

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW082622\
 Data File : VW024404.D
 Acq On : 27 Aug 2022 16:32
 Operator : SY/VA
 Sample : VIBLK542
 Misc : 5.00g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 VIBLK542

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\SFAMWLM082622SMA.M
 Title : SFAM01.0

Signal : TIC: VW024404.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	47	58	59	rBV9	13538	40339	4.27%	0.543%
2	2.337	67	71	82	rVB	142056	230802	24.44%	3.109%
3	2.867	154	158	168	rVB	83610	168776	17.87%	2.273%
4	3.745	300	302	304	rBV3	2081	2213	0.23%	0.030%
5	4.007	336	345	357	rBV2	67501	195063	20.66%	2.628%
6	4.239	381	383	385	rBV3	2189	1585	0.17%	0.021%
7	4.525	428	430	432	rBV3	1762	2028	0.21%	0.027%
8	4.769	468	470	473	rBV3	1834	1802	0.19%	0.024%
9	5.434	576	579	580	rBV3	1801	1535	0.16%	0.021%
10	5.580	601	603	605	rBV3	1688	1347	0.14%	0.018%
11	6.427	740	742	746	rBV5	1414	1424	0.15%	0.019%
12	6.623	771	774	775	rBV3	1634	1502	0.16%	0.020%
13	7.080	843	849	856	rBV2	18331	46353	4.91%	0.624%
14	7.427	904	906	907	rBV2	1593	1097	0.12%	0.015%
15	7.647	934	942	952	rVB	122274	295249	31.27%	3.977%
16	7.939	988	990	993	rBV4	1956	1880	0.20%	0.025%
17	8.153	1022	1025	1026	rBV2	1233	1318	0.14%	0.018%
18	8.275	1035	1045	1060	rBV2	247883	763295	80.83%	10.282%
19	8.665	1107	1109	1110	rBV2	1649	1454	0.15%	0.020%
20	8.842	1130	1138	1148	rVB	266426	519531	55.02%	6.998%
21	9.165	1190	1191	1193	rVB2	1837	1076	0.11%	0.014%
22	9.274	1199	1209	1217	rBV	203924	417805	44.24%	5.628%
23	9.390	1227	1228	1230	rBV2	1469	862	0.09%	0.012%
24	9.531	1249	1251	1253	rBV3	1586	1168	0.12%	0.016%
25	9.598	1260	1262	1265	rBV3	1099	1345	0.14%	0.018%
26	9.652	1269	1271	1273	rBV3	825	667	0.07%	0.009%
27	9.671	1273	1274	1275	rVB	1302	476	0.05%	0.006%
28	9.689	1275	1277	1280	rBV4	1455	1259	0.13%	0.017%
29	9.720	1280	1282	1283	rVB2	1181	855	0.09%	0.012%
30	9.738	1283	1285	1286	rVB2	1227	675	0.07%	0.009%
31	9.768	1286	1290	1292	rBV4	1723	2911	0.31%	0.039%
32	9.927	1314	1316	1317	rBV2	1153	813	0.09%	0.011%
33	10.037	1324	1334	1343	rBV	126099	236579	25.05%	3.187%
34	10.201	1359	1361	1363	rBV3	1527	1685	0.18%	0.023%
35	10.323	1373	1381	1389	rBV	485569	834353	88.36%	11.239%
36	10.579	1416	1423	1431	rBV2	82128	151329	16.03%	2.038%

