

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW071522\
 Data File : VW023776.D
 Acq On : 16 Jul 2022 04:23
 Operator : SY/VA
 Sample : N3701-03RE
 Misc : 5.86g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 F5B64RE

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: VW023776.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.367	238	240	243	rBV4	1687	1529	0.93%	0.137%
2	3.471	255	257	259	rVB3	1404	892	0.54%	0.080%
3	3.855	319	320	325	rBV5	1551	1734	1.05%	0.156%
4	4.007	338	345	356	rVB2	17261	44743	27.09%	4.013%
5	4.275	388	389	393	rBV3	1151	1384	0.84%	0.124%
6	4.348	400	401	403	rVB2	1394	773	0.47%	0.069%
7	4.470	420	421	424	rBV3	1537	1620	0.98%	0.145%
8	4.574	436	438	440	rBV3	1910	1595	0.97%	0.143%
9	4.708	458	460	462	rVB3	1339	1027	0.62%	0.092%
10	4.732	462	464	466	rBV2	1081	874	0.53%	0.078%
11	4.793	472	474	475	rBV2	1434	844	0.51%	0.076%
12	4.989	504	506	508	rBV3	847	731	0.44%	0.066%
13	5.062	517	518	521	rBV3	1677	1308	0.79%	0.117%
14	5.348	564	565	566	rBV	1164	789	0.48%	0.071%
15	5.574	600	602	605	rVB3	1412	1158	0.70%	0.104%
16	5.616	605	609	610	rBV4	1015	1296	0.78%	0.116%
17	5.696	620	622	625	rBV4	1162	1140	0.69%	0.102%
18	5.909	655	657	658	rBV	1402	1003	0.61%	0.090%
19	6.135	689	694	697	rVV7	1659	3317	2.01%	0.298%
20	6.214	705	707	708	rBV2	1439	966	0.58%	0.087%
21	6.519	754	757	760	rBV4	1701	2542	1.54%	0.228%
22	6.726	788	791	792	rBV3	1281	1381	0.84%	0.124%
23	6.793	800	802	804	rBV3	1224	974	0.59%	0.087%
24	6.866	812	814	816	rVB3	916	872	0.53%	0.078%
25	6.958	827	829	832	rVB4	2041	2226	1.35%	0.200%
26	6.994	832	835	837	rBV4	2152	2559	1.55%	0.230%
27	7.506	915	919	924	rBV7	1731	3360	2.03%	0.301%
28	7.647	935	942	950	rVB2	27830	67801	41.05%	6.082%
29	7.842	972	974	977	rVB4	808	844	0.51%	0.076%
30	8.134	1019	1022	1023	rBV3	1042	1081	0.65%	0.097%
31	8.275	1036	1045	1058	rBV3	51730	165167	100.00%	14.815%
32	8.713	1115	1117	1119	rBV2	1015	892	0.54%	0.080%
33	8.842	1131	1138	1145	rVB2	51020	105299	63.75%	9.445%
34	8.982	1160	1161	1164	rVB3	1524	1333	0.81%	0.120%
35	9.024	1166	1168	1169	rBV2	1453	1044	0.63%	0.094%
36	9.274	1202	1209	1218	rVV2	37714	80843	48.95%	7.252%

