

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW071822\
 Data File : VW023855.D
 Acq On : 18 Jul 2022 23:36
 Operator : SY/VA
 Sample : N3721-20
 Misc : 5.00g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 F5C62

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: VW023855.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.678	286	291	293	rBV5	1687	2988	2.55%	0.270%
2	3.818	312	314	316	rVB3	1184	969	0.83%	0.088%
3	3.855	316	320	322	rBV4	1746	2801	2.39%	0.253%
4	4.129	360	365	378	rVB2	8522	22843	19.48%	2.065%
5	4.349	395	401	402	rBV5	2125	3659	3.12%	0.331%
6	4.733	462	464	469	rVB6	1272	2126	1.81%	0.192%
7	4.775	469	471	475	rBV5	1270	2070	1.76%	0.187%
8	4.903	486	492	505	rVB5	6109	18975	16.18%	1.715%
9	5.086	516	522	524	rBV7	2513	4283	3.65%	0.387%
10	5.178	535	537	540	rVB4	1273	1109	0.95%	0.100%
11	5.269	549	552	555	rBV4	1767	2191	1.87%	0.198%
12	5.385	567	571	572	rBV4	1499	2057	1.75%	0.186%
13	5.635	611	612	616	rBV3	996	872	0.74%	0.079%
14	5.665	616	617	619	rVB	1850	941	0.80%	0.085%
15	5.720	621	626	629	rBV6	1303	1656	1.41%	0.150%
16	6.129	691	693	696	rBV4	1013	1050	0.90%	0.095%
17	6.348	727	729	731	rVB3	1450	1245	1.06%	0.113%
18	6.379	731	734	735	rBV2	1128	1125	0.96%	0.102%
19	6.470	748	749	751	rVB2	1769	904	0.77%	0.082%
20	6.519	755	757	759	rBV3	1053	971	0.83%	0.088%
21	6.543	759	761	763	rBV3	1224	1088	0.93%	0.098%
22	6.623	772	774	776	rBV3	1239	1005	0.86%	0.091%
23	6.653	778	779	784	rVB5	2415	2232	1.90%	0.202%
24	6.696	784	786	789	rBV2	1652	1780	1.52%	0.161%
25	6.726	789	791	793	rBV3	1149	1035	0.88%	0.094%
26	6.836	806	809	810	rBV3	1035	992	0.85%	0.090%
27	6.994	831	835	837	rBV5	1307	1719	1.47%	0.155%
28	7.080	843	849	854	rBV	12775	34832	29.70%	3.149%
29	7.446	906	909	910	rBV3	919	910	0.78%	0.082%
30	7.647	935	942	954	rVV2	24795	63164	53.85%	5.710%
31	7.799	965	967	968	rBV2	863	914	0.78%	0.083%
32	8.171	1025	1028	1031	rVB4	2197	2371	2.02%	0.214%
33	8.281	1036	1046	1047	rBV	36082	74316	63.36%	6.718%
34	8.842	1131	1138	1145	rVV2	36257	71403	60.88%	6.454%
35	8.970	1155	1159	1164	rVB7	1027	1916	1.63%	0.173%
36	9.086	1173	1178	1184	rVB10	3128	6936	5.91%	0.627%

