

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW121323\
 Data File : VW027601.D
 Acq On : 13 Dec 2023 17:50
 Operator : SY/MD
 Sample : 05806-09
 Misc : 4.23g/10mL/MSVOA_W/SOIL
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 E0LQ9

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\SFAMWLM120623SMA.M
 Title : SFAM01.0

Signal : TIC: VW027601.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.357	74	77	84	rVB	18427	34292	16.85%	2.730%
2	3.308	231	233	236	rBV4	1972	2802	1.38%	0.223%
3	3.643	286	288	293	rVB6	1516	2653	1.30%	0.211%
4	3.686	293	295	298	rBV4	986	1374	0.68%	0.109%
5	4.027	342	351	360	rBV2	26820	72998	35.87%	5.811%
6	4.289	391	394	395	rBV3	1762	1368	0.67%	0.109%
7	4.814	479	480	481	rBV	1414	884	0.43%	0.070%
8	4.850	485	486	487	rBV	1242	892	0.44%	0.071%
9	5.100	524	527	530	rBV5	1844	2703	1.33%	0.215%
10	5.320	560	563	565	rBV4	1804	2269	1.11%	0.181%
11	5.393	574	575	577	rBV2	864	757	0.37%	0.060%
12	5.661	618	619	625	rVB6	1624	2461	1.21%	0.196%
13	5.704	625	626	627	rBV	1136	671	0.33%	0.053%
14	5.990	671	673	675	rBV3	1114	1144	0.56%	0.091%
15	6.130	693	696	697	rBV3	1939	1922	0.94%	0.153%
16	6.563	763	767	768	rBV4	1097	1311	0.64%	0.104%
17	6.679	784	786	788	rBV2	1085	1042	0.51%	0.083%
18	6.795	803	805	807	rBV3	1025	913	0.45%	0.073%
19	7.008	839	840	843	rBV3	1347	1136	0.56%	0.090%
20	7.088	846	853	854	rBV	7128	11622	5.71%	0.925%
21	7.648	938	945	954	rVB	35455	85823	42.17%	6.832%
22	7.868	979	981	982	rBV2	1542	1247	0.61%	0.099%
23	8.008	1003	1004	1006	rVB2	1412	917	0.45%	0.073%
24	8.100	1018	1019	1022	rBV3	1244	814	0.40%	0.065%
25	8.130	1022	1024	1026	rVB2	1398	1126	0.55%	0.090%
26	8.185	1031	1033	1034	rBV2	1268	979	0.48%	0.078%
27	8.276	1041	1048	1060	rVB2	71784	203529	100.00%	16.203%
28	8.593	1098	1100	1103	rBV4	1741	1755	0.86%	0.140%
29	8.636	1105	1107	1108	rBV2	1492	1228	0.60%	0.098%
30	8.758	1125	1127	1129	rBV2	1302	1787	0.88%	0.142%
31	8.843	1135	1141	1150	rVV	53864	105273	51.72%	8.381%
32	8.929	1153	1155	1158	rBV3	1330	1946	0.96%	0.155%
33	9.026	1170	1171	1172	rBV	1485	1031	0.51%	0.082%
34	9.270	1205	1211	1222	rVB2	50143	106078	52.12%	8.445%
35	9.422	1234	1236	1239	rVB4	1017	1083	0.53%	0.086%
36	9.453	1239	1241	1242	rBV2	1266	1005	0.49%	0.080%

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM120623SMA.M
 Title : SFAM01.0

