

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW071922\
 Data File : VW023938.D
 Acq On : 20 Jul 2022 15:28
 Operator : SY/VA
 Sample : N3744-15
 Misc : 5.88g/10mL/MSVOA_W/SOIL
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 F5D01

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: VW023938.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	rBV7	11820	35505	2.67%	0.342%
2	2.343	68	72	83	rVB	137267	242847	18.25%	2.341%
3	2.879	154	160	174	rVB	92872	208441	15.66%	2.010%
4	3.495	259	261	264	rBV4	1113	1251	0.09%	0.012%
5	3.538	264	268	269	rBV4	1388	1255	0.09%	0.012%
6	3.739	298	301	302	rBV3	1113	1200	0.09%	0.012%
7	3.812	310	313	316	rBV5	853	907	0.07%	0.009%
8	4.007	335	345	360	rBV2	76864	260987	19.61%	2.516%
9	4.409	408	411	412	rBV3	1338	1496	0.11%	0.014%
10	5.104	523	525	527	rBV3	1128	1152	0.09%	0.011%
11	5.208	540	542	544	rVB4	1570	1033	0.08%	0.010%
12	5.232	544	546	550	rVB5	1023	1145	0.09%	0.011%
13	5.391	565	572	574	rBV5	1950	3411	0.26%	0.033%
14	5.866	648	650	653	rBV4	866	1112	0.08%	0.011%
15	6.086	684	686	691	rVB4	1073	1365	0.10%	0.013%
16	6.220	703	708	709	rBV4	765	1167	0.09%	0.011%
17	6.312	720	723	727	rBV4	1029	1443	0.11%	0.014%
18	6.354	727	730	733	rVB4	1511	1867	0.14%	0.018%
19	6.464	746	748	750	rBV2	750	954	0.07%	0.009%
20	6.598	767	770	774	rBV4	1458	2731	0.21%	0.026%
21	6.763	794	797	800	rVB5	937	1362	0.10%	0.013%
22	7.019	836	839	840	rBV3	1616	1469	0.11%	0.014%
23	7.080	841	849	855	rVV	31395	91200	6.85%	0.879%
24	7.165	855	863	879	rVB2	199668	545865	41.02%	5.263%
25	7.445	906	909	913	rBV4	989	1428	0.11%	0.014%
26	7.647	932	942	955	rBV2	178043	447837	33.65%	4.318%
27	7.817	968	970	972	rVB2	1552	936	0.07%	0.009%
28	7.848	972	975	978	rBV5	1914	2197	0.17%	0.021%
29	7.951	984	992	993	rBV5	1804	3854	0.29%	0.037%
30	8.122	1017	1020	1023	rBV5	1075	1560	0.12%	0.015%
31	8.275	1034	1045	1064	rBV2	350541	1052960	79.13%	10.152%
32	8.744	1121	1122	1125	rBV3	912	974	0.07%	0.009%
33	8.842	1129	1138	1150	rVV	335251	656921	49.37%	6.334%
34	9.091	1171	1179	1192	rVB	320164	624878	46.96%	6.025%
35	9.274	1200	1209	1219	rBV	241532	494429	37.16%	4.767%
36	9.433	1233	1235	1238	rBV4	668	916	0.07%	0.009%

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 Title : SFAM01.0

37	9.482	1241	1243	1244	rBV2	1225	1086	0.08%	0.010%
38	9.622	1264	1266	1269	rBV3	1463	1586	0.12%	0.015%
39	9.646	1269	1270	1271	rBV	1523	1106	0.08%	0.011%
40	9.713	1279	1281	1285	rVB3	1111	1137	0.09%	0.011%

41	9.902	1308	1312	1314	rBV5	767	992	0.07%	0.010%
42	9.939	1316	1318	1321	rBV4	1182	1145	0.09%	0.011%
43	9.988	1321	1326	1327	rBV5	1065	1583	0.12%	0.015%
44	10.036	1327	1334	1343	rVV	114646	206673	15.53%	1.993%
45	10.201	1358	1361	1364	rBV5	1322	2135	0.16%	0.021%

46	10.274	1369	1373	1374	rBV3	783	977	0.07%	0.009%
47	10.323	1374	1381	1387	rVV	505840	861563	64.75%	8.307%
48	10.384	1387	1391	1400	rVB	46065	82211	6.18%	0.793%
49	10.579	1417	1423	1432	rVB	78320	135242	10.16%	1.304%
50	10.786	1455	1457	1459	rVB2	1197	935	0.07%	0.009%