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

37	9.140	1184	1187	1191	rVB5	1403	2123	1.81%	0.192%
38	9.189	1194	1195	1198	rBV3	1162	867	0.74%	0.078%
39	9.274	1202	1209	1217	rVV2	38339	78119	66.60%	7.062%
40	9.463	1238	1240	1244	rVB5	2102	2219	1.89%	0.201%
41	9.506	1244	1247	1248	rBV3	935	1118	0.95%	0.101%
42	9.567	1254	1257	1259	rBV2	802	880	0.75%	0.080%
43	9.628	1265	1267	1269	rVB3	1033	845	0.72%	0.076%
44	9.744	1284	1286	1289	rVB3	1327	1380	1.18%	0.125%
45	9.781	1289	1292	1294	rBV4	2343	1839	1.57%	0.166%
46	9.811	1294	1297	1300	rVB4	1349	1886	1.61%	0.170%
47	9.860	1302	1305	1306	rVB3	1063	1030	0.88%	0.093%
48	9.976	1322	1324	1327	rBV4	1400	1535	1.31%	0.139%
49	10.030	1327	1333	1342	rVB2	15635	33060	28.19%	2.988%
50	10.146	1350	1352	1355	rVB4	1007	947	0.81%	0.086%
51	10.207	1359	1362	1363	rBV3	1340	1812	1.54%	0.164%
52	10.323	1374	1381	1389	rBV	36385	66789	56.94%	6.037%
53	10.506	1409	1411	1413	rVB3	1343	988	0.84%	0.089%
54	10.579	1418	1423	1428	rVV2	12312	22866	19.50%	2.067%
55	10.823	1462	1463	1467	rBV3	868	1069	0.91%	0.097%
56	10.884	1471	1473	1474	rBV2	972	964	0.82%	0.087%
57	10.927	1474	1480	1489	rVV2	34655	67372	57.44%	6.090%
58	11.061	1498	1502	1509	rBV5	7682	12673	10.81%	1.146%
59	11.274	1536	1537	1540	rVB2	1311	944	0.80%	0.085%
60	11.317	1541	1544	1546	rBV4	865	953	0.81%	0.086%
61	11.494	1571	1573	1576	rBV3	1140	1136	0.97%	0.103%
62	11.567	1582	1585	1586	rBV3	1184	1358	1.16%	0.123%
63	11.628	1589	1595	1605	rVB	63401	110334	94.07%	9.974%
64	11.756	1613	1616	1617	rBV2	946	875	0.75%	0.079%
65	11.847	1628	1631	1633	rVB4	1498	1569	1.34%	0.142%
66	11.866	1633	1634	1637	rBV3	1258	1117	0.95%	0.101%
67	11.987	1651	1654	1657	rBV4	1020	1458	1.24%	0.132%
68	12.122	1675	1676	1678	rVB2	1578	840	0.72%	0.076%
69	12.152	1678	1681	1685	rBV5	1682	2485	2.12%	0.225%
70	12.256	1697	1698	1701	rVB3	1675	881	0.75%	0.080%
71	12.317	1704	1708	1709	rBV2	1722	1770	1.51%	0.160%
72	12.347	1711	1713	1714	rVV2	1543	881	0.75%	0.080%
73	12.390	1718	1720	1722	rVB2	984	891	0.76%	0.081%
74	12.518	1739	1741	1744	rVB3	1158	978	0.83%	0.088%
75	12.603	1752	1755	1762	rVB7	2974	6185	5.27%	0.559%
76	12.689	1763	1769	1777	rVB2	68226	117288	100.00%	10.602%

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 Title : SFAM01.0

77	13.188	1846	1851	1852	rBV4	1678	2274	1.94%	0.206%
78	13.249	1858	1861	1863	rBV4	1377	1692	1.44%	0.153%
79	13.408	1884	1887	1891	rVV6	2355	3542	3.02%	0.320%
80	13.554	1906	1911	1917	rBV2	52035	85653	73.03%	7.743%
81	13.670	1928	1930	1934	rVB4	1251	1637	1.40%	0.148%
82	13.707	1934	1936	1938	rVB3	1261	985	0.84%	0.089%
83	13.755	1941	1944	1945	rBV2	1264	1289	1.10%	0.117%
84	13.853	1953	1960	1968	rBV2	53194	92605	78.96%	8.371%
85	14.286	2029	2031	2034	rBV4	1154	1244	1.06%	0.112%
86	14.322	2034	2037	2038	rBV3	1679	1256	1.07%	0.114%
87	14.426	2053	2054	2060	rVB5	1757	1934	1.65%	0.175%
88	14.914	2131	2134	2135	rBV3	1133	1083	0.92%	0.098%
89	15.347	2204	2205	2207	rBV2	1322	1156	0.99%	0.104%
90	15.395	2211	2213	2215	rVV3	1433	994	0.85%	0.090%
91	15.597	2245	2246	2248	rBV2	1187	930	0.79%	0.084%
92	15.779	2273	2276	2277	rBV3	1767	1712	1.46%	0.155%
93	15.828	2282	2284	2285	rBV2	915	862	0.73%	0.078%
94	16.011	2312	2314	2315	rBV2	1267	1218	1.04%	0.110%
95	16.127	2329	2333	2334	rBV4	2257	2863	2.44%	0.259%
96	16.285	2357	2359	2363	rBV5	1225	1497	1.28%	0.135%
97	16.407	2377	2379	2381	rVB3	1268	851	0.73%	0.077%
98	16.426	2381	2382	2384	rBV2	1873	1204	1.03%	0.109%
99	16.468	2387	2389	2393	rVV4	1439	1110	0.95%	0.100%
100	16.499	2393	2394	2398	rBV4	1033	897	0.76%	0.081%

