM01.0

37	8.496	1082	1084	1086	rBV4	1211	1191	2.28%	0.252%
38	8.532	1086	1090	1091	rBV4	932	1299	2.49%	0.275%
39	8.666	1110	1112	1115	rBV4	811	801	1.54%	0.170%
40	8.843	1132	1141	1150	rBV	17006	40229	77.10%	8.517%
41	8.977	1161	1163	1167	rVV5	933	1085	2.08%	0.230%
42	9.014	1167	1169	1171	rVB3	1367	850	1.63%	0.180%
43	9.087	1171	1181	1188	rBV6	10883	29315	56.18%	6.206%
44	9.276	1204	1212	1219	rBV2	13279	29601	56.73%	6.267%
45	9.557	1256	1258	1264	rVB7	1206	1562	2.99%	0.331%
46	9.642	1270	1272	1276	rVB4	1177	1450	2.78%	0.307%
47	9.691	1278	1280	1283	rVB3	836	738	1.41%	0.156%
48	9.727	1283	1286	1289	rBV5	838	1081	2.07%	0.229%
49	9.758	1289	1291	1292	rBV2	891	802	1.54%	0.170%
50	9.843	1302	1305	1306	rBV2	1312	1256	2.41%	0.266%
51	10.038	1332	1337	1342	rVV5	4099	8887	17.03%	1.881%
52	10.325	1378	1384	1391	rBV	19527	37305	71.50%	7.898%
53	10.502	1411	1413	1415	rBV2	1446	1345	2.58%	0.285%
54	10.581	1422	1426	1431	rVB7	3113	4595	8.81%	0.973%
55	10.861	1469	1472	1475	rBV4	937	1193	2.29%	0.253%
56	10.940	1477	1485	1491	rBV4	3524	9549	18.30%	2.022%
57	11.038	1498	1501	1502	rBV3	786	870	1.67%	0.184%
58	11.172	1521	1523	1527	rBV5	1072	1860	3.56%	0.394%
59	11.270	1537	1539	1542	rBV4	784	816	1.56%	0.173%
60	11.306	1544	1545	1548	rBV3	703	889	1.70%	0.188%
61	11.343	1548	1551	1552	rBV2	685	759	1.45%	0.161%
62	11.629	1591	1598	1605	rBV	25915	47534	91.10%	10.063%
63	11.696	1607	1609	1612	rVV4	1862	2239	4.29%	0.474%
64	11.727	1612	1614	1617	rVB3	1229	1294	2.48%	0.274%
65	11.757	1617	1619	1621	rBV3	1181	918	1.76%	0.194%
66	11.782	1621	1623	1626	rVV4	1282	1191	2.28%	0.252%
67	11.922	1644	1646	1649	rVB4	1006	770	1.48%	0.163%
68	12.074	1669	1671	1673	rBV3	932	948	1.82%	0.201%
69	12.148	1682	1683	1686	rVB3	971	739	1.42%	0.156%
70	12.251	1698	1700	1703	rBV4	1016	1207	2.31%	0.256%
71	12.324	1708	1712	1713	rBV4	902	874	1.68%	0.185%
72	12.391	1720	1723	1725	rVB4	1086	1015	1.95%	0.215%
73	12.428	1725	1729	1731	rBV4	1008	1680	3.22%	0.356%
74	12.532	1744	1746	1747	rBV2	1223	740	1.42%	0.157%
75	12.580	1750	1754	1755	rBV4	1205	1184	2.27%	0.251%
76	12.763	1783	1784	1786	rBV2	1604	1561	2.99%	0.330%

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 Title : SFAM01.0

77	12.873	1799	1802	1804	rBV4	609	837	1.60%	0.177%
78	12.922	1807	1810	1813	rVV5	1074	1626	3.12%	0.344%
79	12.971	1817	1818	1825	rVB7	1083	1176	2.25%	0.249%
80	13.032	1825	1828	1830	rBV3	728	903	1.73%	0.191%
81	13.135	1843	1845	1848	rVB4	1471	1336	2.56%	0.283%
82	13.184	1851	1853	1854	rBV2	1347	785	1.50%	0.166%
83	13.330	1874	1877	1880	rBV5	1078	1533	2.94%	0.325%
84	13.556	1908	1914	1921	rBV	19821	32290	61.89%	6.836%
85	13.708	1938	1939	1941	rVB2	1053	761	1.46%	0.161%
86	13.775	1948	1950	1952	rBV2	768	748	1.43%	0.158%
87	13.806	1952	1955	1956	rVV2	1365	1377	2.64%	0.292%
88	13.848	1956	1962	1970	rVV2	16319	31655	60.67%	6.701%
89	13.909	1970	1972	1974	rVB3	1308	1075	2.06%	0.228%
90	14.056	1993	1996	1998	rBV4	776	1081	2.07%	0.229%
91	14.202	2017	2020	2023	rBV4	910	1196	2.29%	0.253%
92	14.300	2035	2036	2040	rBV4	955	780	1.49%	0.165%
93	14.336	2040	2042	2044	rBV2	1183	1019	1.95%	0.216%
94	14.586	2080	2083	2085	rBV4	921	1021	1.96%	0.216%
95	14.611	2085	2087	2091	rVB5	941	1091	2.09%	0.231%
96	14.641	2091	2092	2095	rBV3	1704	1467	2.81%	0.311%
97	14.672	2095	2097	2100	rVB4	956	1063	2.04%	0.225%
98	14.714	2100	2104	2111	rBV7	3116	6692	12.83%	1.417%
99	14.824	2120	2122	2131	rVB9	2073	3979	7.63%	0.842%
100	16.427	2383	2385	2387	rVB3	1262	841	1.61%	0.178%