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 Title : SFAM01.0

37	9.469	1239	1241	1243	rBV3	1032	856	0.52%	0.077%
38	9.744	1283	1286	1288	rBV3	1743	1708	1.03%	0.153%
39	9.884	1307	1309	1315	rVB7	1137	1444	0.87%	0.130%
40	10.036	1327	1334	1341	rBV3	11896	24130	14.61%	2.164%
41	10.140	1349	1351	1354	rVB4	1361	1018	0.62%	0.091%
42	10.323	1374	1381	1387	rBV	59183	107802	65.27%	9.670%
43	10.573	1418	1422	1430	rVB3	7862	16126	9.76%	1.446%
44	10.640	1430	1433	1435	rVB3	1046	1171	0.71%	0.105%
45	10.695	1438	1442	1448	rBV5	2456	5054	3.06%	0.453%
46	10.847	1459	1467	1469	rBV8	2140	2867	1.74%	0.257%
47	10.872	1469	1471	1473	rVB3	1241	912	0.55%	0.082%
48	10.927	1473	1480	1487	rBV	16007	34198	20.71%	3.068%
49	11.335	1545	1547	1548	rBV	928	842	0.51%	0.076%
50	11.433	1561	1563	1567	rBV5	1982	2238	1.35%	0.201%
51	11.628	1587	1595	1602	rBV2	69850	123273	74.64%	11.057%
52	11.829	1626	1628	1630	rBV3	1249	1443	0.87%	0.129%
53	11.963	1647	1650	1654	rBV5	1353	2099	1.27%	0.188%
54	12.024	1659	1660	1663	rVB3	1143	726	0.44%	0.065%
55	12.067	1663	1667	1669	rBV4	1492	1958	1.19%	0.176%
56	12.115	1673	1675	1678	rVB5	824	876	0.53%	0.079%
57	12.298	1702	1705	1708	rVB5	1175	1676	1.01%	0.150%
58	12.335	1708	1711	1713	rBV3	1073	1066	0.65%	0.096%
59	12.359	1713	1715	1718	rBV4	1308	869	0.53%	0.078%
60	12.426	1724	1726	1729	rVV4	1009	1152	0.70%	0.103%
61	12.463	1731	1732	1734	rVV	1417	946	0.57%	0.085%
62	12.481	1734	1735	1738	rVB3	1821	1332	0.81%	0.119%
63	12.518	1738	1741	1742	rBV3	1032	1153	0.70%	0.103%
64	12.566	1745	1749	1750	rBV3	1968	2435	1.47%	0.218%
65	12.603	1750	1755	1759	rVV5	3924	7239	4.38%	0.649%
66	12.688	1763	1769	1777	rVB	31112	56667	34.31%	5.083%
67	12.762	1777	1781	1783	rBV5	1500	2489	1.51%	0.223%
68	12.804	1786	1788	1792	rVB5	1080	1369	0.83%	0.123%
69	12.932	1802	1809	1812	rBV8	2523	5995	3.63%	0.538%
70	13.024	1822	1824	1827	rBV4	1352	1576	0.95%	0.141%
71	13.170	1843	1848	1849	rVV5	1201	1609	0.97%	0.144%
72	13.243	1858	1860	1864	rBV5	1248	1348	0.82%	0.121%
73	13.554	1906	1911	1916	rBV	48280	78957	47.80%	7.082%
74	13.664	1927	1929	1930	rBV2	1320	898	0.54%	0.081%
75	13.853	1954	1960	1967	rBV	41297	74187	44.92%	6.655%
76	14.164	2009	2011	2013	rBV3	1055	1117	0.68%	0.100%

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 Title : SFAM01.0

77	14.347	2037	2041	2042	rBV4	1112	1565	0.95%	0.140%
78	14.408	2049	2051	2055	rBV5	745	1030	0.62%	0.092%
79	14.493	2062	2065	2070	rVB7	1633	2760	1.67%	0.248%
80	14.719	2098	2102	2104	rVB5	1437	1879	1.14%	0.169%
81	14.840	2121	2122	2125	rBV3	1014	942	0.57%	0.084%
82	15.017	2148	2151	2152	rBV3	961	832	0.50%	0.075%
83	15.054	2154	2157	2158	rVV3	1019	1241	0.75%	0.111%
84	15.109	2164	2166	2169	rVV3	1218	968	0.59%	0.087%
85	15.133	2169	2170	2173	rVB3	1197	731	0.44%	0.066%
86	15.170	2173	2176	2179	rBV4	1048	1421	0.86%	0.127%
87	15.212	2179	2183	2186	rBV6	1087	1734	1.05%	0.156%
88	15.328	2200	2202	2205	rVB4	1077	1116	0.68%	0.100%
89	15.407	2213	2215	2217	rBV3	1074	1101	0.67%	0.099%
90	15.560	2238	2240	2242	rVB2	1273	960	0.58%	0.086%
91	15.712	2263	2265	2268	rBV4	1099	1441	0.87%	0.129%
92	15.816	2280	2282	2284	rBV3	986	824	0.50%	0.074%
93	15.926	2297	2300	2301	rBV3	1328	1327	0.80%	0.119%
94	16.285	2357	2359	2363	rVB4	1755	2089	1.26%	0.187%
95	16.413	2378	2380	2381	rBV2	965	790	0.48%	0.071%
96	16.493	2392	2393	2397	rVB4	1593	1380	0.84%	0.124%
97	16.541	2397	2401	2403	rBV4	1536	2125	1.29%	0.191%
98	16.700	2424	2427	2431	rBV4	1793	1981	1.20%	0.178%
99	16.736	2431	2433	2435	rVV3	1518	1346	0.81%	0.121%
100	16.767	2435	2438	2440	rVB4	1493	1494	0.90%	0.134%