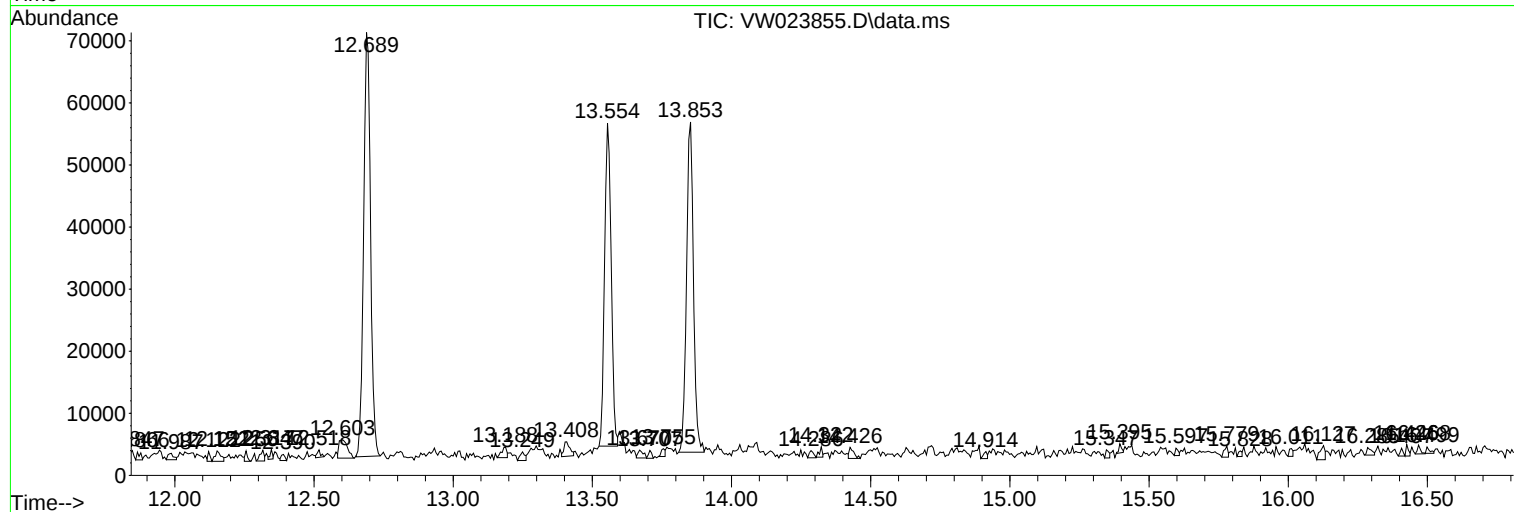
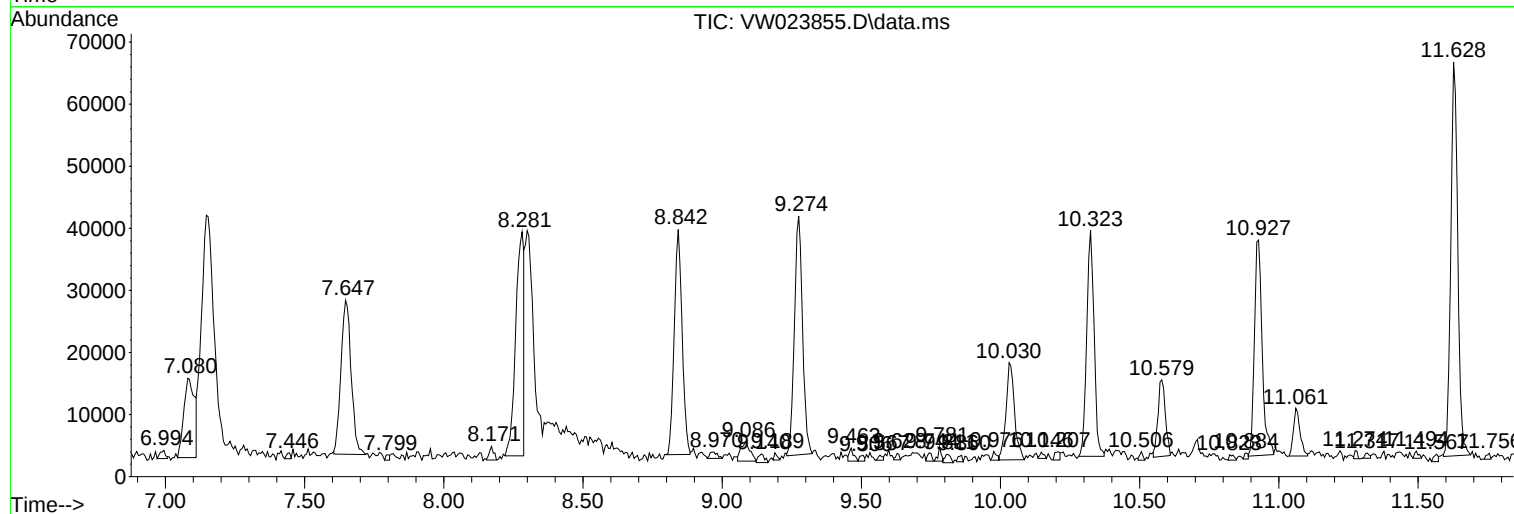