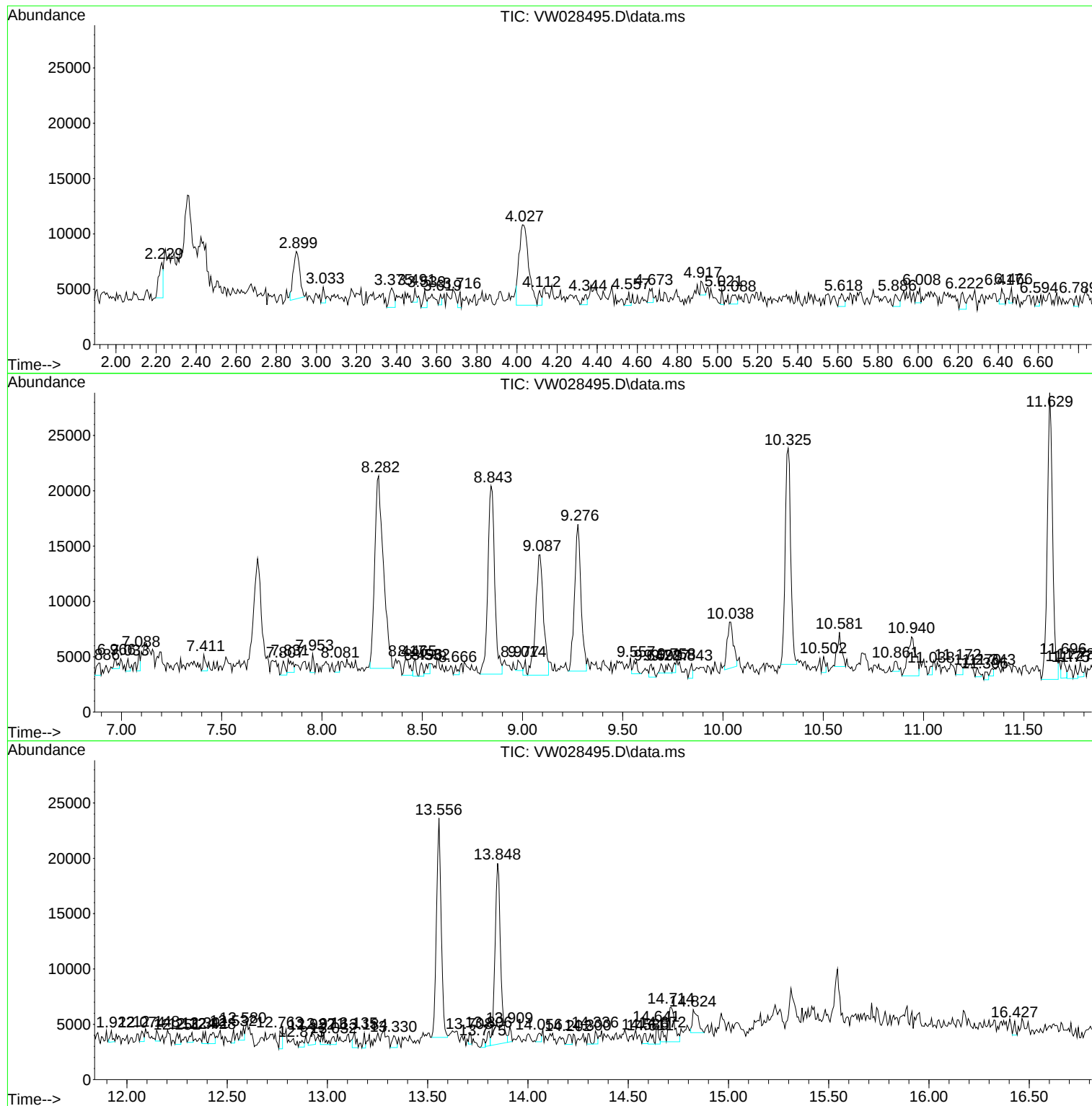
Sum of corrected areas: 472357

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Instrument :
MSVOA_W
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM040824SMA.M
Quant Title : SFAM01.0

