

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW071522\
 Data File : VW023747.D
 Acq On : 15 Jul 2022 16:07
 Operator : SY/VA
 Sample : N3678-20
 Misc : 5.04g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 VHBLK001

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: VW023747.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.245	48	56	60	rBV5	11808	37673	5.29%	0.702%
2	2.349	68	73	86	rVB	119887	221588	31.11%	4.131%
3	2.879	155	160	172	rVB	70775	156469	21.97%	2.917%
4	3.885	323	325	326	rBV2	1303	735	0.10%	0.014%
5	4.013	337	346	358	rBV2	51421	165533	23.24%	3.086%
6	4.690	455	457	460	rBV4	1707	1924	0.27%	0.036%
7	5.098	521	524	525	rBV3	2734	2939	0.41%	0.055%
8	5.208	540	542	547	rVB6	1488	1879	0.26%	0.035%
9	5.257	547	550	552	rBV4	1285	1536	0.22%	0.029%
10	5.373	567	569	570	rBV2	1306	852	0.12%	0.016%
11	5.537	594	596	598	rBV3	1078	1140	0.16%	0.021%
12	5.720	624	626	629	rBV4	1896	2413	0.34%	0.045%
13	5.873	648	651	653	rBV4	801	969	0.14%	0.018%
14	5.934	653	661	670	rVB4	3403	12452	1.75%	0.232%
15	6.080	684	685	688	rBV3	1041	1104	0.16%	0.021%
16	6.123	691	692	695	rBV3	1331	1154	0.16%	0.022%
17	6.147	695	696	700	rBV3	1317	1703	0.24%	0.032%
18	6.336	725	727	728	rBV2	1202	1089	0.15%	0.020%
19	6.525	754	758	762	rVB7	1431	1989	0.28%	0.037%
20	6.562	762	764	765	rBV2	1396	1194	0.17%	0.022%
21	6.629	772	775	777	rVB4	1216	1213	0.17%	0.023%
22	6.720	788	790	793	rBV3	1403	1763	0.25%	0.033%
23	6.824	805	807	808	rBV2	904	823	0.12%	0.015%
24	6.915	820	822	826	rBV5	1331	1517	0.21%	0.028%
25	6.970	829	831	834	rBV4	1068	1204	0.17%	0.022%
26	7.080	845	849	855	rBV	13259	26106	3.67%	0.487%
27	7.330	888	890	894	rVB5	1592	1917	0.27%	0.036%
28	7.366	894	896	901	rBV6	1149	2209	0.31%	0.041%
29	7.500	915	918	921	rBV5	1087	1812	0.25%	0.034%
30	7.647	933	942	953	rBV	115293	284147	39.90%	5.297%
31	7.915	985	986	988	rVB2	1589	1124	0.16%	0.021%
32	7.958	988	993	998	rBV8	1938	3280	0.46%	0.061%
33	8.043	1006	1007	1010	rBV3	1277	1379	0.19%	0.026%
34	8.183	1029	1030	1033	rBV2	1304	1372	0.19%	0.026%
35	8.275	1033	1045	1060	rVV2	233878	712193	100.00%	13.277%
36	8.555	1089	1091	1094	rBV3	1501	1233	0.17%	0.023%

