

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW071322\
 Data File : VW023694.D
 Acq On : 14 Jul 2022 11:39
 Operator : SY/VA
 Sample : N3679-05RE
 Misc : 6.09g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 F5B45RE

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: VW023694.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.257	48	58	59	rBV7	11443	30763	24.29%	3.246%
2	3.556	270	271	273	rBV2	2083	1558	1.23%	0.164%
3	3.684	289	292	294	rBV3	1459	2166	1.71%	0.229%
4	4.001	338	344	355	rVB2	13910	36761	29.02%	3.879%
5	4.556	432	435	436	rBV3	1281	1027	0.81%	0.108%
6	4.574	436	438	440	rBV3	1525	1450	1.14%	0.153%
7	4.659	451	452	454	rBV2	1017	832	0.66%	0.088%
8	4.684	454	456	457	rVV2	1114	679	0.54%	0.072%
9	4.757	466	468	471	rVV3	1215	1148	0.91%	0.121%
10	4.800	474	475	478	rVB3	1508	930	0.73%	0.098%
11	5.080	519	521	524	rBV4	1337	1466	1.16%	0.155%
12	5.104	524	525	526	rBV	1618	782	0.62%	0.083%
13	5.220	542	544	545	rBV2	1185	697	0.55%	0.074%
14	5.330	561	562	563	rBV	1373	788	0.62%	0.083%
15	5.495	588	589	591	rBV2	1126	942	0.74%	0.099%
16	5.549	595	598	599	rBV3	1465	1715	1.35%	0.181%
17	5.617	606	609	612	rBV5	1169	1515	1.20%	0.160%
18	5.665	615	617	621	rBV5	1244	1745	1.38%	0.184%
19	5.909	654	657	658	rBV3	1599	1685	1.33%	0.178%
20	6.251	711	713	716	rBV4	1352	1322	1.04%	0.140%
21	6.281	716	718	720	rBV2	1178	1287	1.02%	0.136%
22	6.799	801	803	804	rBV2	1074	795	0.63%	0.084%
23	7.000	834	836	838	rBV3	1101	1005	0.79%	0.106%
24	7.086	843	850	853	rBV2	5280	12154	9.60%	1.283%
25	7.348	891	893	894	rBV2	1353	852	0.67%	0.090%
26	7.647	933	942	950	rBV2	25073	64385	50.83%	6.794%
27	7.769	960	962	967	rVB6	1329	1695	1.34%	0.179%
28	7.927	987	988	991	rBV3	1215	1046	0.83%	0.110%
29	8.159	1024	1026	1027	rVB3	1564	964	0.76%	0.102%
30	8.177	1027	1029	1031	rBV2	1418	1337	1.06%	0.141%
31	8.275	1038	1045	1057	rVB4	42674	126667	100.00%	13.367%
32	8.768	1125	1126	1129	rBV3	1635	1359	1.07%	0.143%
33	8.842	1131	1138	1146	rVV	42194	88093	69.55%	9.296%
34	8.951	1155	1156	1157	rBV	1815	800	0.63%	0.084%
35	9.274	1202	1209	1217	rVB2	32833	67713	53.46%	7.145%
36	9.488	1243	1244	1245	rBV	1486	762	0.60%	0.080%