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW041924\
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ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_W
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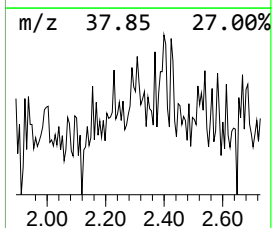
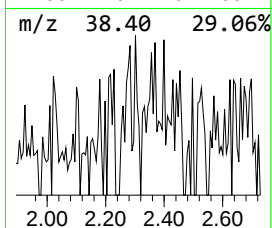
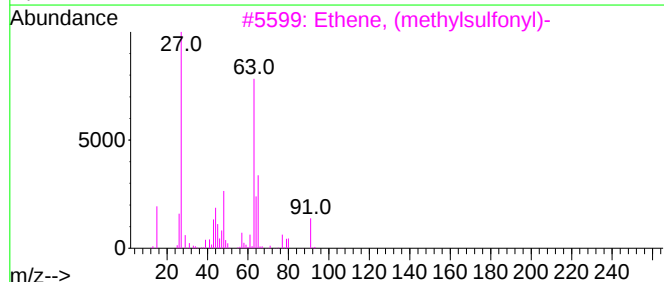
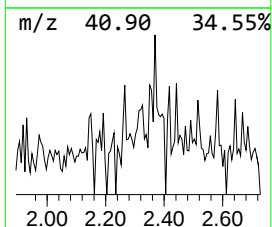
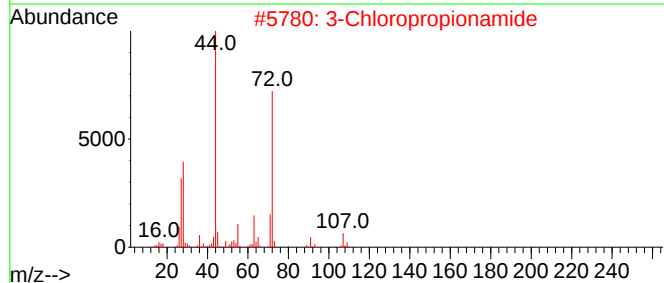
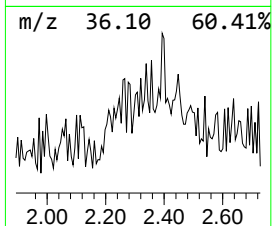
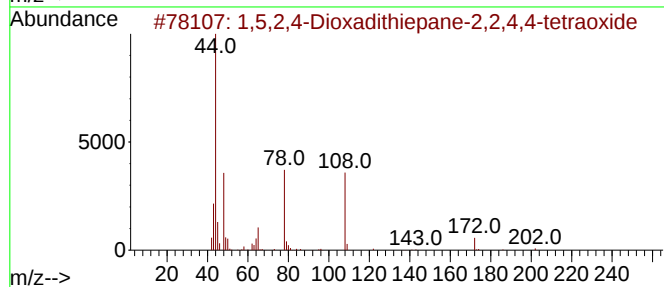
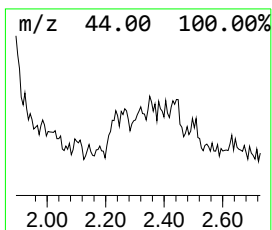
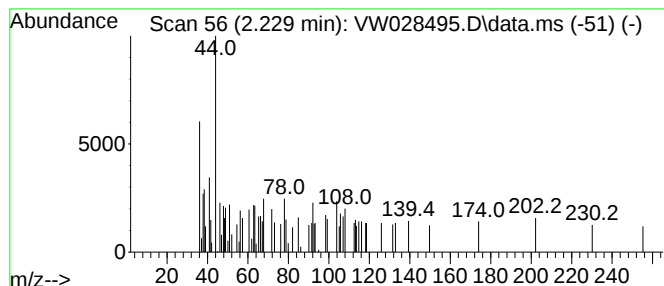
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM040824SMA.M
Quant Title : SFAM01.0

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

Peak Number 1 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.229	3.00 ug/L	4820	1,4-Difluorobenzene	8.849

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,5,2,4-Dioxadithiepane-2,2,4,4-...	202	C3H6O6S2	099591-73-8	14		
2	3-Chloropropionamide	107	C3H6ClNO	005875-24-1	10		
3	Ethene, (methylsulfonyl)-	106	C3H6O2S	003680-02-2	9		
4	dl-Allo-cystathionine	222	C7H14N2O4S	000056-88-2	9		
5	2-(3-Chlorophenyl)ethylamine	155	C8H10ClN	013078-79-0	9		