51	10.859	1461	1469	1475	rBV	790674	1330690	100.00%	12.830%
52	10.927	1475	1480	1491	rVB	148041	255276	19.18%	2.461%
53	11.061	1498	1502	1507	rVV4	5515	8231	0.62%	0.079%
54	11.128	1511	1513	1516	rVB5	1810	1670	0.13%	0.016%
55	11.292	1537	1540	1543	rBV4	1010	1438	0.11%	0.014%

56	11.433	1559	1563	1564	rBV4	1283	1635	0.12%	0.016%
57	11.500	1573	1574	1577	rVB2	1207	1030	0.08%	0.010%
58	11.628	1585	1595	1606	rBV	499000	839797	63.11%	8.097%
59	11.829	1625	1628	1633	rVV7	1811	3031	0.23%	0.029%
60	12.103	1670	1673	1674	rBV2	937	1129	0.08%	0.011%

61	12.182	1681	1686	1690	rBV8	1389	2620	0.20%	0.025%
62	12.243	1695	1696	1699	rVV3	1116	1167	0.09%	0.011%
63	12.359	1713	1715	1720	rVV6	660	1215	0.09%	0.012%
64	12.463	1729	1732	1735	rBV4	1102	1627	0.12%	0.016%
65	12.597	1748	1754	1762	rBV8	5726	14959	1.12%	0.144%

66	12.688	1762	1769	1777	rBV	226860	381717	28.69%	3.680%
67	12.835	1790	1793	1795	rBV4	967	1447	0.11%	0.014%
68	12.932	1805	1809	1812	rBV4	3830	5028	0.38%	0.048%
69	13.158	1844	1846	1848	rBV3	975	1036	0.08%	0.010%
70	13.243	1858	1860	1864	rBV4	2135	2131	0.16%	0.021%

71	13.402	1882	1886	1890	rVV6	3871	6199	0.47%	0.060%
72	13.487	1898	1900	1902	rBV3	1465	1879	0.14%	0.018%
73	13.554	1904	1911	1924	rVV	472471	753037	56.59%	7.260%
74	13.761	1942	1945	1951	rVB6	4326	6997	0.53%	0.067%
75	13.853	1953	1960	1967	rBV	440184	713376	53.61%	6.878%

76	14.237	2021	2023	2025	rBV3	1368	1203	0.09%	0.012%
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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM071322SMA.M
 Title : SFAM01.0

77	14.298	2032	2033	2035	rBV2	853	898	0.07%	0.009%
78	14.322	2035	2037	2041	rVB5	1470	1468	0.11%	0.014%
79	14.408	2048	2051	2052	rBV2	1098	1150	0.09%	0.011%
80	14.487	2061	2064	2065	rBV3	1444	1444	0.11%	0.014%
81	14.633	2086	2088	2092	rVB5	1197	1303	0.10%	0.013%
82	14.719	2098	2102	2106	rVB5	3657	5728	0.43%	0.055%
83	14.877	2125	2128	2130	rVB3	1284	1545	0.12%	0.015%
84	14.914	2130	2134	2137	rBV4	839	1691	0.13%	0.016%
85	15.072	2158	2160	2161	rBV2	970	980	0.07%	0.009%
86	15.127	2167	2169	2170	rBV2	1034	1038	0.08%	0.010%
87	15.225	2183	2185	2187	rBV3	944	1081	0.08%	0.010%
88	15.261	2189	2191	2195	rBV5	868	983	0.07%	0.009%
89	15.389	2210	2212	2214	rVB3	1103	899	0.07%	0.009%
90	15.407	2214	2215	2217	rBV2	2088	1514	0.11%	0.015%
91	15.749	2269	2271	2274	rBV5	1108	1519	0.11%	0.015%
92	15.895	2292	2295	2298	rBV4	909	1201	0.09%	0.012%
93	15.926	2298	2300	2302	rVV2	1322	1259	0.09%	0.012%
94	15.974	2306	2308	2311	rVB4	1111	1267	0.10%	0.012%
95	16.285	2357	2359	2362	rVB3	1233	1227	0.09%	0.012%
96	16.310	2362	2363	2366	rBV2	1152	1138	0.09%	0.011%
97	16.413	2376	2380	2381	rBV4	857	1231	0.09%	0.012%
98	16.627	2411	2415	2417	rVB5	972	1318	0.10%	0.013%
99	16.645	2417	2418	2424	rBV4	1134	1278	0.10%	0.012%
100	16.761	2435	2437	2440	rBV4	794	917	0.07%	0.009%