37	9.514	1248	1251	1252	rBV3	1509	1524	0.75%	0.121%
38	9.618	1266	1268	1269	rBV2	1684	1200	0.59%	0.096%
39	9.764	1291	1292	1293	rBV	1218	703	0.35%	0.056%
40	10.032	1331	1336	1345	rBV2	20616	40944	20.12%	3.260%
41	10.203	1360	1364	1366	rBV5	1215	1583	0.78%	0.126%
42	10.227	1366	1368	1370	rBV3	880	777	0.38%	0.062%
43	10.325	1377	1384	1392	rBV	77813	141499	69.52%	11.265%
44	10.495	1409	1412	1414	rBV4	1144	1254	0.62%	0.100%
45	10.581	1420	1426	1432	rBV2	10859	20068	9.86%	1.598%
46	10.703	1441	1446	1451	rVB2	7404	13419	6.59%	1.068%
47	10.849	1467	1470	1476	rBV8	3088	5384	2.65%	0.429%
48	11.239	1532	1534	1536	rBV3	1414	1206	0.59%	0.096%
49	11.410	1555	1562	1563	rBV6	2338	3527	1.73%	0.281%
50	11.562	1584	1587	1588	rBV3	1713	1384	0.68%	0.110%
51	11.581	1588	1590	1591	rVV2	1186	1025	0.50%	0.082%
52	11.629	1591	1598	1608	rVB	57463	104708	51.45%	8.336%
53	11.696	1608	1609	1610	rBV	1996	964	0.47%	0.077%
54	11.904	1640	1643	1644	rBV3	1736	1309	0.64%	0.104%
55	11.946	1649	1650	1655	rBV5	983	687	0.34%	0.055%
56	12.001	1658	1659	1662	rBV3	1122	1077	0.53%	0.086%
57	12.062	1666	1669	1670	rBV3	1025	1016	0.50%	0.081%
58	12.178	1685	1688	1690	rBV3	1367	2069	1.02%	0.165%
59	12.245	1698	1699	1700	rVV	1202	499	0.25%	0.040%
60	12.263	1700	1702	1703	rVB2	1334	864	0.42%	0.069%
61	12.300	1704	1708	1710	rBV5	896	947	0.47%	0.075%
62	12.337	1712	1714	1717	rBV4	950	989	0.49%	0.079%
63	12.367	1717	1719	1721	rVB3	2071	1352	0.66%	0.108%
64	12.385	1721	1722	1726	rBV4	1242	1608	0.79%	0.128%
65	12.538	1744	1747	1752	rBV7	1714	2872	1.41%	0.229%
66	12.605	1752	1758	1764	rVV3	13833	25726	12.64%	2.048%
67	12.690	1766	1772	1780	rVV2	30057	54240	26.65%	4.318%
68	12.745	1780	1781	1783	rVV2	1461	940	0.46%	0.075%
69	12.794	1787	1789	1794	rVB6	1248	2191	1.08%	0.174%
70	12.843	1794	1797	1798	rBV3	958	1003	0.49%	0.080%
71	12.861	1798	1800	1803	rVB3	1361	1206	0.59%	0.096%
72	12.885	1803	1804	1807	rBV3	1323	1340	0.66%	0.107%
73	12.916	1807	1809	1810	rBV2	1124	685	0.34%	0.055%
74	13.086	1835	1837	1839	rVB2	1558	1271	0.62%	0.101%
75	13.135	1843	1845	1847	rBV3	1328	1498	0.74%	0.119%
76	13.227	1857	1860	1863	rBV4	1056	1348	0.66%	0.107%

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 Title : SFAM01.0

77	13.269	1865	1867	1868	rBV2	1508	1536	0.75%	0.122%
78	13.458	1896	1898	1900	rBV3	1461	1373	0.67%	0.109%
79	13.556	1908	1914	1927	rVB	27704	51450	25.28%	4.096%
80	13.678	1932	1934	1936	rVB3	1210	1123	0.55%	0.089%
81	13.702	1936	1938	1939	rBV2	1119	976	0.48%	0.078%
82	13.751	1943	1946	1950	rBV6	2091	2650	1.30%	0.211%
83	13.849	1956	1962	1968	rBV	34266	59349	29.16%	4.725%
84	14.056	1993	1996	2001	rVB4	2554	4225	2.08%	0.336%
85	14.159	2012	2013	2014	rBV	818	595	0.29%	0.047%
86	14.208	2019	2021	2023	rVV3	1208	1169	0.57%	0.093%
87	14.269	2028	2031	2034	rBV5	1487	1884	0.93%	0.150%
88	14.294	2034	2035	2037	rBV2	885	751	0.37%	0.060%
89	14.373	2046	2048	2049	rVB2	969	618	0.30%	0.049%
90	14.409	2052	2054	2056	rVB3	1555	925	0.45%	0.074%
91	14.452	2059	2061	2063	rVB3	1264	1109	0.54%	0.088%
92	14.483	2063	2066	2067	rBV3	1322	1576	0.77%	0.125%
93	14.525	2072	2073	2074	rBV	1521	796	0.39%	0.063%
94	14.574	2079	2081	2085	rBV5	1271	1245	0.61%	0.099%
95	14.604	2085	2086	2088	rBV2	950	551	0.27%	0.044%
96	14.757	2109	2111	2112	rBV2	948	546	0.27%	0.043%
97	14.940	2140	2141	2142	rBV	1634	861	0.42%	0.069%
98	15.421	2215	2220	2225	rVB5	4909	9074	4.46%	0.722%
99	15.684	2261	2263	2266	rVB4	1566	1278	0.63%	0.102%
100	16.494	2393	2396	2399	rBV5	1156	1700	0.84%	0.135%