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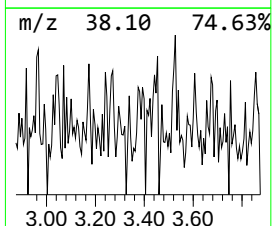
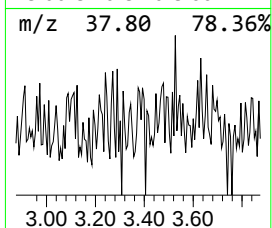
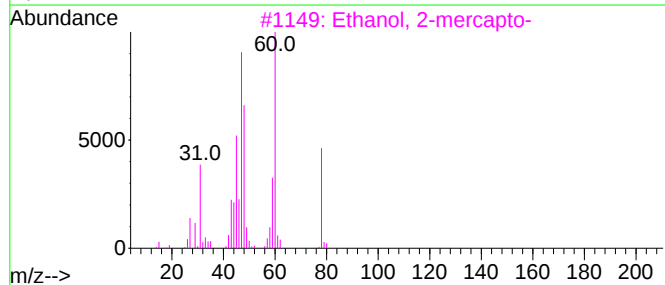
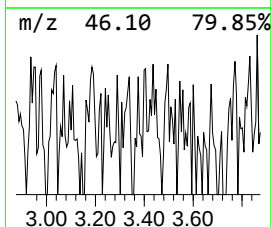
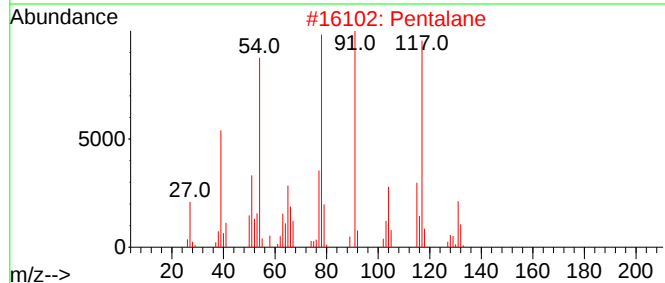
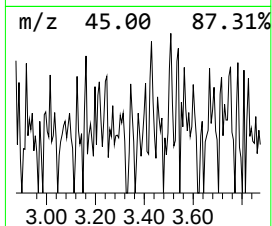
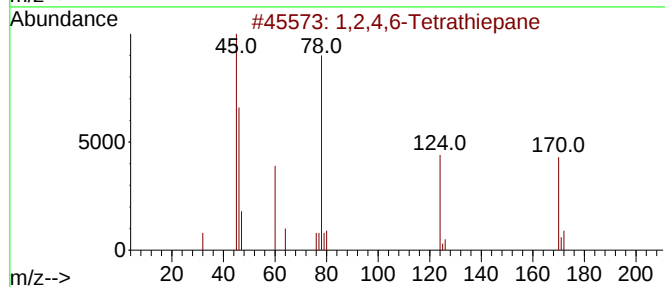
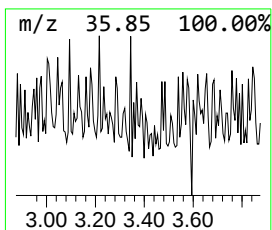
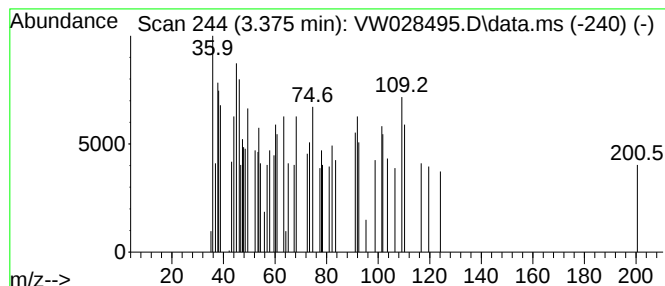
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM040824SMA.M
Quant Title : SFAM01.0

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

Peak Number 2 unknown-02 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.375	1.79 ug/L	2876	1,4-Difluorobenzene	8.849

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,2,4,6-Tetrathiepane	170	C3H6S4	000292-45-5	14
2		Pentalane	132	C10H12	1000221-91-2	10
3		Ethanol, 2-mercapto-	78	C2H6OS	000060-24-2	10
4		Methyl 12,13-tetradecadienoate	238	C15H26O2	1000336-33-7	10
5		2-Oxiran-2-ylpyridine 1-oxide	137	C7H7NO2	069062-54-0	10



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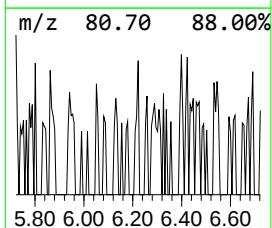
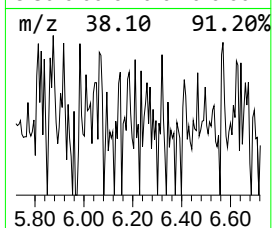
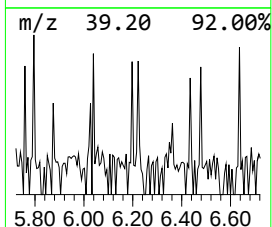
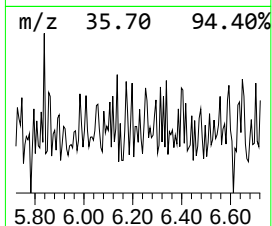
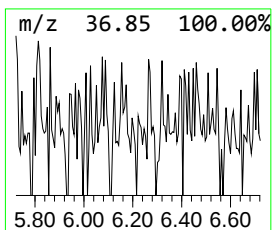
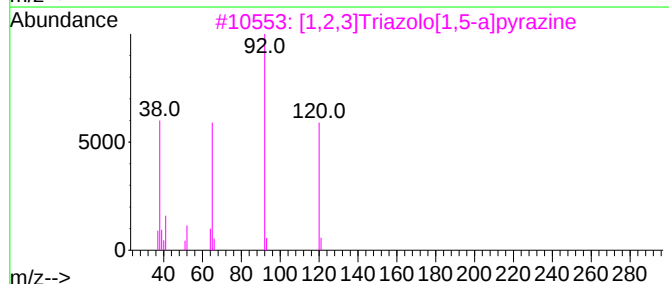
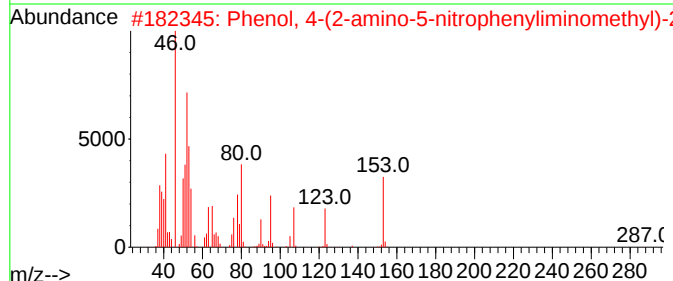
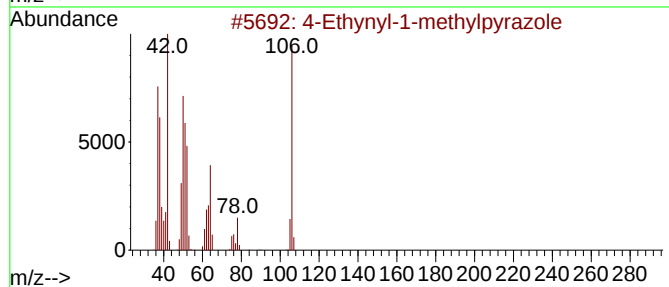
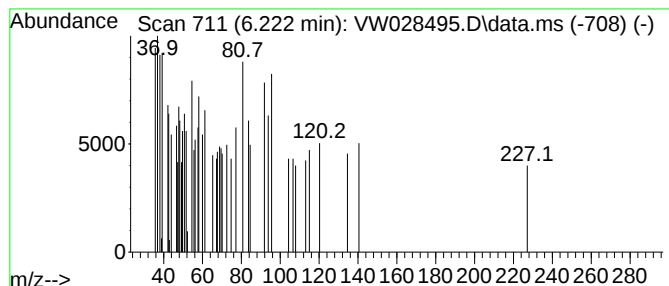
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM040824SMA.M
Quant Title : SFAM01.0

