

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW082622\
 Data File : VW024402.D
 Acq On : 27 Aug 2022 15:43
 Operator : SY/VA
 Sample : N4345-21
 Misc : 6.27g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 DBVT9

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: VW024402.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.337	67	71	78	rVB	88738	126019	30.09%	3.573%
2	4.001	336	344	357	rVB2	42863	122287	29.20%	3.467%
3	4.897	486	491	502	rVB3	10225	29490	7.04%	0.836%
4	5.202	539	541	543	rBV3	1789	1347	0.32%	0.038%
5	6.111	687	690	692	rBV3	1109	1333	0.32%	0.038%
6	6.324	723	725	726	rBV2	1353	748	0.18%	0.021%
7	6.348	726	729	730	rBV3	1158	1120	0.27%	0.032%
8	6.726	790	791	795	rVB4	1656	1439	0.34%	0.041%
9	6.787	800	801	804	rBV2	1114	599	0.14%	0.017%
10	6.842	806	810	812	rBV5	1744	2910	0.69%	0.083%
11	7.080	842	849	852	rBV2	11187	24443	5.84%	0.693%
12	7.647	934	942	951	rVB2	70583	172814	41.26%	4.899%
13	8.092	1012	1015	1017	rBV4	1119	1246	0.30%	0.035%
14	8.183	1028	1030	1031	rBV2	1724	1049	0.25%	0.030%
15	8.275	1037	1045	1059	rBV2	135688	398754	95.21%	11.305%
16	8.756	1120	1124	1127	rBV5	1714	3163	0.76%	0.090%
17	8.842	1130	1138	1146	rVV	149900	303646	72.50%	8.609%
18	9.226	1199	1201	1202	rBV2	2055	1772	0.42%	0.050%
19	9.275	1202	1209	1217	rVB	99664	201444	48.10%	5.711%
20	9.537	1250	1252	1253	rVB2	1210	533	0.13%	0.015%
21	9.573	1256	1258	1260	rVV3	1618	1524	0.36%	0.043%
22	9.622	1264	1266	1268	rBV3	1534	1583	0.38%	0.045%
23	9.744	1284	1286	1288	rBV3	1758	1627	0.39%	0.046%
24	9.866	1304	1306	1307	rBV2	1163	520	0.12%	0.015%
25	9.970	1321	1323	1326	rBV3	1078	1041	0.25%	0.030%
26	10.031	1326	1333	1342	rBV2	49718	94572	22.58%	2.681%
27	10.323	1374	1381	1389	rBV	195984	344828	82.34%	9.776%
28	10.573	1417	1422	1430	rBV2	33016	57634	13.76%	1.634%
29	10.695	1441	1442	1449	rVB4	4497	5958	1.42%	0.169%
30	10.860	1463	1469	1475	rBV2	73622	123776	29.56%	3.509%
31	10.921	1475	1479	1491	rVB	42565	81123	19.37%	2.300%
32	11.067	1497	1503	1513	rVB3	13346	29201	6.97%	0.828%
33	11.530	1576	1579	1581	rBV4	1826	2197	0.52%	0.062%
34	11.549	1581	1582	1583	rBV	1567	745	0.18%	0.021%
35	11.628	1588	1595	1603	rVV	249943	418797	100.00%	11.873%
36	12.000	1654	1656	1657	rBV2	1069	1030	0.25%	0.029%