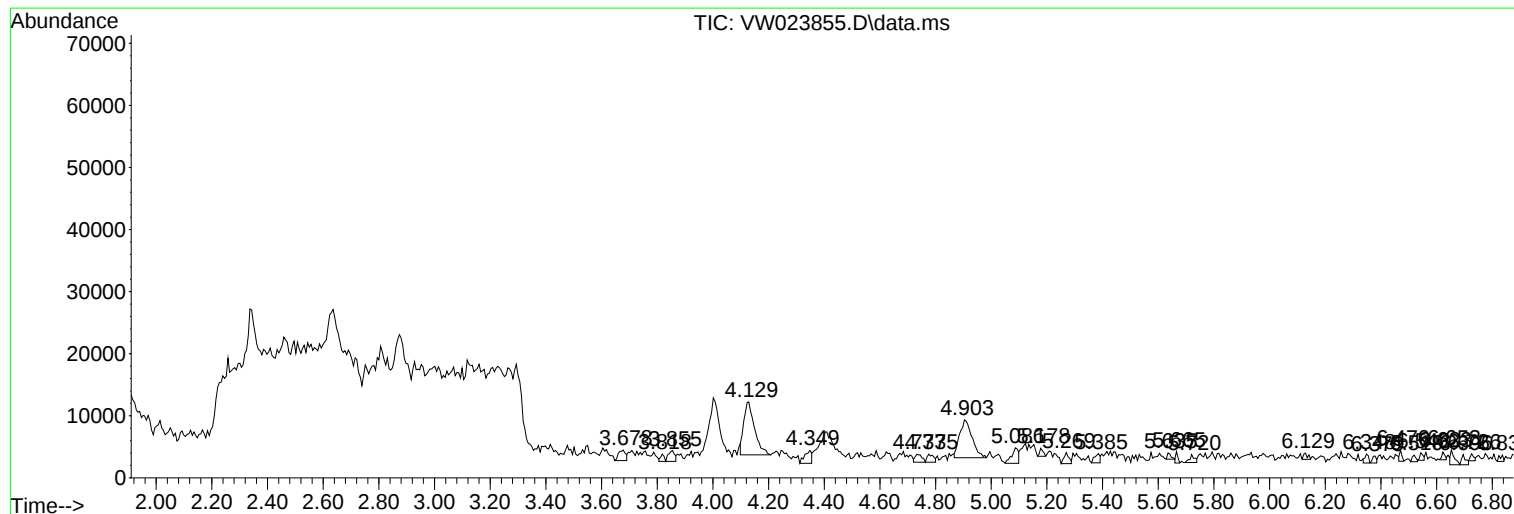
Sum of corrected areas: 1106260