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

37	9.585	1256	1260	1261	rBV3	1369	1086	0.86%	0.115%
38	9.658	1270	1272	1276	rBV5	1159	1528	1.21%	0.161%
39	9.921	1313	1315	1317	rBV3	1454	1266	1.00%	0.134%
40	10.030	1328	1333	1343	rVB2	13958	28090	22.18%	2.964%
41	10.128	1348	1349	1351	rBV2	1152	1028	0.81%	0.108%
42	10.323	1375	1381	1388	rBV	46530	81775	64.56%	8.629%
43	10.579	1418	1423	1431	rVB3	9649	17740	14.01%	1.872%
44	10.762	1449	1453	1454	rBV4	1986	2696	2.13%	0.284%
45	10.853	1465	1468	1471	rVB5	1392	1453	1.15%	0.153%
46	10.927	1475	1480	1486	rVV	16012	30578	24.14%	3.227%
47	11.061	1500	1502	1510	rVB7	4270	5970	4.71%	0.630%
48	11.628	1589	1595	1604	rVB	55157	96152	75.91%	10.146%
49	11.725	1609	1611	1614	rBV4	1195	927	0.73%	0.098%
50	11.762	1614	1617	1618	rBV3	1095	1421	1.12%	0.150%
51	12.000	1651	1656	1659	rBV7	1923	3168	2.50%	0.334%
52	12.121	1673	1676	1678	rBV3	996	1368	1.08%	0.144%
53	12.140	1678	1679	1684	rVB5	1829	1392	1.10%	0.147%
54	12.182	1684	1686	1687	rBV	1311	958	0.76%	0.101%
55	12.201	1687	1689	1691	rBV3	934	1054	0.83%	0.111%
56	12.256	1697	1698	1701	rBV3	981	686	0.54%	0.072%
57	12.298	1703	1705	1707	rBV3	1010	809	0.64%	0.085%
58	12.414	1722	1724	1725	rBV2	1332	998	0.79%	0.105%
59	12.469	1730	1733	1734	rBV3	948	797	0.63%	0.084%
60	12.603	1752	1755	1759	rVB5	2087	3183	2.51%	0.336%
61	12.695	1763	1770	1778	rVB	30751	52664	41.58%	5.557%
62	12.755	1778	1780	1784	rBV5	996	1189	0.94%	0.125%
63	12.786	1784	1785	1790	rVB5	1524	1875	1.48%	0.198%
64	13.036	1825	1826	1828	rBV2	1193	823	0.65%	0.087%
65	13.176	1846	1849	1852	rBV5	1844	2834	2.24%	0.299%
66	13.475	1897	1898	1903	rBV5	1401	1841	1.45%	0.194%
67	13.518	1903	1905	1906	rBV2	1018	853	0.67%	0.090%
68	13.554	1906	1911	1917	rBV3	34268	56364	44.50%	5.948%
69	13.853	1954	1960	1967	rVB	28755	47846	37.77%	5.049%
70	13.987	1980	1982	1984	rBV3	1245	936	0.74%	0.099%
71	14.066	1993	1995	1997	rBV3	1258	1013	0.80%	0.107%
72	14.365	2042	2044	2046	rVB	1650	1041	0.82%	0.110%
73	14.383	2046	2047	2050	rBV2	1308	1176	0.93%	0.124%
74	14.420	2050	2053	2057	rVV5	1279	1959	1.55%	0.207%
75	14.456	2057	2059	2062	rVB4	1248	1243	0.98%	0.131%
76	14.499	2062	2066	2068	rBV4	1122	1621	1.28%	0.171%

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

77	14.688	2095	2097	2099	rBV3	1273	1021	0.81%	0.108%
78	14.706	2099	2100	2101	rBV	1450	719	0.57%	0.076%
79	14.767	2108	2110	2112	rBV3	951	1012	0.80%	0.107%
80	15.060	2156	2158	2162	rBV5	1408	1518	1.20%	0.160%
81	15.121	2162	2168	2171	rBV7	1025	2010	1.59%	0.212%
82	15.450	2220	2222	2227	rBV6	848	1427	1.13%	0.151%
83	15.535	2234	2236	2239	rVB4	969	820	0.65%	0.087%
84	15.572	2239	2242	2244	rVB2	1148	1228	0.97%	0.130%
85	15.627	2249	2251	2255	rVB4	968	978	0.77%	0.103%
86	15.718	2263	2266	2268	rVB4	1212	1300	1.03%	0.137%
87	15.755	2268	2272	2273	rBV4	988	1212	0.96%	0.128%
88	15.871	2290	2291	2295	rVB4	1419	1370	1.08%	0.145%
89	15.907	2295	2297	2298	rBV2	817	720	0.57%	0.076%
90	16.060	2320	2322	2324	rBV3	960	829	0.65%	0.087%
91	16.279	2356	2358	2360	rBV3	916	1008	0.80%	0.106%
92	16.377	2371	2374	2375	rVB3	1376	1310	1.03%	0.138%
93	16.395	2375	2377	2380	rVB4	963	865	0.68%	0.091%
94	16.426	2380	2382	2385	rBV4	751	845	0.67%	0.089%
95	16.456	2385	2387	2390	rBV4	1376	1236	0.98%	0.130%
96	16.511	2395	2396	2398	rVB2	1528	691	0.55%	0.073%
97	16.535	2398	2400	2402	rVB3	1039	803	0.63%	0.085%
98	16.572	2404	2406	2407	rBV2	1131	841	0.66%	0.089%
99	16.627	2413	2415	2417	rVB3	1466	883	0.70%	0.093%
100	16.694	2425	2426	2428	rBV2	880	713	0.56%	0.075%