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

37	12.055	1664	1665	1667	rBV2	1026	517	0.12%	0.015%
38	12.097	1670	1672	1674	rBV3	1298	960	0.23%	0.027%
39	12.323	1705	1709	1710	rBV3	1038	1553	0.37%	0.044%
40	12.494	1736	1737	1739	rBV2	1096	1055	0.25%	0.030%
41	12.542	1743	1745	1749	rBV5	1058	1502	0.36%	0.043%
42	12.689	1762	1769	1777	rBV	86394	145064	34.64%	4.113%
43	13.012	1821	1822	1824	rVB2	1264	483	0.12%	0.014%
44	13.042	1824	1827	1830	rBV4	1806	2993	0.71%	0.085%
45	13.073	1830	1832	1836	rVV5	1070	1538	0.37%	0.044%
46	13.140	1841	1843	1844	rVV2	1137	723	0.17%	0.020%
47	13.189	1848	1851	1854	rVV4	1861	1594	0.38%	0.045%
48	13.274	1863	1865	1866	rBV2	1737	844	0.20%	0.024%
49	13.438	1891	1892	1893	rBV	1153	479	0.11%	0.014%
50	13.463	1893	1896	1898	rBV4	1481	1906	0.46%	0.054%
51	13.554	1905	1911	1920	rVB	239084	387662	92.57%	10.991%
52	13.847	1953	1959	1969	rBV	180283	312351	74.58%	8.855%
53	13.987	1981	1982	1985	rBV3	1602	1334	0.32%	0.038%
54	14.054	1991	1993	1996	rBV3	2866	3099	0.74%	0.088%
55	14.146	2006	2008	2010	rBV3	1418	1014	0.24%	0.029%
56	14.213	2017	2019	2021	rVB3	1852	1615	0.39%	0.046%
57	14.237	2021	2023	2024	rBV2	1249	949	0.23%	0.027%
58	14.268	2026	2028	2030	rBV3	1278	1071	0.26%	0.030%
59	14.481	2059	2063	2067	rBV6	1964	3705	0.88%	0.105%
60	14.554	2074	2075	2076	rBV	1274	794	0.19%	0.023%
61	14.621	2081	2086	2091	rVV8	4776	8712	2.08%	0.247%
62	14.707	2098	2100	2109	rVB10	2149	3474	0.83%	0.098%
63	14.865	2123	2126	2128	rBV4	1803	2569	0.61%	0.073%
64	14.944	2136	2139	2141	rBV4	1265	1503	0.36%	0.043%
65	14.999	2145	2148	2149	rBV2	1829	1824	0.44%	0.052%
66	15.072	2156	2160	2161	rBV3	1399	1640	0.39%	0.046%
67	15.127	2166	2169	2173	rVB6	4322	6758	1.61%	0.192%
68	15.237	2185	2187	2189	rBV3	975	1203	0.29%	0.034%
69	15.359	2200	2207	2213	rBV3	6407	14062	3.36%	0.399%
70	15.432	2214	2219	2223	rVB5	7311	13115	3.13%	0.372%
71	15.554	2233	2239	2245	rVB9	6425	12067	2.88%	0.342%
72	15.645	2252	2254	2255	rBV2	927	664	0.16%	0.019%
73	15.780	2275	2276	2278	rVB2	1308	806	0.19%	0.023%
74	15.804	2278	2280	2281	rBV2	1307	1036	0.25%	0.029%
75	15.962	2303	2306	2310	rBV5	1378	1752	0.42%	0.050%
76	16.029	2314	2317	2319	rBV4	996	1266	0.30%	0.036%

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

77	16.048	2319	2320	2322	rVB2	1449	834	0.20%	0.024%
78	16.066	2322	2323	2324	rVB	873	320	0.08%	0.009%
79	16.084	2324	2326	2328	rBV3	1261	1065	0.25%	0.030%
80	16.164	2336	2339	2342	rVB4	1487	1333	0.32%	0.038%
81	16.188	2342	2343	2344	rVB	1017	372	0.09%	0.011%
82	16.212	2344	2347	2349	rBV3	2037	1475	0.35%	0.042%
83	16.249	2349	2353	2355	rBV4	1308	1529	0.37%	0.043%
84	16.389	2373	2376	2377	rVB2	1447	1257	0.30%	0.036%
85	16.426	2380	2382	2383	rBV2	1791	1133	0.27%	0.032%
86	16.511	2395	2396	2399	rVV3	852	508	0.12%	0.014%
87	16.554	2401	2403	2405	rVB3	1451	1309	0.31%	0.037%
88	16.590	2408	2409	2413	rBV4	1196	1434	0.34%	0.041%
89	16.633	2413	2416	2419	rBV4	1220	2070	0.49%	0.059%
90	16.694	2423	2426	2427	rBV3	1614	1652	0.39%	0.047%
91	16.731	2430	2432	2434	rVV3	970	934	0.22%	0.026%
92	16.773	2438	2439	2440	rVB	1131	414	0.10%	0.012%