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 Title : SFAM01.0

37	10.701	1437	1443	1452	rVB3	20031	39306	4.16%	0.529%
38	10.860	1461	1469	1474	rBV2	22103	45484	4.82%	0.613%
39	10.921	1474	1479	1491	rVB	130055	234879	24.87%	3.164%
40	11.061	1498	1502	1512	rVB	23364	39083	4.14%	0.526%
41	11.433	1554	1563	1569	rBV2	13294	27435	2.91%	0.370%
42	11.481	1569	1571	1573	rVB3	1261	697	0.07%	0.009%
43	11.628	1588	1595	1607	rBV	568967	944301	100.00%	12.720%
44	12.024	1656	1660	1662	rBV4	737	1015	0.11%	0.014%
45	12.048	1662	1664	1665	rVV2	1130	539	0.06%	0.007%
46	12.237	1692	1695	1696	rBV3	1009	1058	0.11%	0.014%
47	12.280	1699	1702	1704	rVB3	1090	865	0.09%	0.012%
48	12.402	1720	1722	1726	rVB5	1216	1504	0.16%	0.020%
49	12.439	1726	1728	1730	rBV3	1477	1557	0.16%	0.021%
50	12.493	1735	1737	1739	rVB3	961	772	0.08%	0.010%
51	12.524	1741	1742	1743	rVB	1180	440	0.05%	0.006%
52	12.603	1749	1755	1759	rBV2	15457	26115	2.77%	0.352%
53	12.689	1763	1769	1778	rVV	219383	364187	38.57%	4.906%
54	12.817	1788	1790	1792	rVB2	952	647	0.07%	0.009%
55	12.859	1795	1797	1799	rVB2	1860	1631	0.17%	0.022%
56	12.884	1799	1801	1803	rBV3	1508	1744	0.18%	0.023%
57	12.926	1803	1808	1813	rVB8	2794	5906	0.63%	0.080%
58	12.963	1813	1814	1818	rVB4	1439	1400	0.15%	0.019%
59	13.018	1819	1823	1824	rBV4	860	1152	0.12%	0.016%
60	13.066	1830	1831	1832	rBV	851	519	0.05%	0.007%
61	13.164	1845	1847	1849	rBV3	1801	1395	0.15%	0.019%
62	13.231	1856	1858	1859	rBV2	1567	1139	0.12%	0.015%
63	13.335	1873	1875	1877	rBV3	820	473	0.05%	0.006%
64	13.402	1881	1886	1890	rBV6	2278	3957	0.42%	0.053%
65	13.438	1890	1892	1894	rVB3	1659	1429	0.15%	0.019%
66	13.475	1896	1898	1899	rBV2	969	704	0.07%	0.009%
67	13.554	1904	1911	1924	rVV	555023	879242	93.11%	11.844%
68	13.798	1949	1951	1952	rBV2	1434	906	0.10%	0.012%
69	13.847	1952	1959	1967	rVV	463672	768911	81.43%	10.357%
70	13.987	1980	1982	1984	rBV3	1831	1651	0.17%	0.022%
71	14.066	1991	1995	2002	rVB4	5194	9937	1.05%	0.134%
72	14.237	2022	2023	2024	rBV	1350	970	0.10%	0.013%
73	14.316	2030	2036	2046	rVB	3667	11240	1.19%	0.151%
74	14.396	2046	2049	2050	rBV3	1022	1050	0.11%	0.014%
75	14.414	2050	2052	2053	rBV2	956	818	0.09%	0.011%
76	14.469	2059	2061	2062	rBV2	1305	922	0.10%	0.012%

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Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM082622SMA.M
 Title : SFAM01.0

77	14.487	2062	2064	2066	rVV2	1129	1005	0.11%	0.014%
78	14.536	2071	2072	2073	rVB	1815	666	0.07%	0.009%
79	14.554	2073	2075	2076	rBV2	621	366	0.04%	0.005%
80	14.719	2098	2102	2107	rVB7	4164	7526	0.80%	0.101%
81	14.755	2107	2108	2111	rBV3	868	1223	0.13%	0.016%
82	14.798	2113	2115	2116	rVB	1271	627	0.07%	0.008%
83	14.883	2127	2129	2131	rVB3	1436	923	0.10%	0.012%
84	14.926	2134	2136	2137	rBV2	1198	1069	0.11%	0.014%
85	15.036	2152	2154	2155	rBV2	1261	953	0.10%	0.013%
86	15.054	2155	2157	2158	rVV2	1410	856	0.09%	0.012%
87	15.097	2162	2164	2166	rVV2	1735	1783	0.19%	0.024%
88	15.133	2166	2170	2174	rVV7	2420	4103	0.43%	0.055%
89	15.170	2174	2176	2181	rVV6	1556	2379	0.25%	0.032%
90	15.310	2196	2199	2201	rBV4	1501	1731	0.18%	0.023%
91	15.359	2203	2207	2210	rVV6	1512	2499	0.26%	0.034%
92	15.432	2214	2219	2224	rVB3	14707	25422	2.69%	0.342%
93	15.542	2233	2237	2238	rBV4	2363	3211	0.34%	0.043%
94	15.828	2282	2284	2288	rBV5	1706	2167	0.23%	0.029%
95	16.115	2329	2331	2332	rVB2	995	669	0.07%	0.009%
96	16.182	2340	2342	2343	rBV2	744	596	0.06%	0.008%
97	16.279	2356	2358	2359	rBV	1183	983	0.10%	0.013%
98	16.346	2365	2369	2370	rBV3	1346	1807	0.19%	0.024%
99	16.694	2424	2426	2428	rBV3	1223	1023	0.11%	0.014%
100	16.743	2432	2434	2435	rVB2	1372	778	0.08%	0.010%