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

37	8.842	1130	1138	1147	rBV	215174	414477	58.20%	7.727%
38	9.201	1196	1197	1200	rBV3	1396	1199	0.17%	0.022%
39	9.275	1201	1209	1218	rVV	155164	319535	44.87%	5.957%
40	9.457	1237	1239	1240	rBV2	991	882	0.12%	0.016%
41	9.537	1251	1252	1253	rBV	1204	767	0.11%	0.014%
42	9.671	1271	1274	1277	rVB5	1562	1875	0.26%	0.035%
43	9.707	1278	1280	1282	rBV3	1331	1094	0.15%	0.020%
44	9.799	1294	1295	1299	rVB4	683	688	0.10%	0.013%
45	9.829	1299	1300	1301	rBV	1017	686	0.10%	0.013%
46	10.031	1326	1333	1341	rBV	79483	147337	20.69%	2.747%
47	10.323	1373	1381	1390	rBV	331753	576397	80.93%	10.745%
48	10.579	1415	1423	1435	rVB	55251	101896	14.31%	1.900%
49	10.701	1438	1443	1449	rVB	23684	44323	6.22%	0.826%
50	10.841	1464	1466	1469	rBV4	2054	1420	0.20%	0.026%
51	10.927	1472	1480	1492	rBV	81736	150155	21.08%	2.799%
52	11.061	1497	1502	1508	rBV	28868	47305	6.64%	0.882%
53	11.384	1553	1555	1556	rBV2	1422	959	0.13%	0.018%
54	11.402	1556	1558	1559	rVV2	1516	1212	0.17%	0.023%
55	11.433	1559	1563	1572	rVB3	9417	17711	2.49%	0.330%
56	11.628	1588	1595	1605	rVB	330571	550658	77.32%	10.266%
57	11.701	1605	1607	1610	rBV4	1389	1562	0.22%	0.029%
58	11.951	1646	1648	1652	rVB5	1488	1906	0.27%	0.036%
59	12.250	1693	1697	1702	rBV8	851	1307	0.18%	0.024%
60	12.548	1744	1746	1748	rVB3	1314	998	0.14%	0.019%
61	12.603	1750	1755	1761	rVB2	15184	26781	3.76%	0.499%
62	12.689	1763	1769	1776	rVB	135760	220985	31.03%	4.120%
63	12.926	1803	1808	1813	rBV6	3609	6652	0.93%	0.124%
64	13.225	1855	1857	1858	rBV2	975	797	0.11%	0.015%
65	13.243	1858	1860	1862	rVB3	1435	1013	0.14%	0.019%
66	13.359	1872	1879	1881	rBV8	1715	3859	0.54%	0.072%
67	13.493	1899	1901	1902	rBV2	1274	1006	0.14%	0.019%
68	13.554	1905	1911	1918	rVV	319698	509446	71.53%	9.497%
69	13.755	1942	1944	1947	rVV4	1830	1723	0.24%	0.032%
70	13.847	1953	1959	1969	rVB	290226	483453	67.88%	9.013%
71	14.060	1991	1994	2000	rVB2	7466	11673	1.64%	0.218%
72	14.164	2009	2011	2012	rBV2	975	806	0.11%	0.015%
73	14.280	2027	2030	2033	rBV5	1215	1756	0.25%	0.033%
74	14.322	2033	2037	2044	rVB9	3553	5807	0.82%	0.108%
75	14.463	2055	2060	2063	rBV5	1509	2868	0.40%	0.053%
76	14.542	2069	2073	2074	rBV3	981	1025	0.14%	0.019%

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

77	14.627	2082	2087	2092	rBV9	1995	4662	0.65%	0.087%
78	14.877	2126	2128	2129	rVB2	1370	847	0.12%	0.016%
79	14.902	2129	2132	2135	rBV5	1252	2020	0.28%	0.038%
80	14.938	2135	2138	2143	rVB6	1252	1804	0.25%	0.034%
81	15.024	2150	2152	2158	rBV7	560	921	0.13%	0.017%
82	15.206	2180	2182	2184	rVB3	1119	864	0.12%	0.016%
83	15.341	2202	2204	2205	rBV2	1143	822	0.12%	0.015%
84	15.432	2216	2219	2223	rVB4	2609	3968	0.56%	0.074%
85	15.475	2223	2226	2229	rBV5	2018	2782	0.39%	0.052%
86	15.554	2237	2239	2241	rVB3	1970	1637	0.23%	0.031%
87	15.645	2251	2254	2255	rBV2	1658	1067	0.15%	0.020%
88	15.676	2255	2259	2261	rBV5	926	1690	0.24%	0.032%
89	15.877	2289	2292	2296	rVB4	1128	1867	0.26%	0.035%
90	15.926	2299	2300	2301	rBV	1053	634	0.09%	0.012%
91	15.968	2306	2307	2311	rVB4	1071	640	0.09%	0.012%
92	16.023	2314	2316	2319	rBV3	1037	948	0.13%	0.018%
93	16.103	2327	2329	2331	rBV3	1019	929	0.13%	0.017%
94	16.151	2334	2337	2338	rVB2	1115	977	0.14%	0.018%
95	16.170	2338	2340	2345	rBV6	1219	2108	0.30%	0.039%
96	16.292	2359	2360	2367	rVB7	1588	2191	0.31%	0.041%
97	16.353	2367	2370	2372	rBV3	1707	1751	0.25%	0.033%
98	16.456	2383	2387	2388	rBV3	971	1192	0.17%	0.022%
99	16.499	2392	2394	2395	rBV2	1298	771	0.11%	0.014%
100	16.572	2404	2406	2409	rVB4	1285	1415	0.20%	0.026%