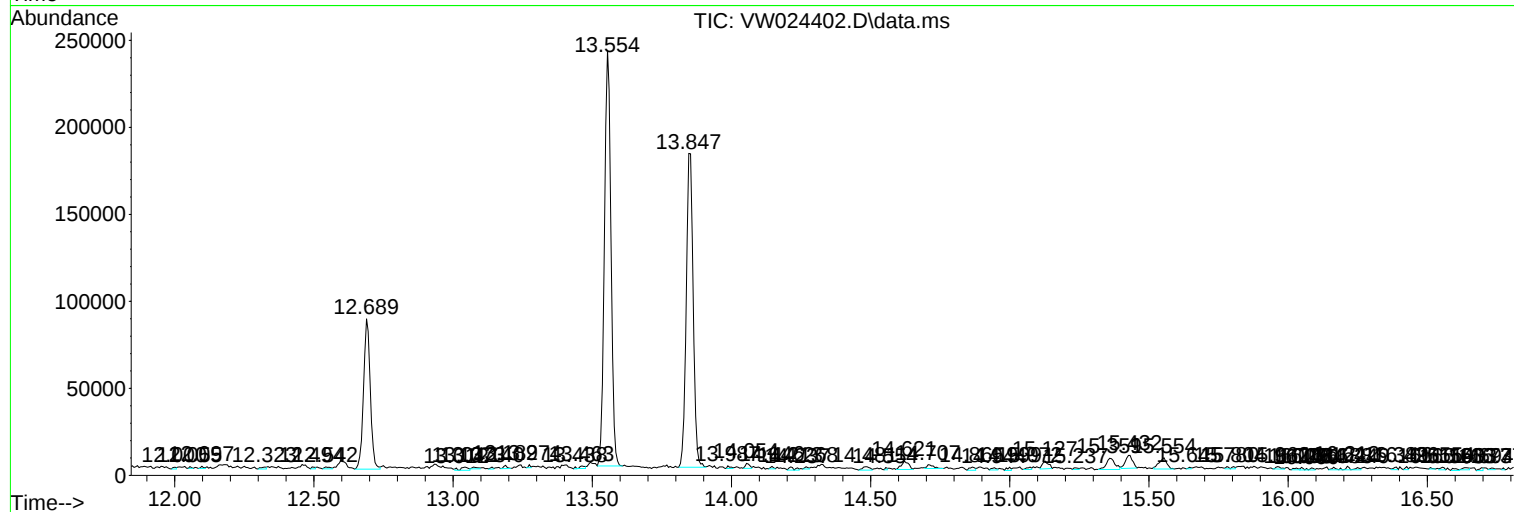
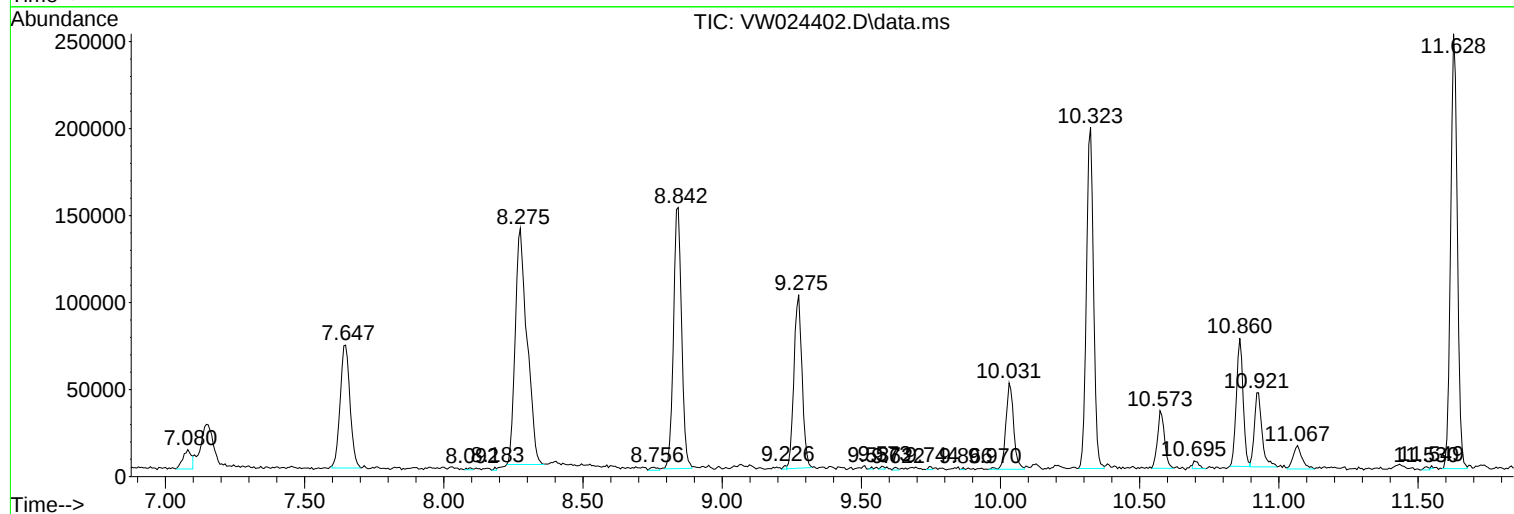