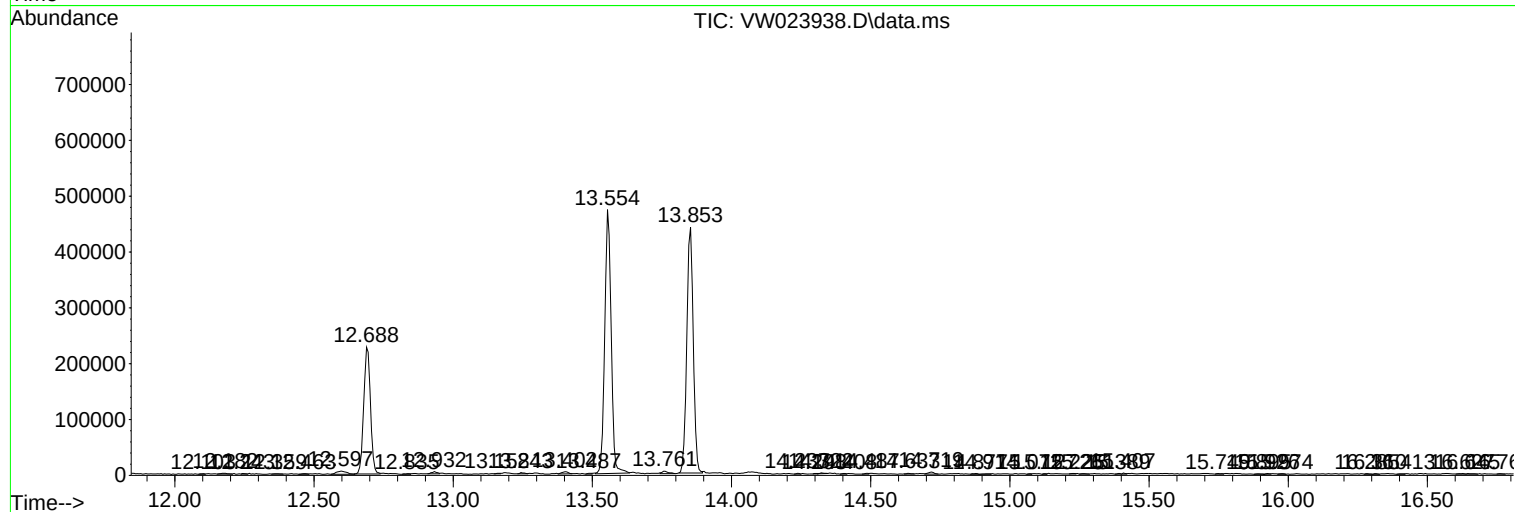
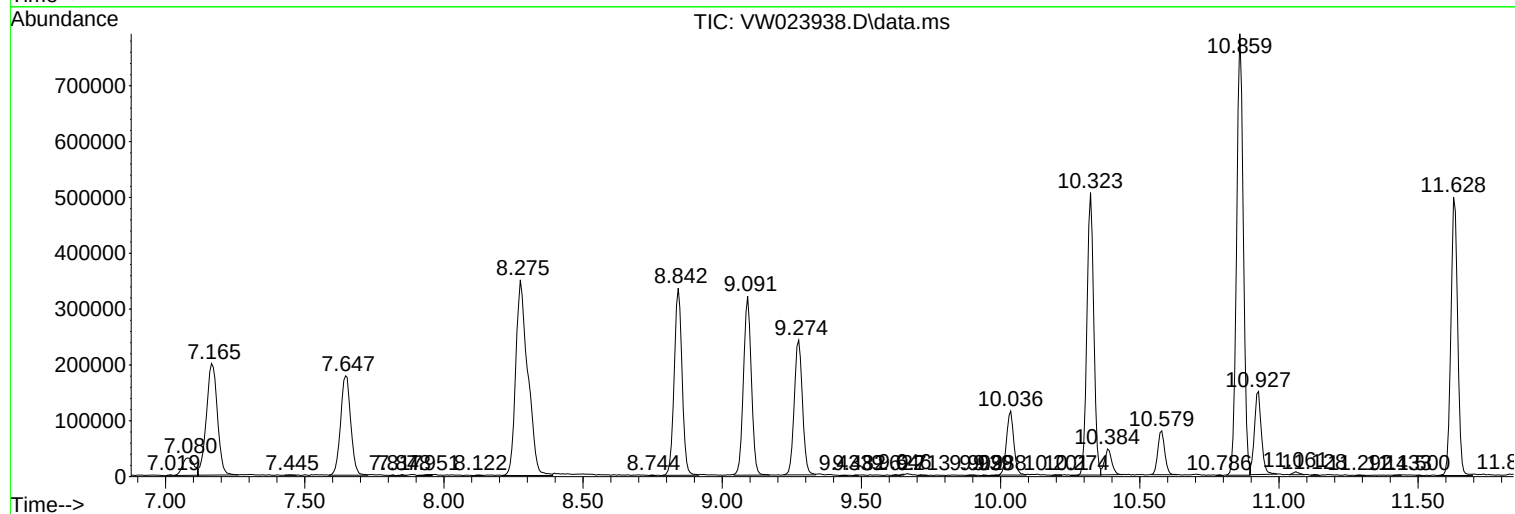