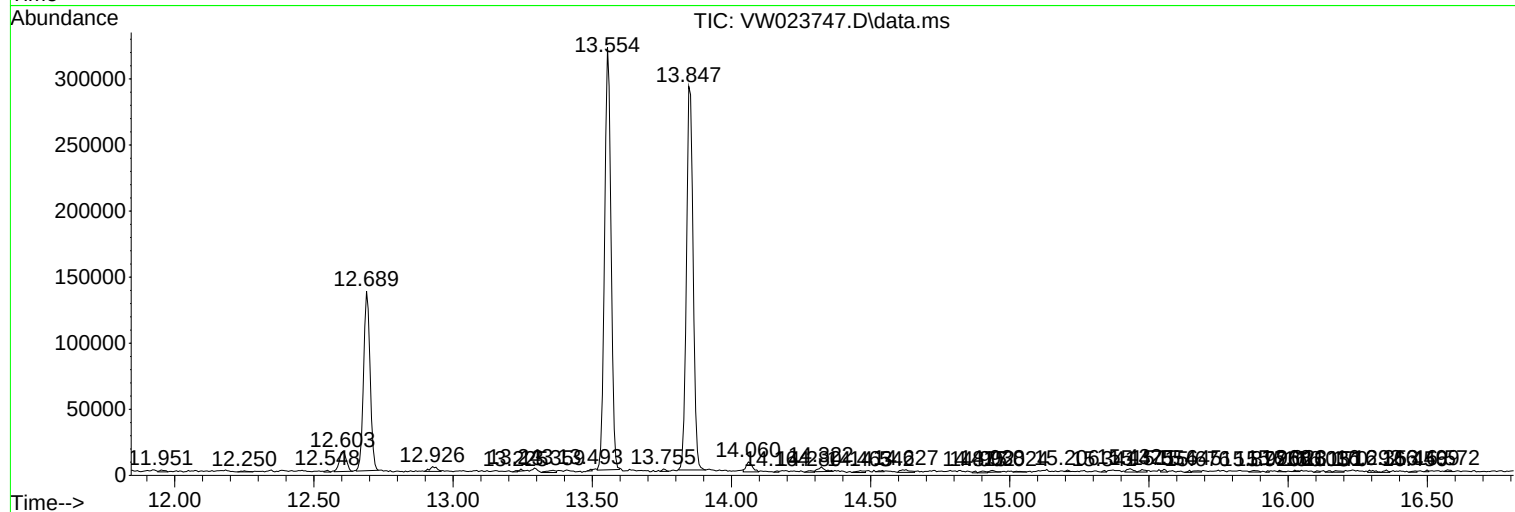
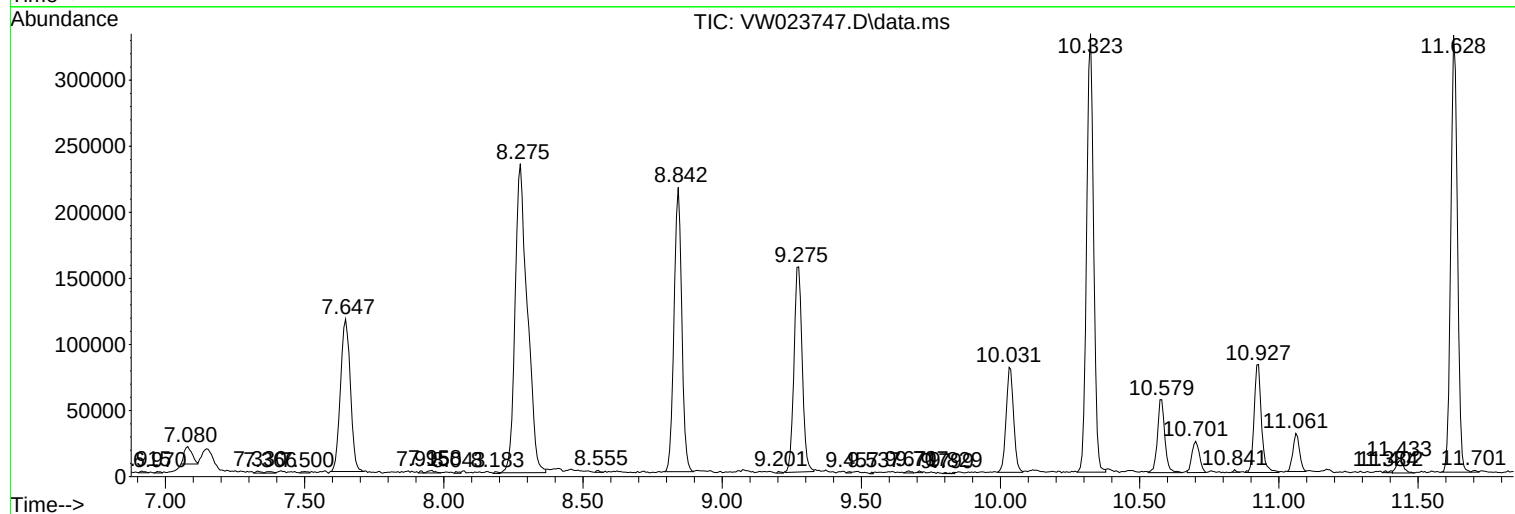