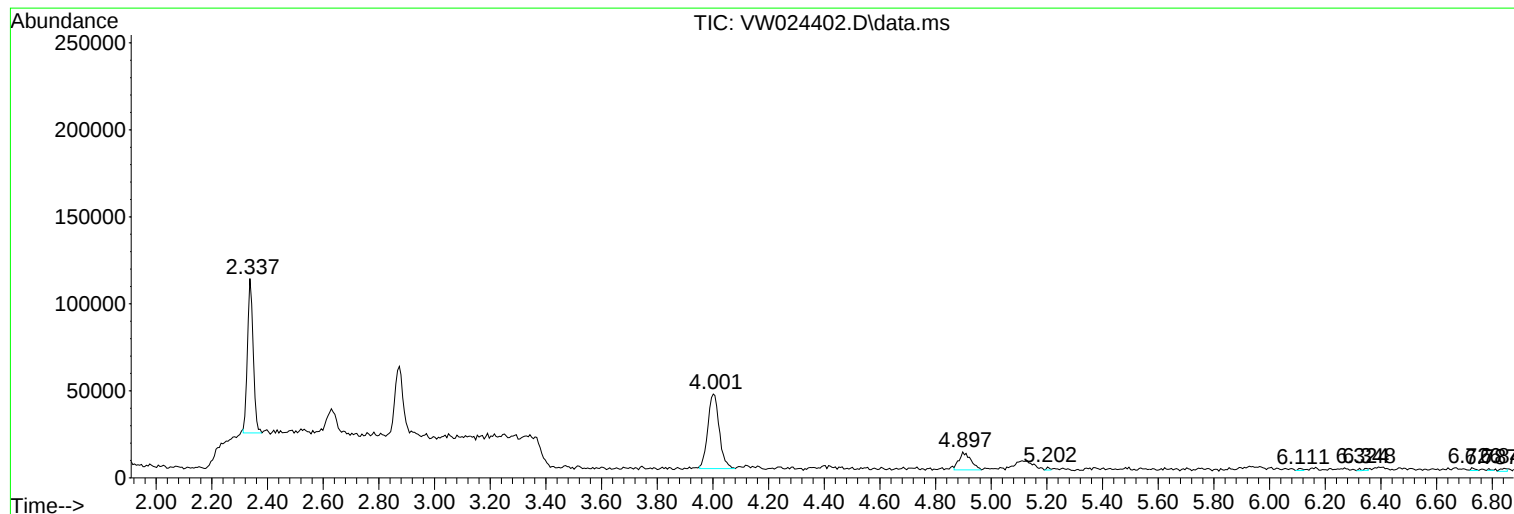
Sum of corrected areas: 3527207