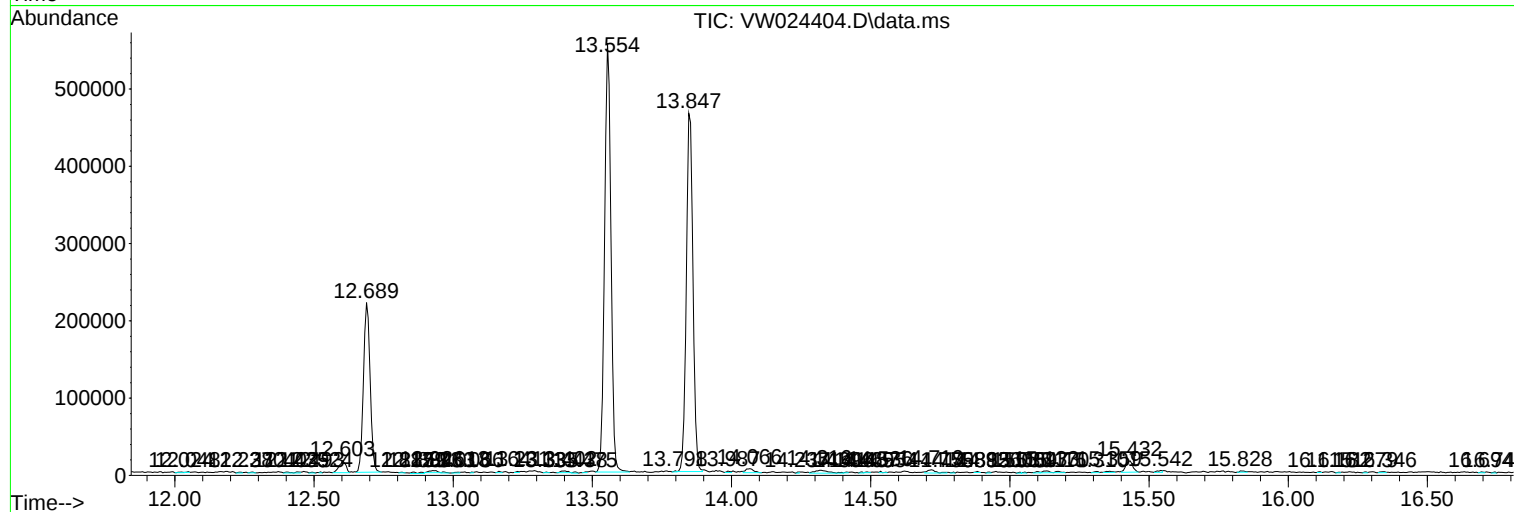
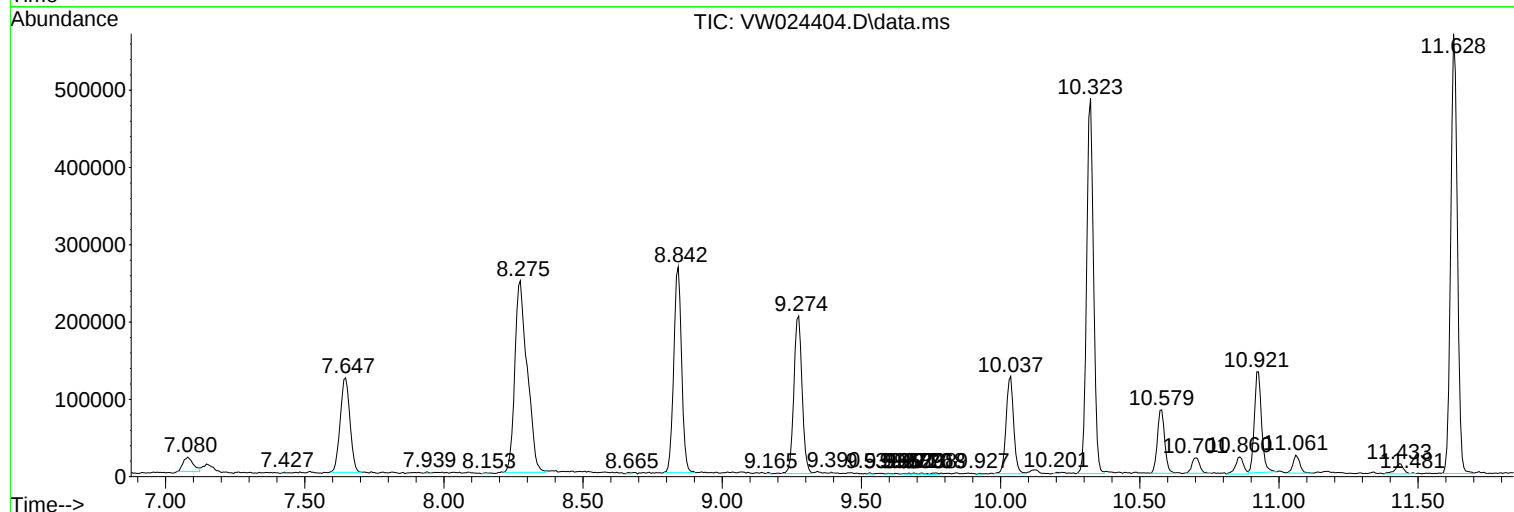