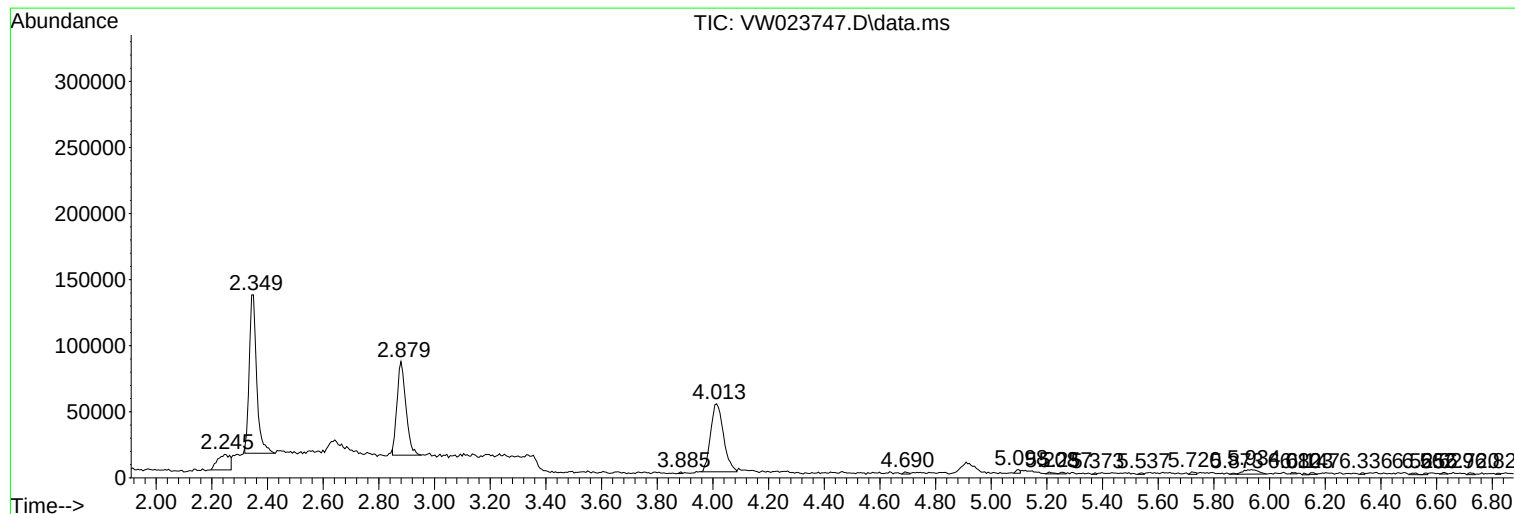
Sum of corrected areas: 5364133