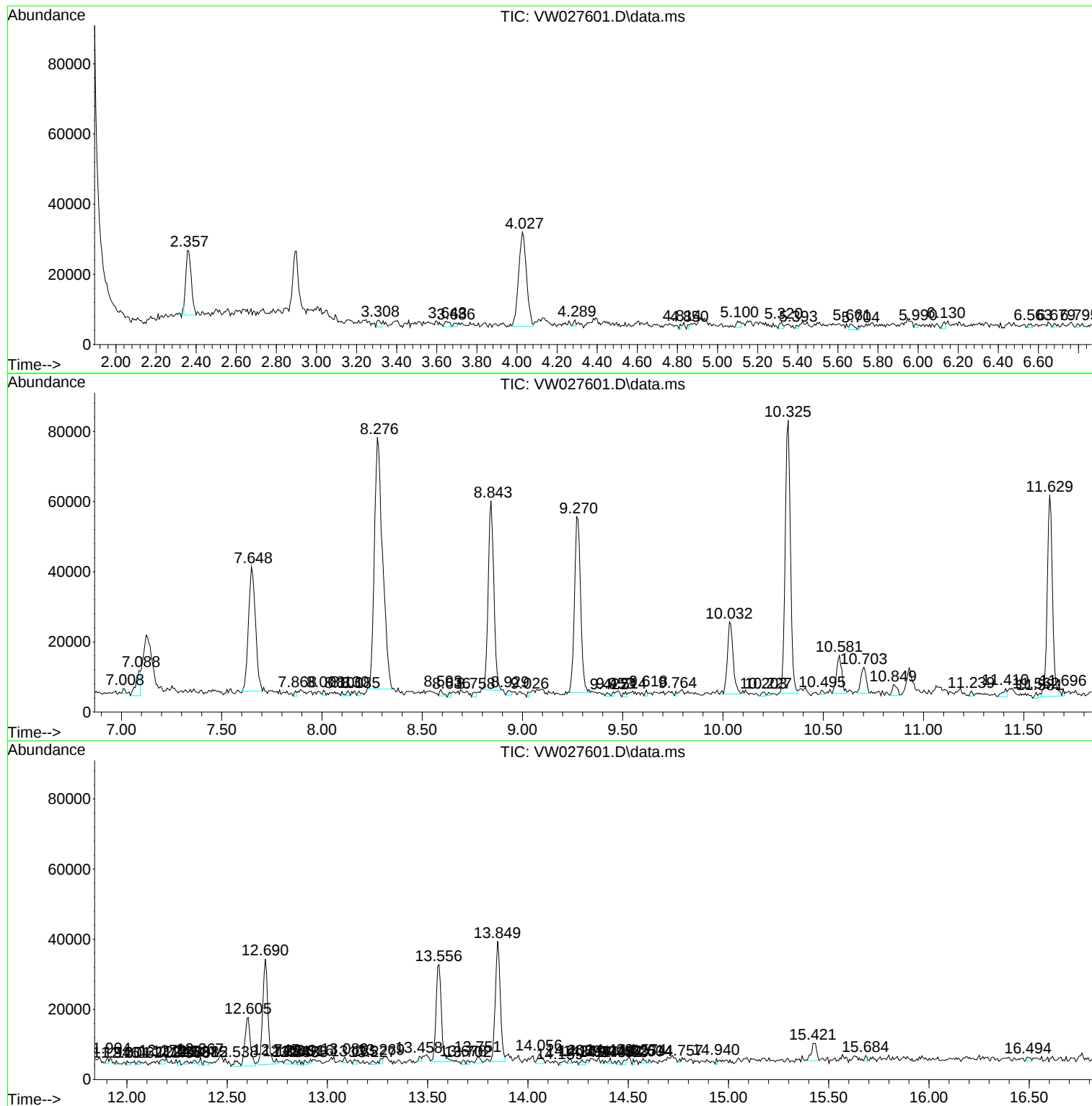
Sum of corrected areas: 1256101

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM120623SMA.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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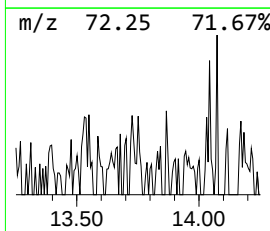
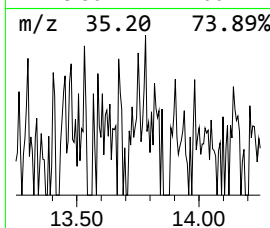
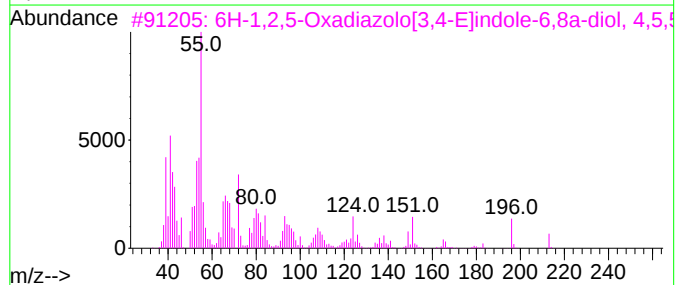
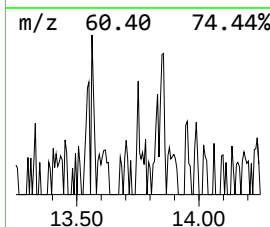
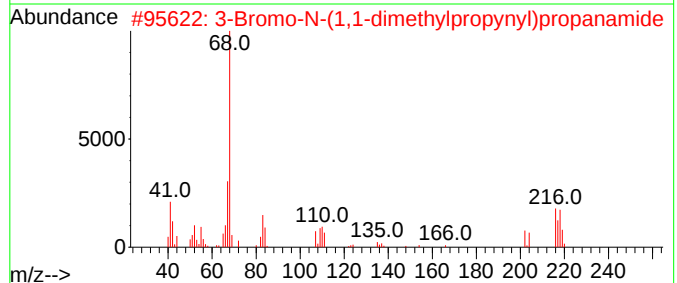
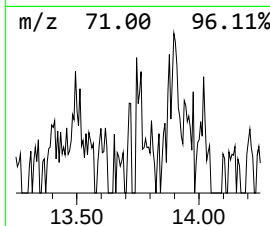
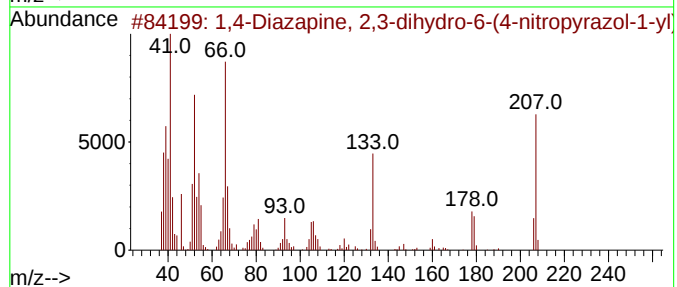
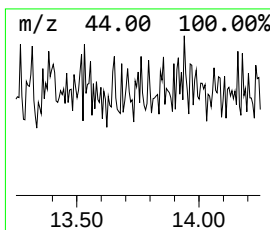
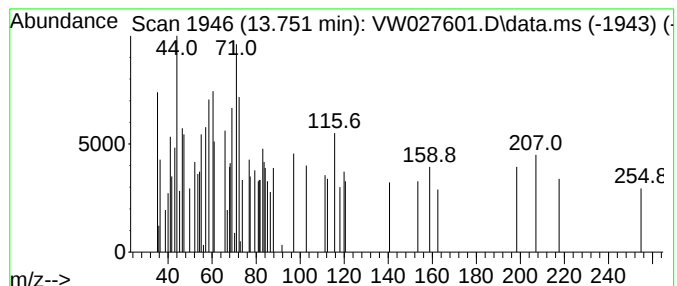
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM120623SMA.M
Quant Title : SFAM01.0

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

Peak Number 4 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.751	1.29 ug/L	2650	1,4-Dichlorobenzene-d4	13.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Diazapine, 2,3-dihydro-6-(4-...	207	C8H9N5O2	108262-29-9	46
2			3-Bromo-N-(1,1-dimethylpropynyl)...	217	C8H12BrNO	1000140-18-6	23
3			6H-1,2,5-Oxadiazolo[3,4-E]indole...	213	C8H11N3O4	331853-25-9	20
4			Propanoic acid, 3-(methylthio)-	120	C4H8O2S	000646-01-5	12
5			Pyrazine, 2-ethenyl-5-methyl-	120	C7H8N2	013925-08-1	9