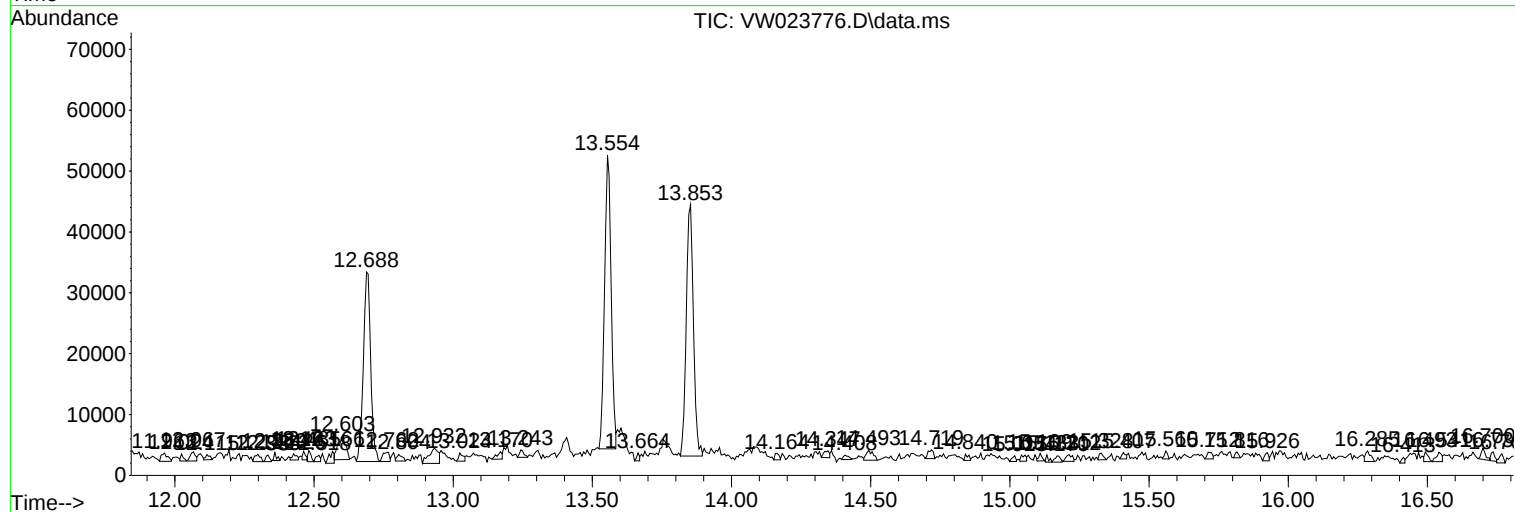
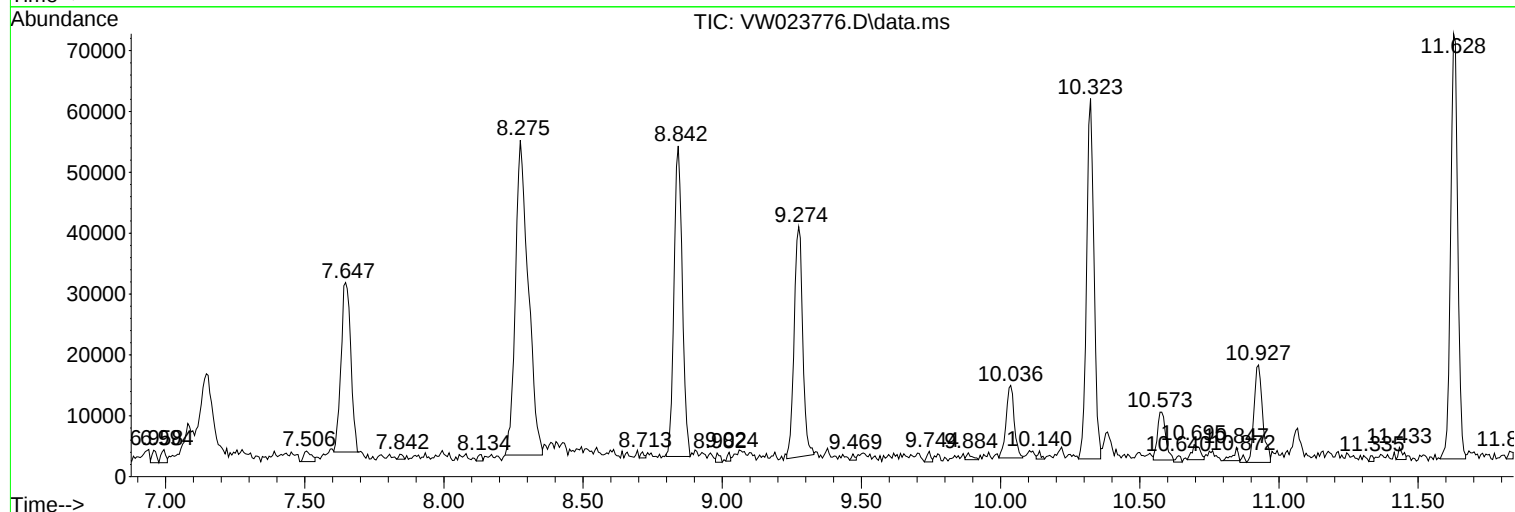