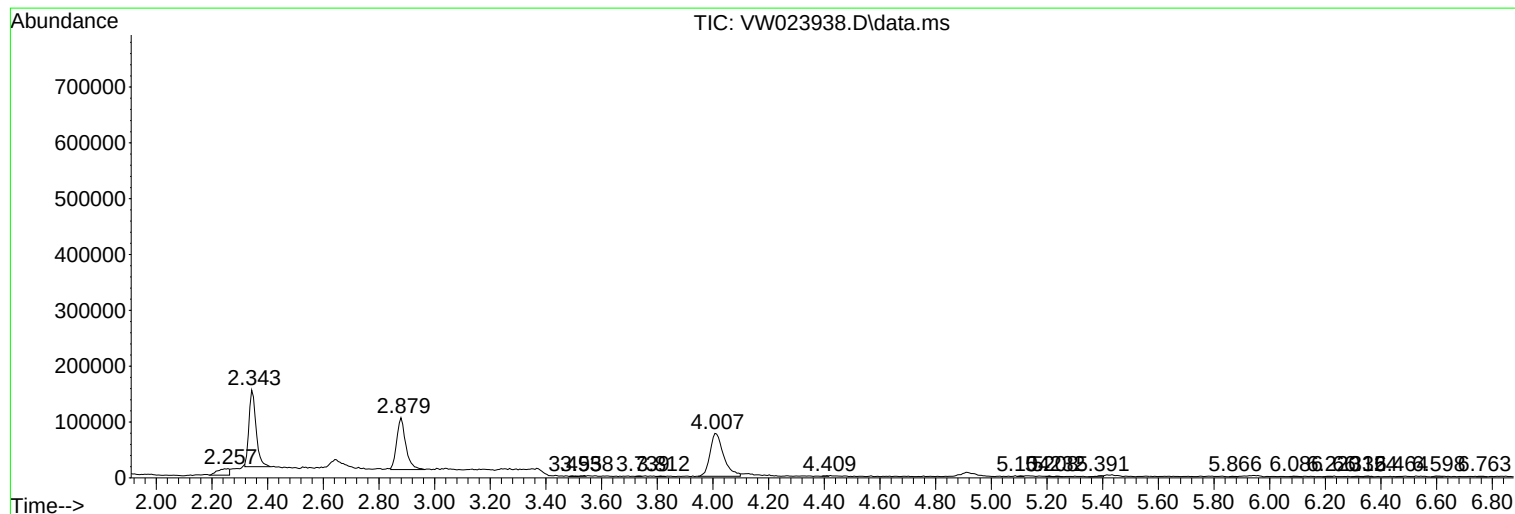
Sum of corrected areas: 10372068