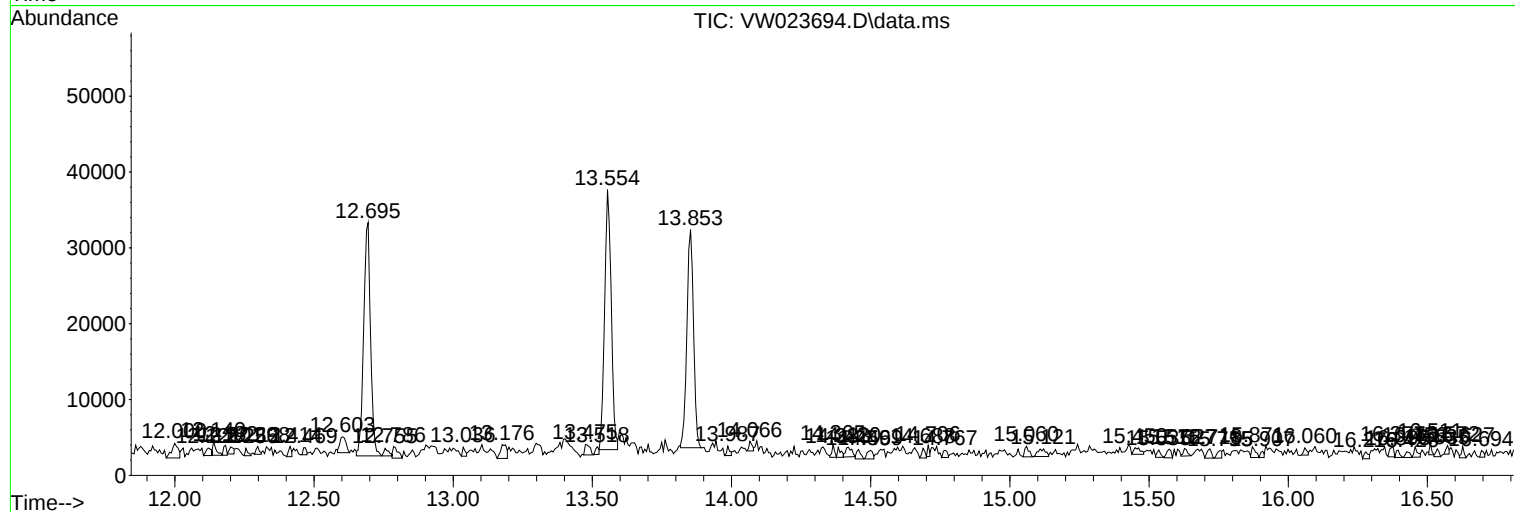
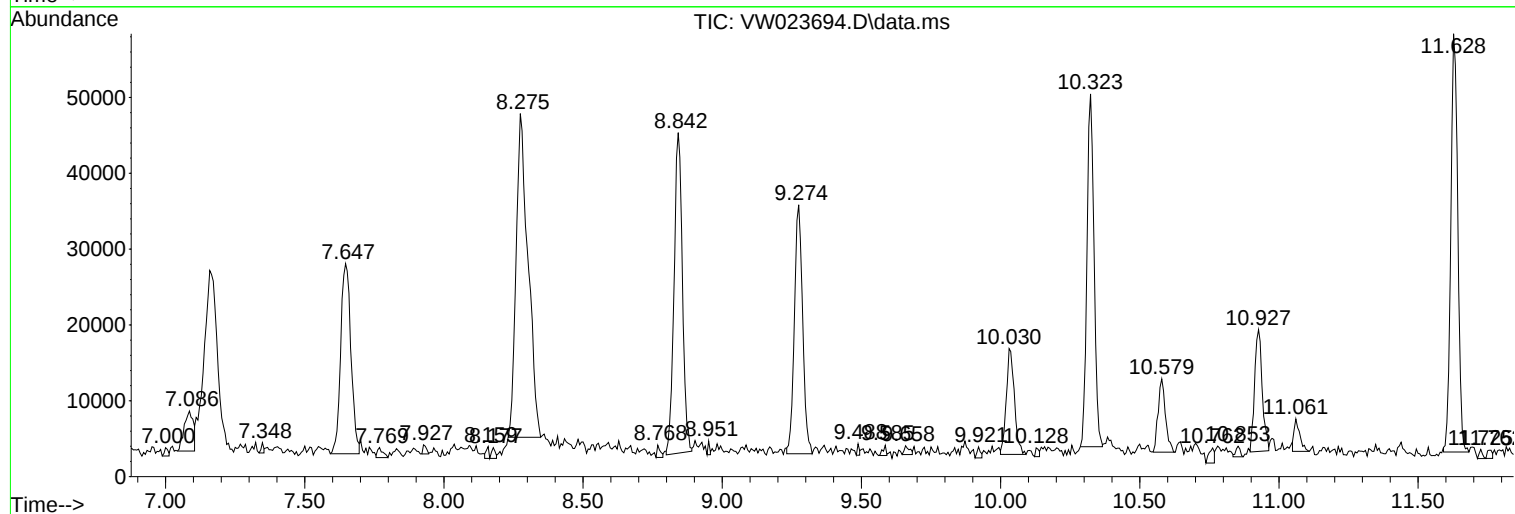