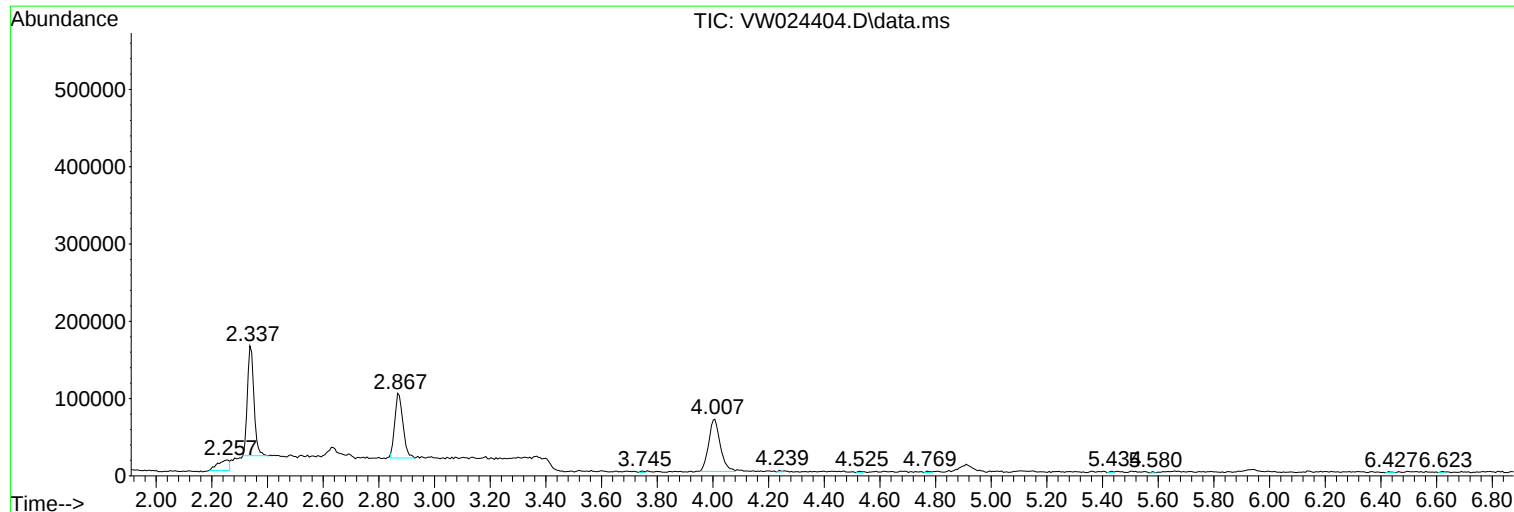
Sum of corrected areas: 7423796