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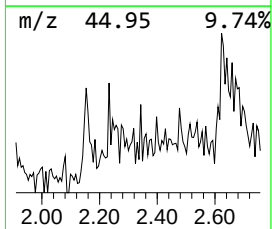
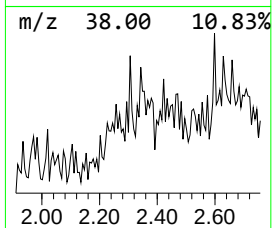
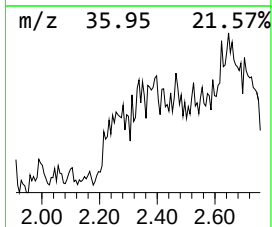
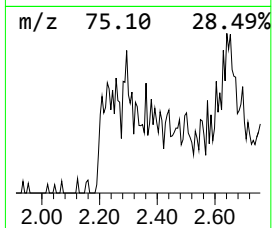
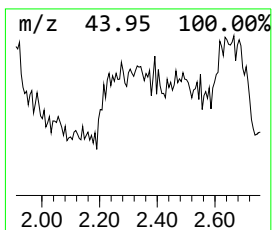
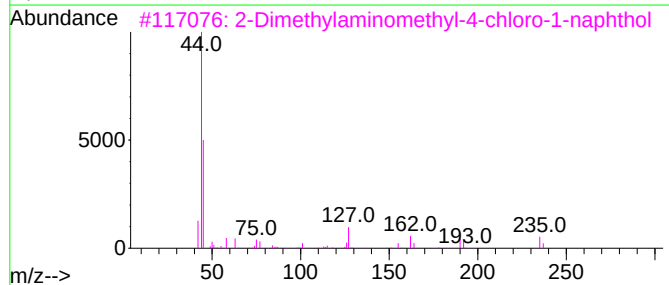
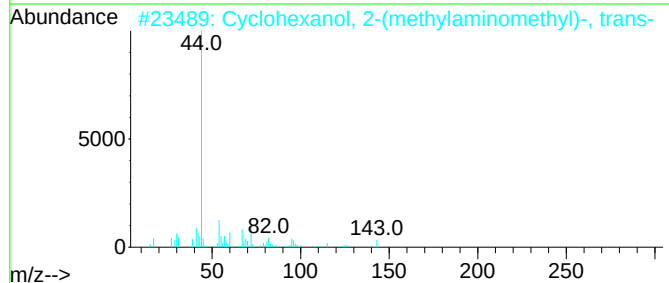
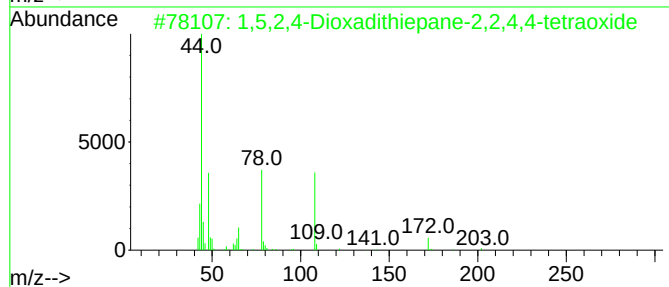
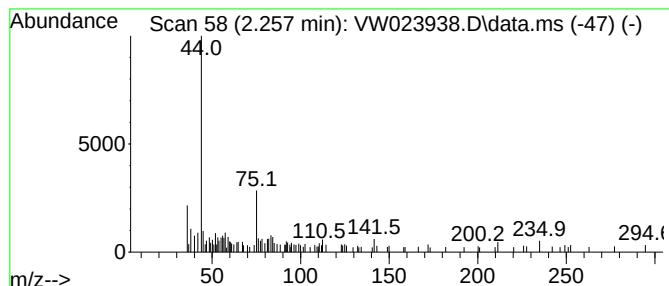
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM071322SMA.M
Quant Title : SFAM01.0

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

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.257	1.35 ug/L	35505	1,4-Difluorobenzene	8.842

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,5,2,4-Dioxadithiepane-2,2,4,4-...	202	C3H6O6S2	099591-73-8	47		
2	Cyclohexanol, 2-(methylaminometh...	143	C8H17NO	077612-16-9	47		
3	2-Dimethylaminomethyl-4-chloro-1...	235	C13H14ClNO	167163-22-6	43		
4	2-Aminopropane-1-thiol	91	C3H9NS	010229-29-5	43		
5	1-Pentanol, 4-amino-	103	C5H13NO	000927-55-9	43		



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	2.257	1.4	ug/L	35505	1	8.842	656921	25.0