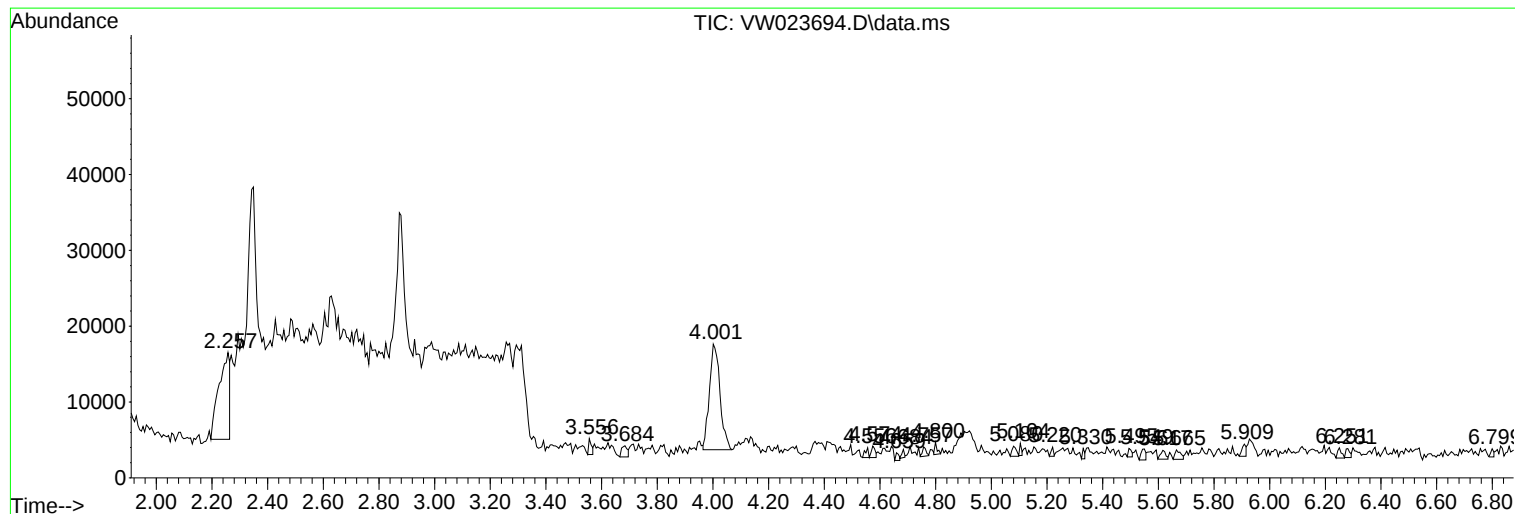
Sum of corrected areas: 947645