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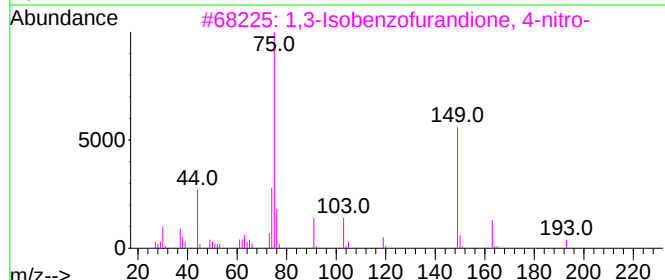
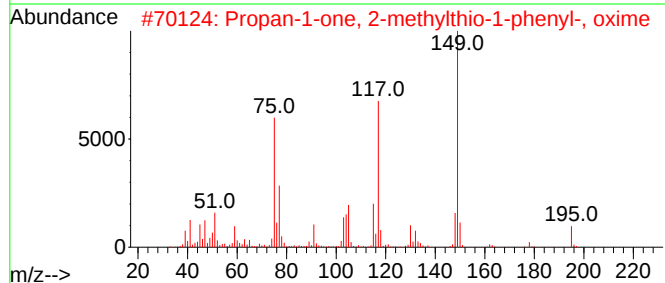
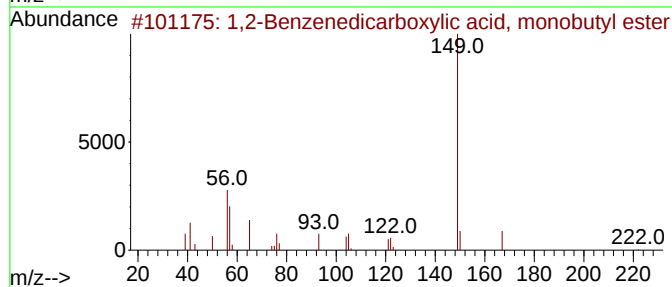
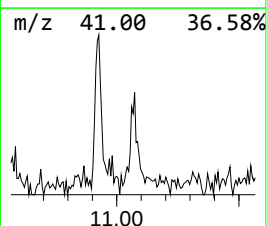
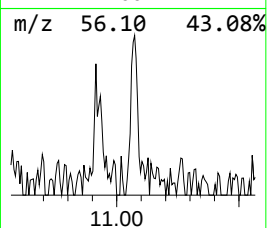
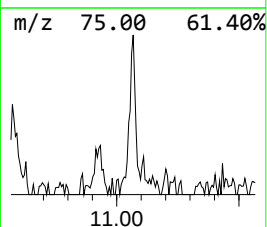
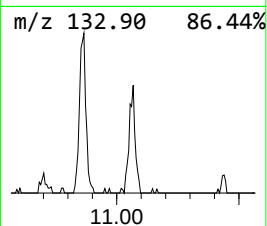
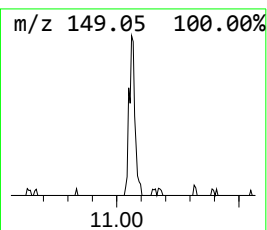
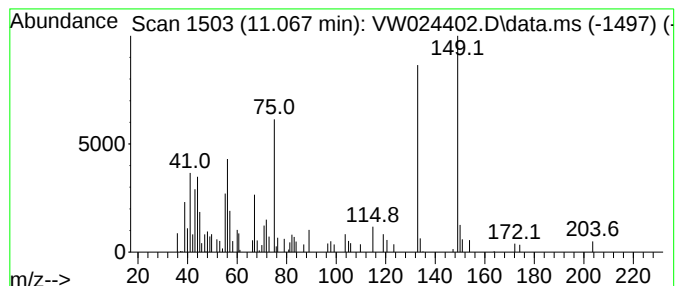
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM082622SMA.M
Quant Title : SFAM01.0

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

Peak Number 3 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.067	1.74 ug/L	29201	Chlorobenzene-d5	11.628

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Benzenedicarboxylic acid, mo...	222	C12H14O4	000131-70-4	35
2			Propan-1-one, 2-methylthio-1-phe...	195	C10H13NOS	274690-11-8	32
3			1,3-Isobenzofurandione, 4-nitro-	193	C8H3NO5	000641-70-3	25
4			3-Methylthiazolidine-2-thione	133	C4H7NS2	001908-87-8	18
5			7-Methylthieno[3,2-b]pyridine	149	C8H7NS	013362-83-9	18



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	11.067	1.7	ug/L	29201	2	11.628	418797	25.0