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

Peak Number 3 unknown-03 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.222	1.30 ug/L	2091	1,4-Difluorobenzene	8.849

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Ethynyl-1-methylpyrazole	106	C6H6N2	039806-89-8	35
2			Phenol, 4-(2-amino-5-nitrophenyl...)	287	C14H13N3O4	306744-56-9	28
3			[1,2,3]Triazolo[1,5-a]pyrazine	120	C5H4N4	051392-75-7	18
4			Borazine, 1-methyl-	95	CH8B3N3	021127-94-6	16
5			Bicyclo[4.1.0]heptane, 2-methyl-	110	C8H14	041977-46-2	14



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW041924\
Data File : VW028495.D
Acq On : 19 Apr 2024 14:44
Operator : SY/MD
Sample : P2203-03
Misc : 5.02g/10mL/MSVOA_W/SOIL/A
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
E1CX3

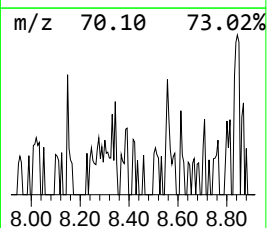
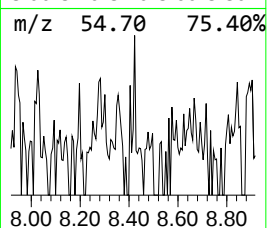
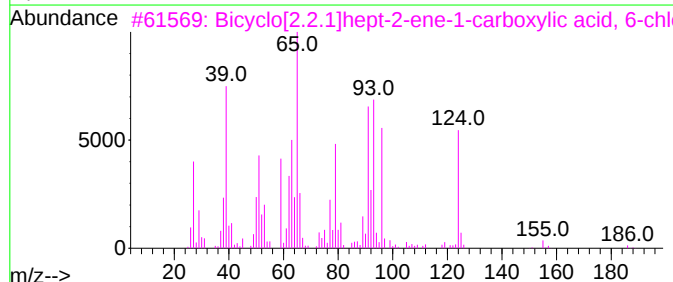
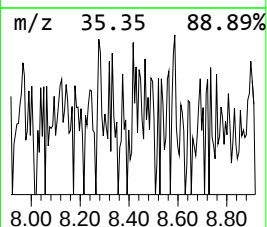
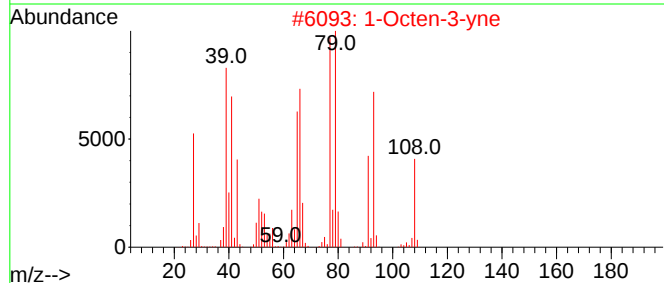
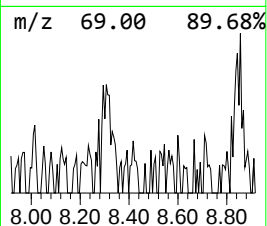
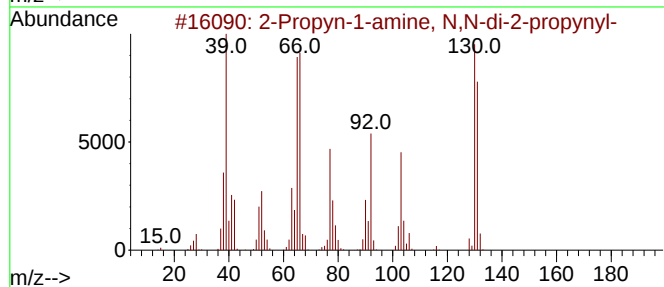
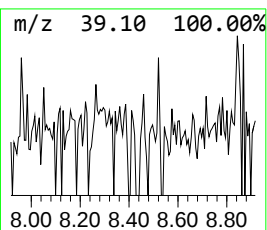
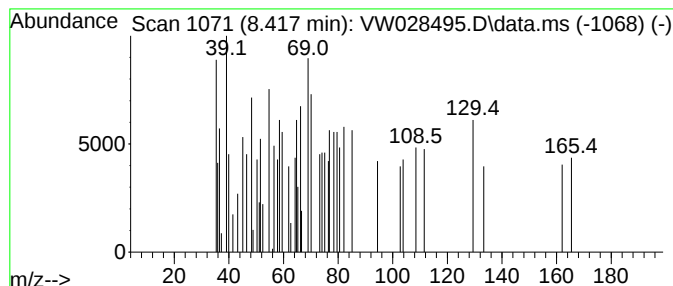
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Quant Title : SFAM01.0