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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



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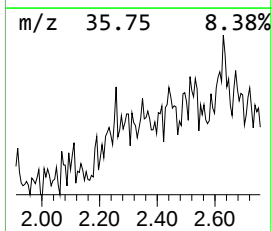
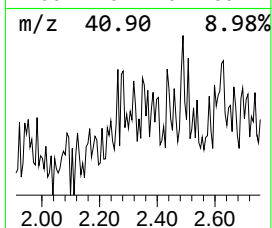
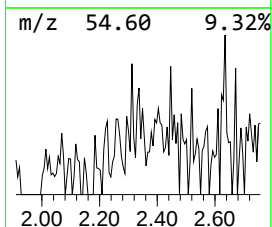
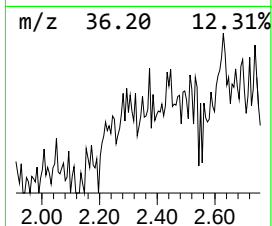
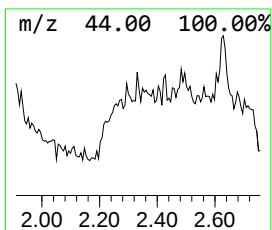
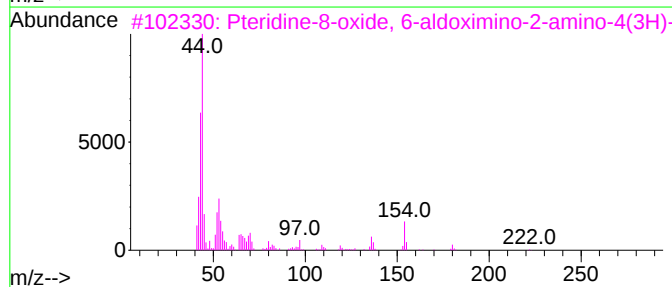
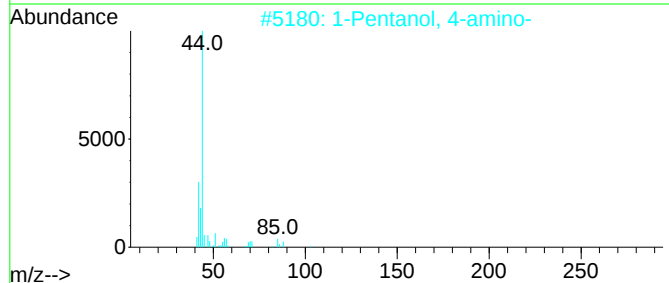
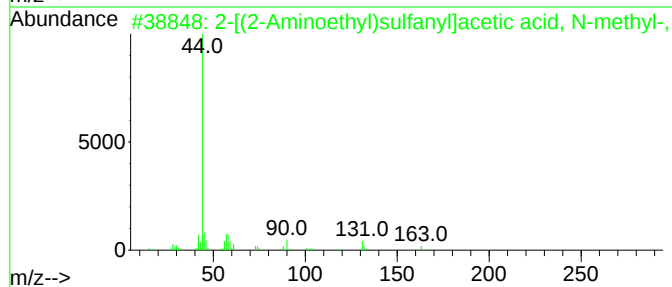
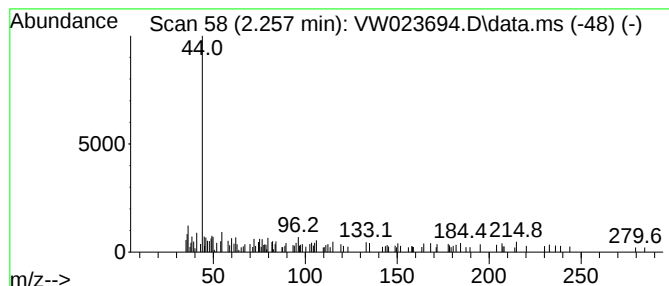
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM071322SMA.M
Quant Title : SFAM01.0

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

Peak Number 1 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.257	8.73 ug/L	30763	1,4-Difluorobenzene	8.842

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-[(2-Aminoethyl)sulfanyl]acetic...	163	C6H13N02S	1249150-80-8	49		
2	1-Pentanol, 4-amino-	103	C5H13NO	000927-55-9	45		
3	Pteridine-8-oxide, 6-aldoximino-	222	C7H6N6O3	023663-23-2	45		
4	Imidazole, 2-amino-5-[(2-carboxy...	153	C6H7N3O2	1000116-74-7	42		
5	Ethyl isopropyl dimethylphosphor...	195	C7H18N03P	099520-56-6	40		