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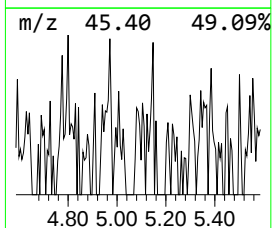
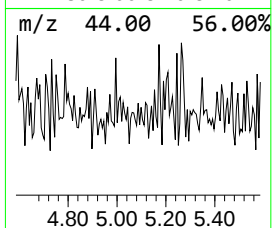
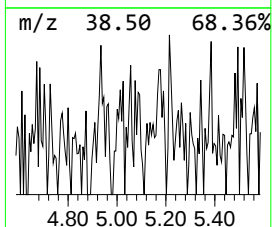
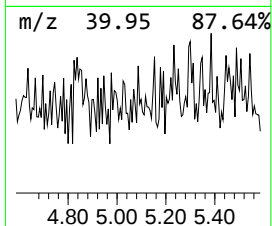
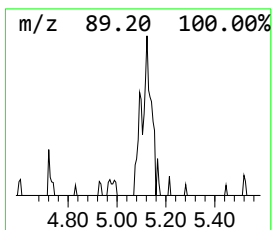
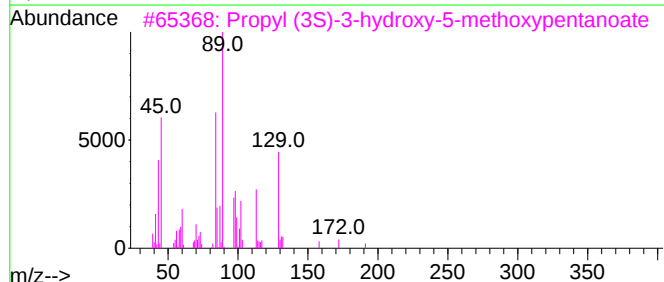
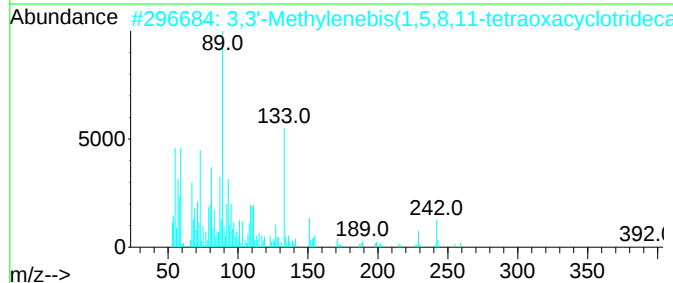
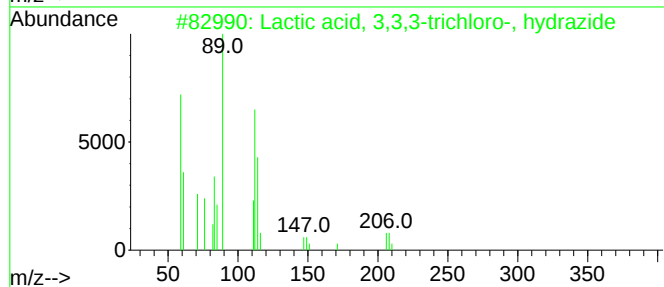
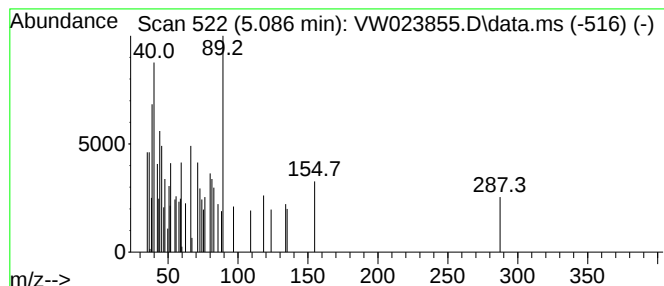
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM071322SMA.M
Quant Title : SFAM01.0