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

Peak Number 4 unknown-04 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.417	1.76 ug/L	2825	1,4-Difluorobenzene	8.849

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propyn-1-amine, N,N-di-2-propy...	131	C9H9N	006921-29-5	35		
2	1-Octen-3-yne	108	C8H12	017679-92-4	25		
3	Bicyclo[2.2.1]hept-2-ene-1-carbo...	186	C9H11ClO2	085173-64-4	16		
4	Propanoic acid, 2-chloro-	108	C3H5ClO2	000598-78-7	12		
5	Furan, 2-(3-imino-3-ethoxyprop-1...	165	C9H11NO2	036878-63-4	12		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW041924\
Data File : VW028495.D
Acq On : 19 Apr 2024 14:44
Operator : SY/MD
Sample : P2203-03
Misc : 5.02g/10mL/MSVOA_W/SOIL/A
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
E1CX3

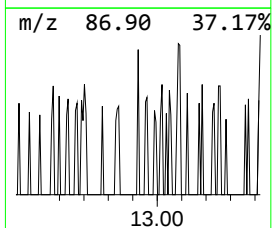
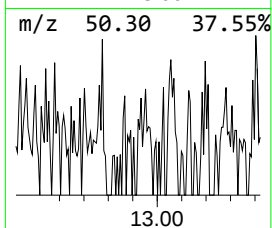
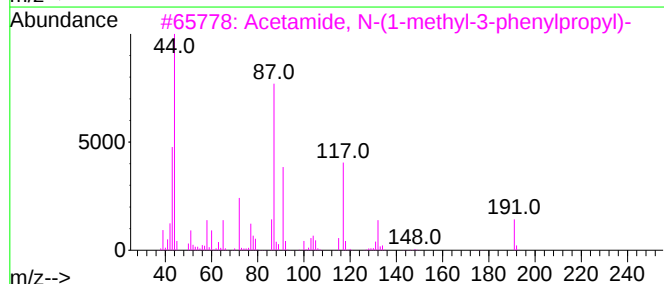
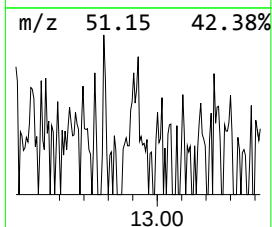
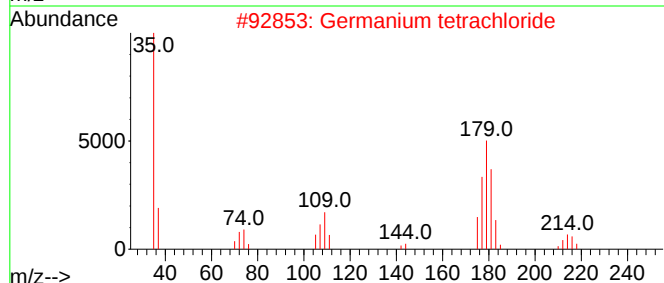
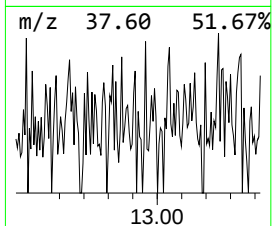
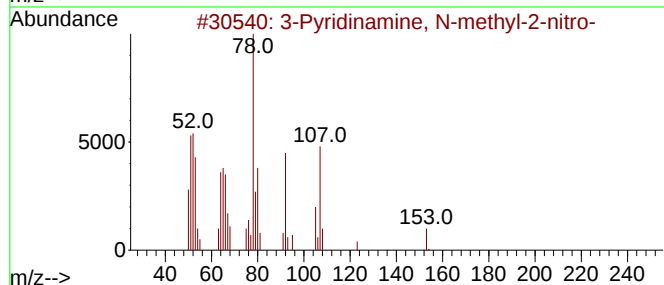
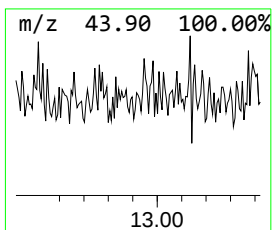
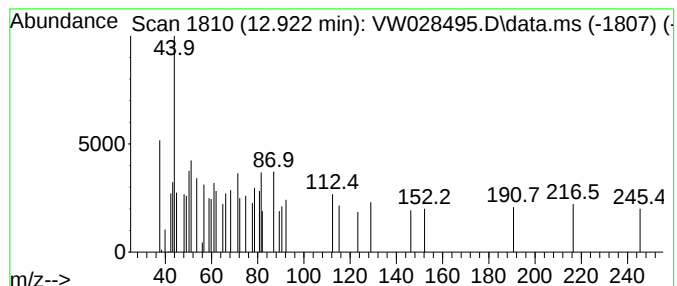
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Quant Title : SFAM01.0