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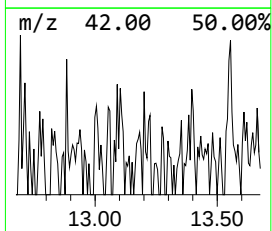
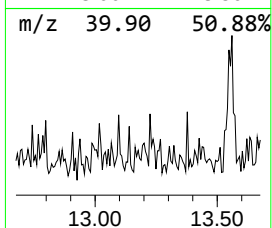
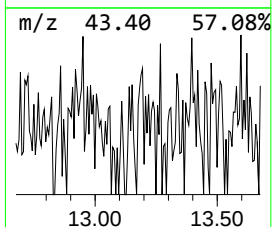
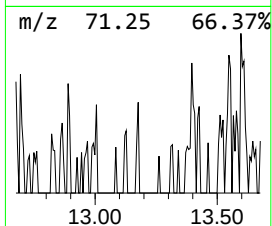
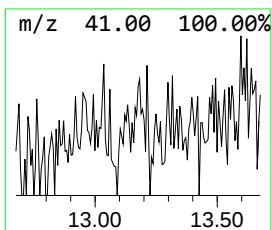
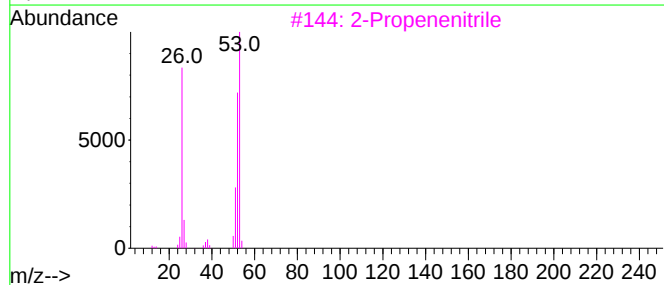
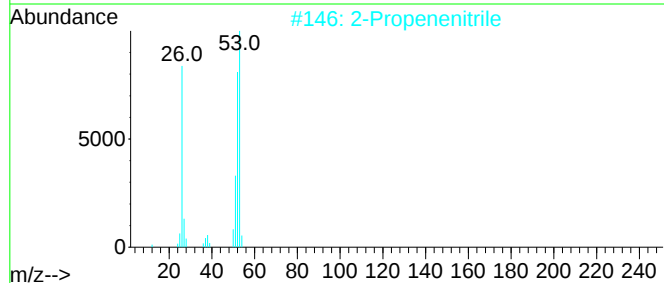
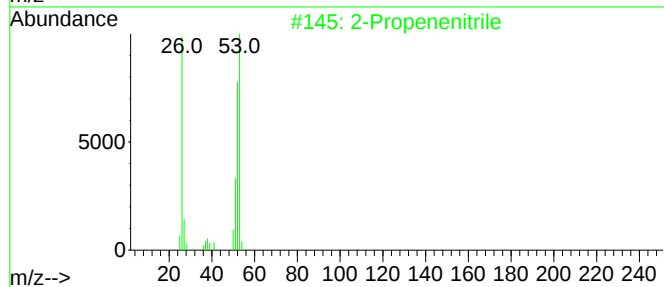
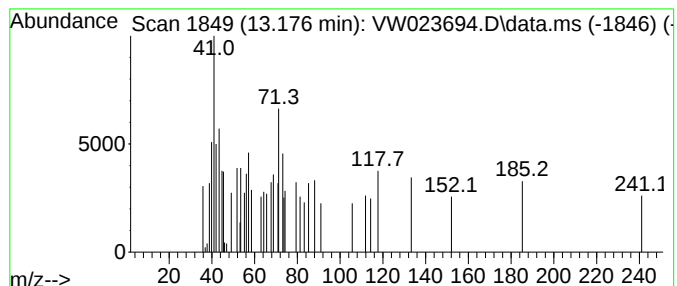
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM071322SMA.M
Quant Title : SFAM01.0

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

Peak Number 5 unknown-02 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.176	1.26 ug/L	2834	1,4-Dichlorobenzene-d4	13.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propenenitrile	53	C3H3N	000107-13-1	25
2			2-Propenenitrile	53	C3H3N	000107-13-1	25
3			2-Propenenitrile	53	C3H3N	000107-13-1	25
4			Chloroacetic acid, 4-methylpenty...	178	C8H15ClO2	1000282-37-7	17
5			2-Hexyn-1-ol	98	C6H10O	000764-60-3	13



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Quant Title : SFAM01.0

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	2.257	8.7	ug/L	30763	1	8.842	88093	25.0
unknown-02	13.176	1.3	ug/L	2834	3	13.554	56364	25.0