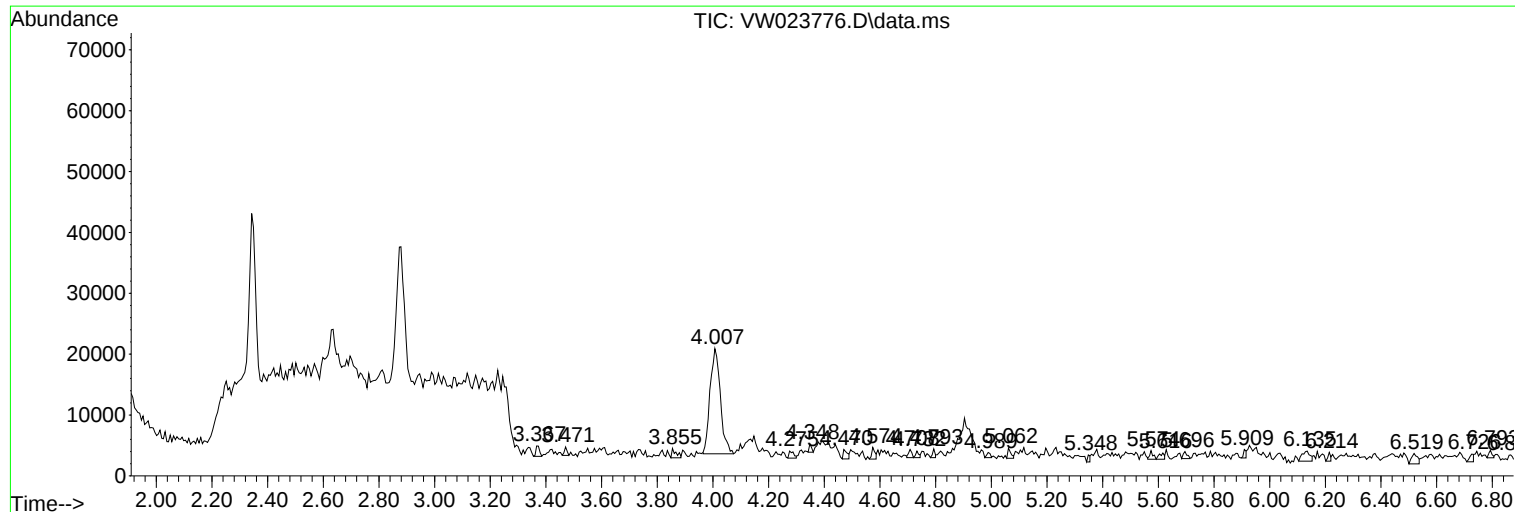
Sum of corrected areas: 1114839