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

Peak Number 6 unknown-05 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.922	1.26 ug/L	1626	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pyridinamine, N-methyl-2-nitro-	153	C6H7N3O2	032605-06-4	10
2			Germanium tetrachloride	214	Cl4Ge	010038-98-9	9
3			Acetamide, N-(1-methyl-3-phenylp...	191	C12H17NO	128442-57-9	9
4			Carbonic acid, dimethyl ester	90	C3H6O3	000616-38-6	9
5			Carbamic acid, (2-chloroethylide...	238	C8H15ClN2O4	005336-13-0	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW041924\
Data File : VW028495.D
Acq On : 19 Apr 2024 14:44
Operator : SY/MD
Sample : P2203-03
Misc : 5.02g/10mL/MSVOA_W/SOIL/A
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
E1CX3

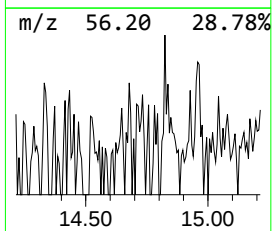
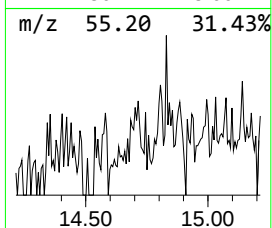
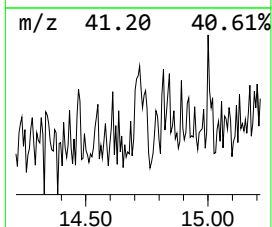
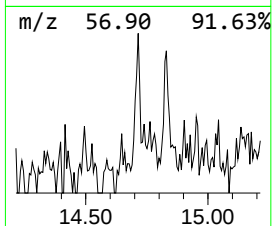
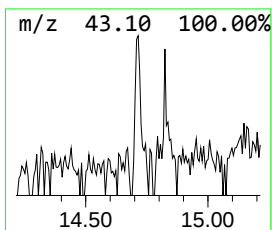
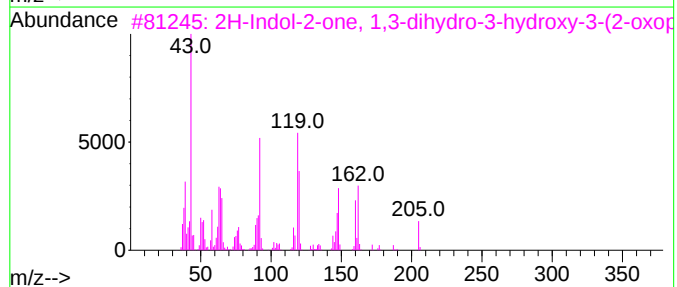
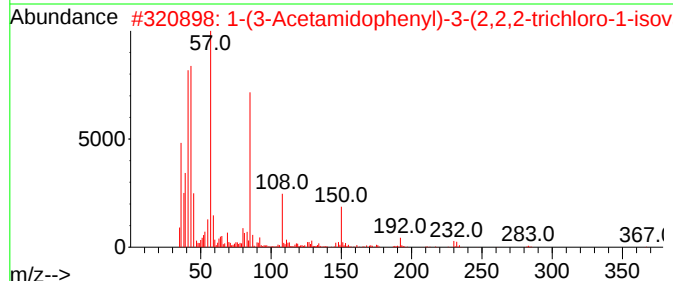
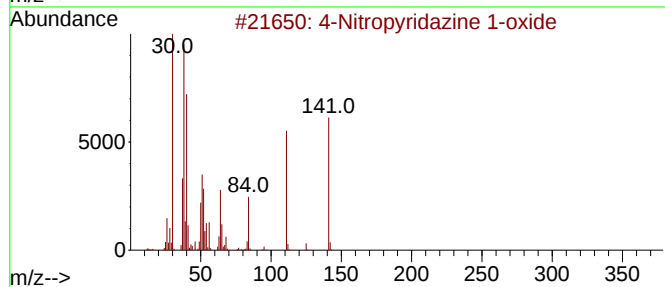
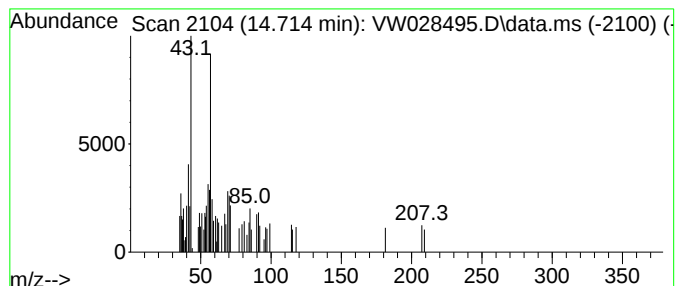
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Quant Title : SFAM01.0

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

Peak Number 7 unknown-06 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.714	5.18 ug/L	6692	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Nitropyridazine 1-oxide	141	C4H3N3O3	028147-45-7	35
2			1-(3-Acetamidophenyl)-3-(2,2,2-t...	438	C16H21Cl3N4O2S	294658-29-0	32
3			2H-Indol-2-one, 1,3-dihydro-3-hy...	205	C11H11NO3	033417-17-3	28
4			Acetoacetic acid, 1-thio-, S-all...	158	C7H10O2S	015780-65-1	25
5			Ethanedial,1,2-dichloro-, bis(0-...	240	C6H6Cl2N2O4	089715-76-4	17



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW041924\
Data File : VW028495.D
Acq On : 19 Apr 2024 14:44
Operator : SY/MD
Sample : P2203-03
Misc : 5.02g/10mL/MSVOA_W/SOIL/A
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
E1CX3