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ALS Vial : 1 Sample Multiplier: 1

Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM082622SMA.M
Quant Title : SFAM01.0

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



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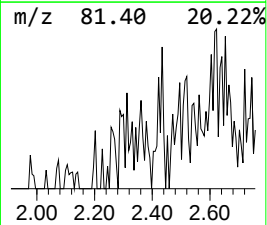
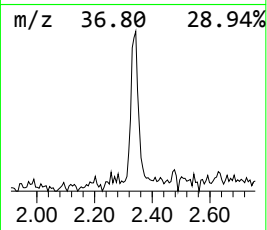
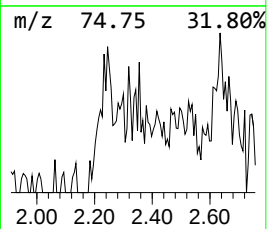
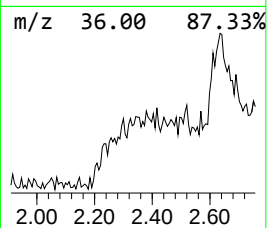
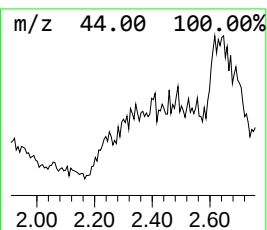
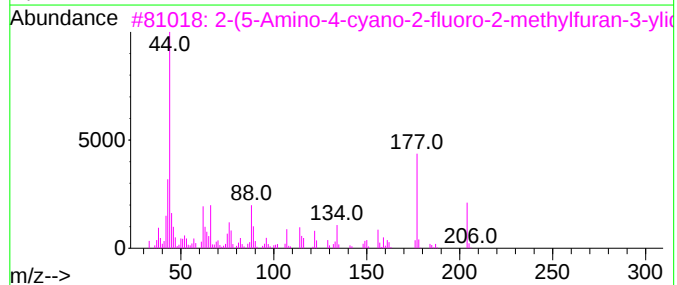
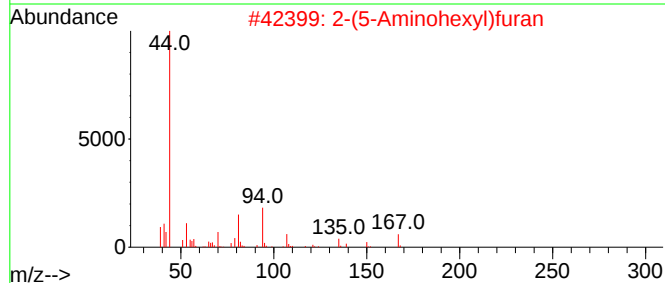
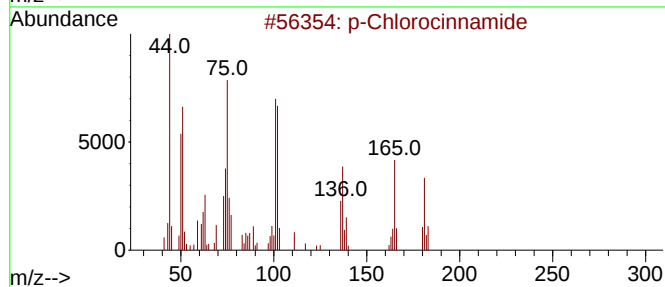
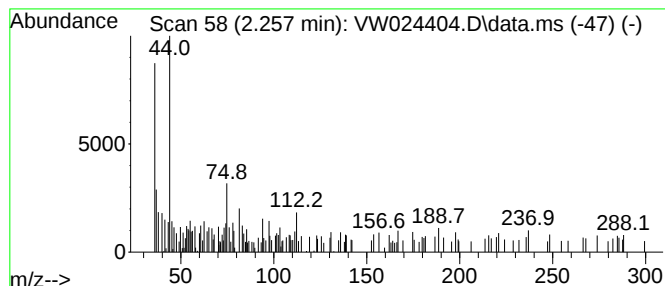
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM082622SMA.M
Quant Title : SFAM01.0

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

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.257	1.94 ug/L	40339	1,4-Difluorobenzene	8.842

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			p-Chlorocinnamide	181	C9H8ClNO	018166-64-8	38
2			2-(5-Aminohexyl)furan	167	C10H17NO	013748-11-3	30
3			2-(5-Amino-4-cyano-2-fluoro-2-me...	204	C9H5FN4O	1000435-15-6	25
4			Atomoxetine	255	C17H21NO	083015-26-3	22
5			2-Chloroprop-2-enamide	105	C3H4ClNO	1000411-34-7	16



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	2.257	1.9	ug/L	40339	1	8.842	519531	25.0