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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



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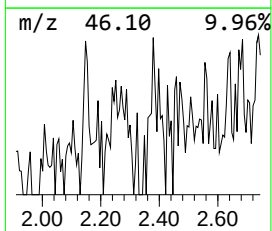
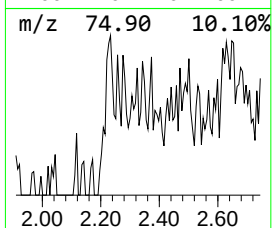
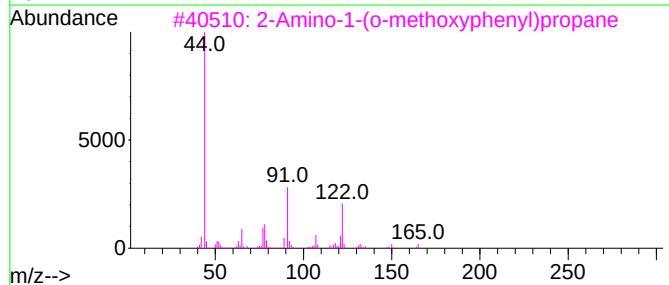
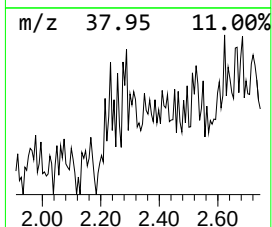
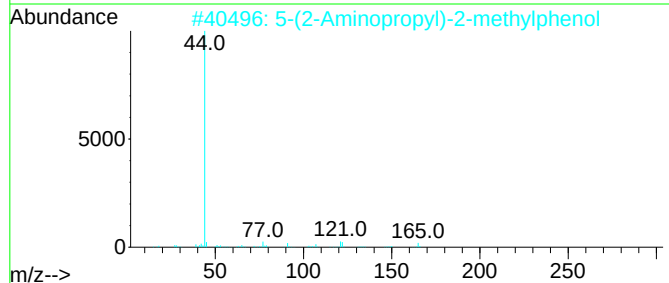
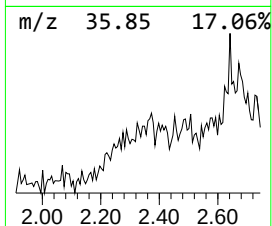
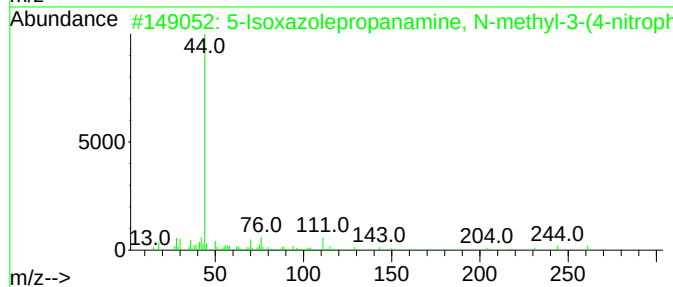
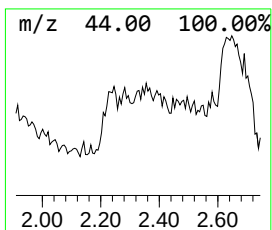
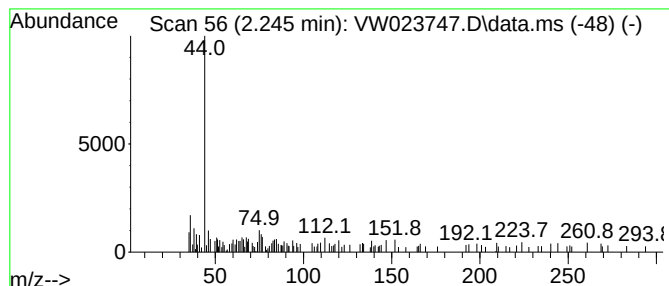
Instrument :
MSVOA_W
ClientSampleId :
VHBLK001

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 5-Isoxazolepropanamine, N-m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
2.245	2.27 ug/L	37673	1,4-Difluorobenzene	8.842	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Isoxazolepropanamine, N-methyl...	261	C13H15N3O3	157170-19-9	50
2	5-(2-Aminopropyl)-2-methylphenol	165	C10H15NO	021618-99-5	47
3	2-Amino-1-(o-methoxyphenyl)propane	165	C10H15NO	015402-84-3	47
4	Pregn-5-en-3-ol, 20-amino-, (3.b...	317	C21H35NO	005035-10-9	47
5	Cyclohexanol, 2-(methylaminometh...	143	C8H17NO	077612-16-9	47



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
5-Isoxazoleprop...	2.245	2.3	ug/L	37673	1	8.842	414477	25.0