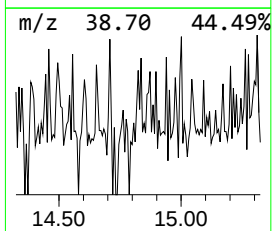
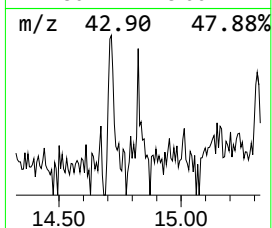
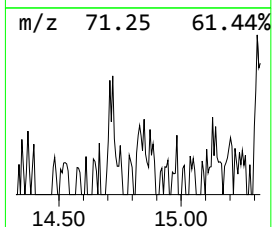
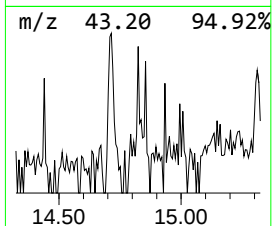
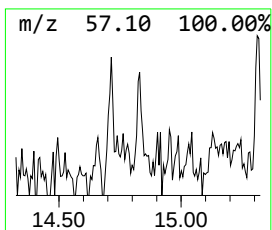
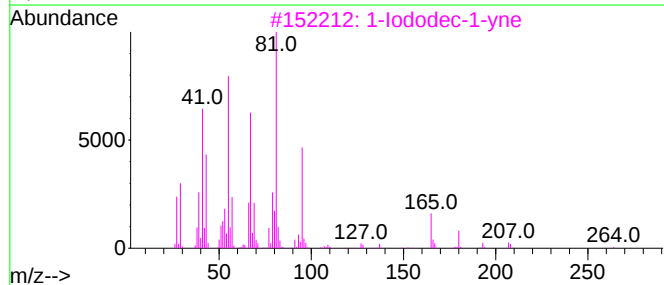
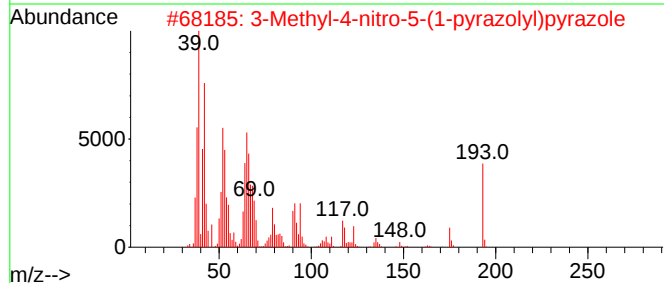
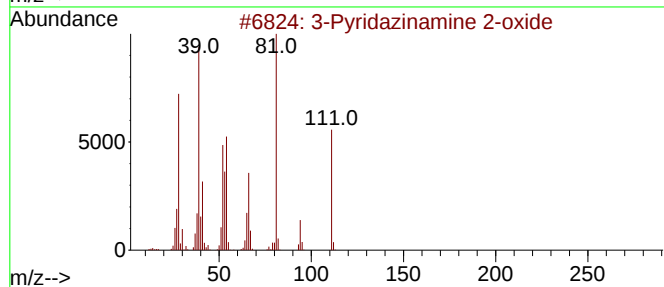
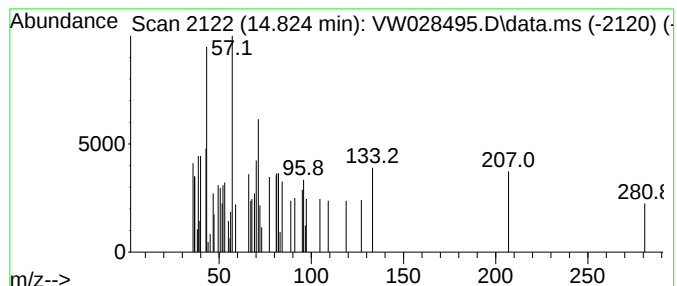
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Quant Title : SFAM01.0

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

Peak Number 8 unknown-07 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.824	3.08 ug/L	3979	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pyridazinamine 2-oxide		111	C4H5N3O	033471-48-6	10	
2	3-Methyl-4-nitro-5-(1-pyrazolyl)...		193	C7H7N5O2	292855-42-6	10	
3	1-Iododec-1-yne		264	C10H17I	067826-81-7	9	
4	Bicyclo[2.2.1]heptane-2-carboxal...		138	C9H14O	015780-37-7	9	
5	6-Methyl-4-propan-2-on-3-propyl-...		265	C11H15N5O3	1010312-00-4	9	



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW041924\
Data File : VW028495.D
Acq On : 19 Apr 2024 14:44
Operator : SY/MD
Sample : P2203-03
Misc : 5.02g/10mL/MSVOA_W/SOIL/A
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
E1CX3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM040824SMA.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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unknown-02	3.375	1.8	ug/L	2876	1	8.849	40229	25.0
unknown-03	6.222	1.3	ug/L	2091	1	8.849	40229	25.0
unknown-04	8.417	1.8	ug/L	2825	1	8.849	40229	25.0
unknown-05	12.922	1.3	ug/L	1626	3	13.556	32290	25.0
unknown-06	14.714	5.2	ug/L	6692	3	13.556	32290	25.0
unknown-07	14.824	3.1	ug/L	3979	3	13.556	32290	25.0