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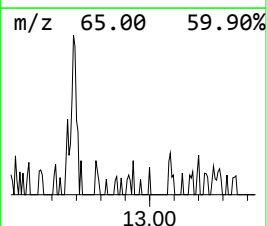
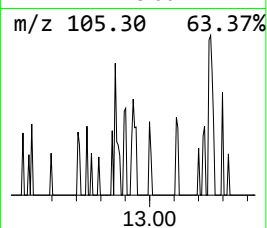
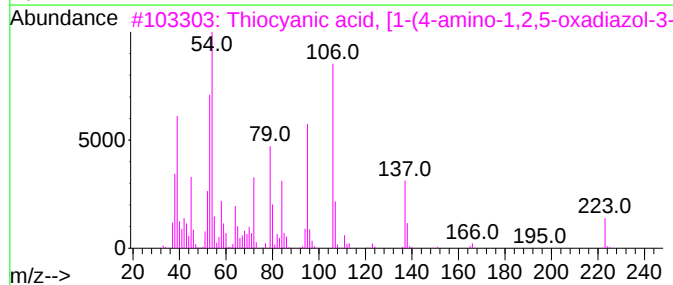
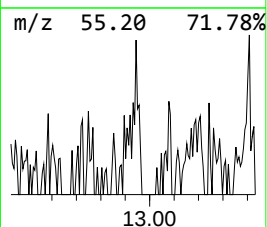
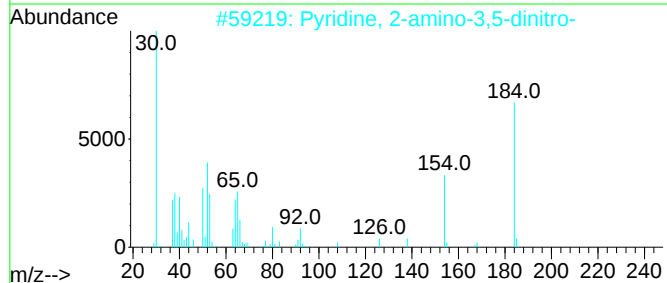
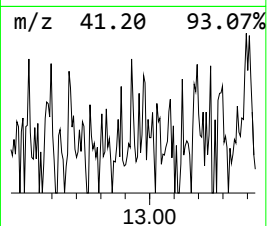
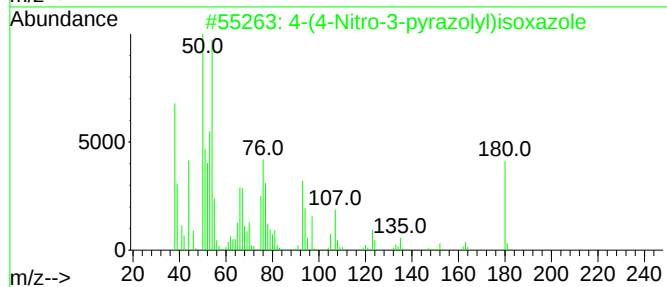
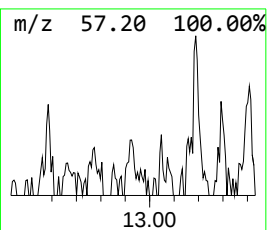
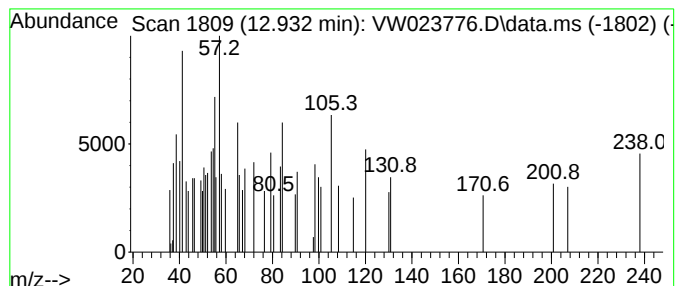
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM071322SMA.M
Quant Title : SFAM01.0

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

Peak Number 3 4-(4-Nitro-3-pyrazolyl)isoxazole... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.932	1.90 ug/L	5995	1,4-Dichlorobenzene-d4	13.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-(4-Nitro-3-pyrazolyl)isoxazole	180	C6H4N4O3	1000225-72-7	50
2			Pyridine, 2-amino-3,5-dinitro-	184	C5H4N4O4	003073-30-1	38
3			Thiocyanic acid, [1-(4-amino-1,2...	223	C6H5N7OS	1000337-65-6	22
4			Cyclohexene, 4-ethenyl-	108	C8H12	000100-40-3	14
5			3-Butenenitrile, 2-methyl-	81	C5H7N	016529-56-9	12



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
4-(4-Nitro-3-py...	12.932	1.9	ug/L	5995	3	13.554	78957	25.0