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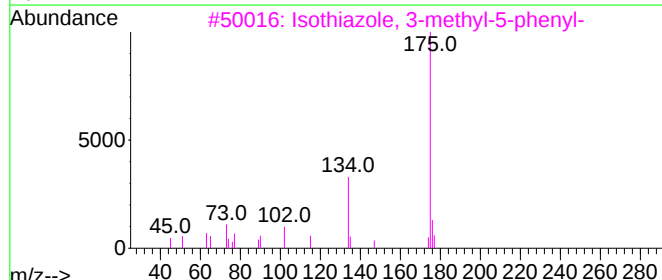
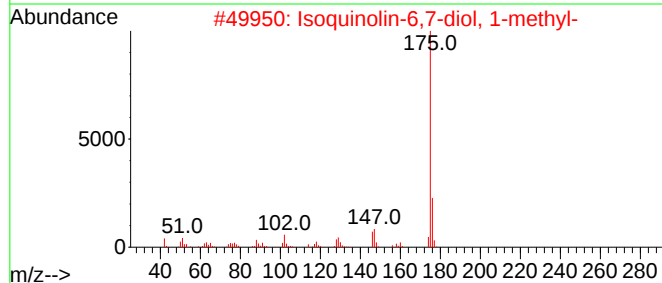
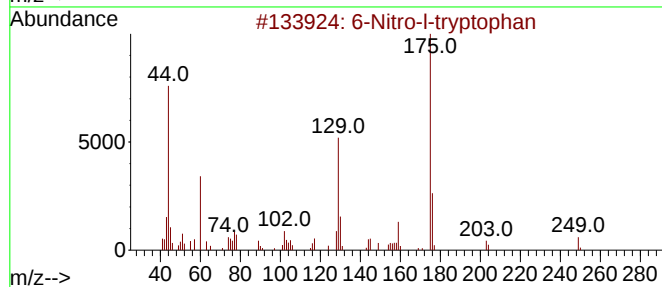
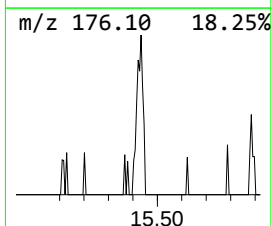
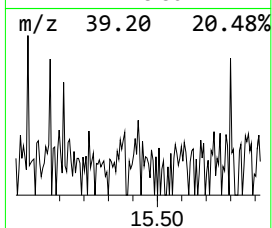
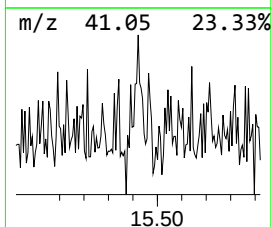
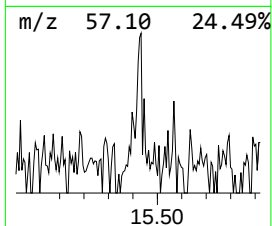
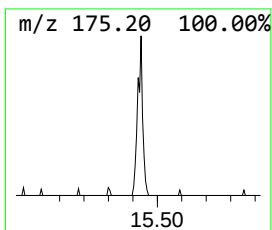
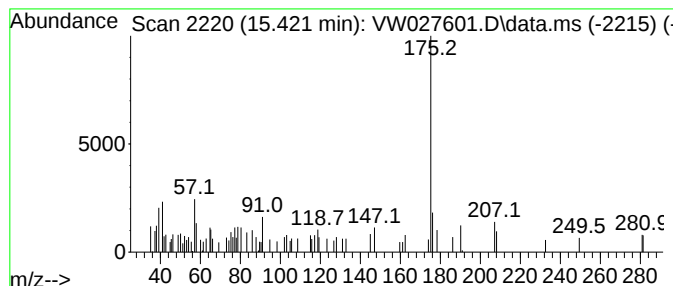
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM120623SMA.M
Quant Title : SFAM01.0

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

Peak Number 6 unknown-02 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.421	4.41 ug/L	9074	1,4-Dichlorobenzene-d4	13.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			6-Nitro-l-tryptophan	249	C11H11N3O4	1000130-45-3	49
2			Isoquinolin-6,7-diol, 1-methyl-	175	C10H9NO2	123438-49-3	49
3			Isothiazole, 3-methyl-5-phenyl-	175	C10H9NS	001732-45-2	47
4			Quinoline, 6-methoxy-, 1-oxide	175	C10H9NO2	006563-13-9	47
5			4-Methyl-2,6-dihydroxyquinoline	175	C10H9NO2	034982-01-9	47



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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	13.751	1.3	ug/L	2650	3	13.550	51450	25.0
unknown-02	15.421	4.4	ug/L	9074	3	13.550	51450	25.0