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

Peak Number 1 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.086	1.50 ug/L	4283	1,4-Difluorobenzene	8.842

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Lactic acid, 3,3,3-trichloro-, h...	206	C3H5Cl3N2O2	019836-22-7	43
2		3,3'-Methylenebis(1,5,8,11-tetra...	392	C19H36O8	120343-85-3	25
3		Propyl (3S)-3-hydroxy-5-methoxyp...	190	C9H18O4	1000429-61-1	12
4		2,5-Anhydrogluconic acid	178	C6H10O6	1000227-00-0	12
5		2,4,6-Trimethyldecane-1,3,10-triol	232	C13H28O3	085887-96-3	12



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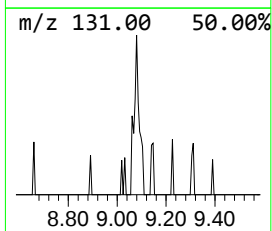
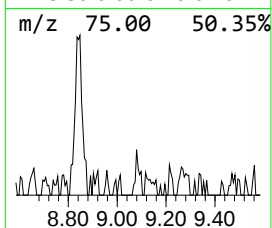
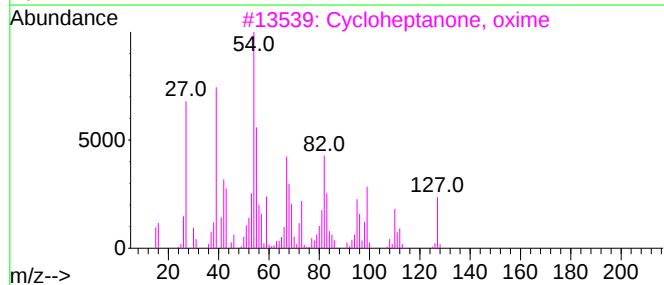
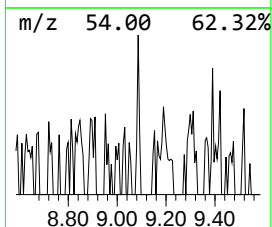
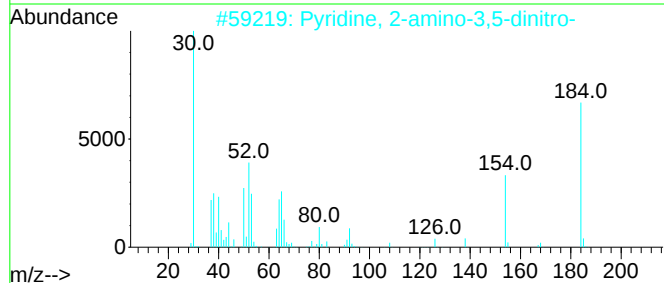
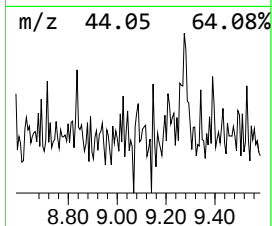
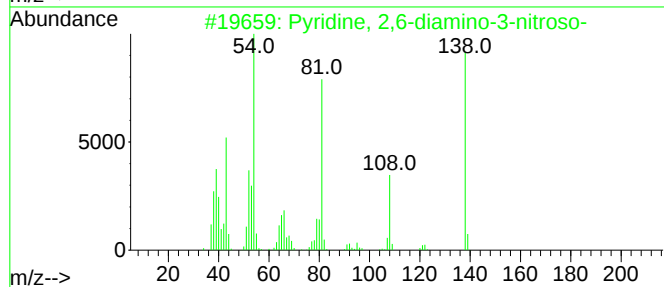
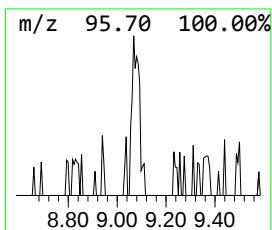
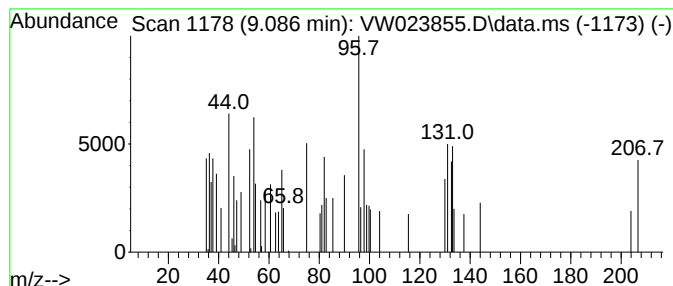
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM071322SMA.M
Quant Title : SFAM01.0

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

Peak Number 2 unknown-02 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.086	2.43 ug/L	6936	1,4-Difluorobenzene	8.842

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyridine, 2,6-diamino-3-nitroso-	138	C5H6N4O	089323-10-4	25
2			Pyridine, 2-amino-3,5-dinitro-	184	C5H4N4O4	003073-30-1	16
3			Cycloheptanone, oxime	127	C7H13NO	002158-31-8	10
4			(E)-2-Pentenitrile	81	C5H7N	026294-98-4	10
5			2-Pentenitrile	81	C5H7N	013284-42-9	10



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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	5.086	1.5	ug/L	4283	1	8.842	71403	25.0
unknown-02	9.086	2.4	ug/L	6936	1	8.842	71403	25.0