

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW050923\
 Data File : VW025910.D
 Acq On : 09 May 2023 16:03
 Operator : SY/MD
 Sample : 02612-38
 Misc : 5.07g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 JREJ2

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\SFAMWLM050123SMA.M
 Title : SFAM01.0

Signal : TIC: VW025910.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.143	38	42	49	rVB	48326	75680	19.43%	2.763%
2	3.442	253	255	257	rBV3	2626	1869	0.48%	0.068%
3	3.832	317	319	320	rVB2	2154	1287	0.33%	0.047%
4	3.905	329	331	332	rBV2	2062	1239	0.32%	0.045%
5	4.015	339	349	359	rBV2	42998	120053	30.82%	4.383%
6	4.380	403	409	410	rBV6	2580	3946	1.01%	0.144%
7	4.557	436	438	440	rBV3	1641	1105	0.28%	0.040%
8	4.624	446	449	451	rBV4	1294	1490	0.38%	0.054%
9	4.868	487	489	490	rBV2	2306	2012	0.52%	0.073%
10	4.905	493	495	503	rVB7	5128	13287	3.41%	0.485%
11	5.021	512	514	516	rVB3	1990	1858	0.48%	0.068%
12	5.063	516	521	523	rBV6	1939	3149	0.81%	0.115%
13	5.331	563	565	570	rBV6	1797	2344	0.60%	0.086%
14	5.472	586	588	589	rBV2	1675	1441	0.37%	0.053%
15	5.520	595	596	599	rBV3	1953	1714	0.44%	0.063%
16	5.697	624	625	627	rBV2	1724	1129	0.29%	0.041%
17	5.758	633	635	636	rBV2	1362	1436	0.37%	0.052%
18	5.923	658	662	663	rBV4	2911	3508	0.90%	0.128%
19	6.014	675	677	681	rVB5	1593	2038	0.52%	0.074%
20	6.356	731	733	736	rVB4	1728	1727	0.44%	0.063%
21	6.398	736	740	741	rBV4	1761	2225	0.57%	0.081%
22	6.569	767	768	771	rBV3	1223	1287	0.33%	0.047%
23	6.661	779	783	786	rVB6	2026	2207	0.57%	0.081%
24	6.685	786	787	791	rBV4	1432	1282	0.33%	0.047%
25	6.795	804	805	808	rBV3	1480	1698	0.44%	0.062%
26	6.868	816	817	822	rVB5	2069	3264	0.84%	0.119%
27	6.953	825	831	834	rBV6	2647	3711	0.95%	0.135%
28	7.087	841	853	855	rBV2	12645	29803	7.65%	1.088%
29	7.343	893	895	898	rVV4	1989	1439	0.37%	0.053%
30	7.569	929	932	935	rVB5	3132	3490	0.90%	0.127%
31	7.648	935	945	956	rBV2	65521	172158	44.20%	6.286%
32	7.825	972	974	976	rBV3	1113	1345	0.35%	0.049%
33	7.983	998	1000	1002	rBV2	1168	1140	0.29%	0.042%
34	8.099	1015	1019	1021	rBV5	2501	3685	0.95%	0.135%
35	8.124	1021	1023	1026	rVB4	1637	1535	0.39%	0.056%
36	8.154	1026	1028	1031	rBV4	1428	1565	0.40%	0.057%

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM050123SMA.M
 Title : SFAM01.0

37	8.221	1037	1039	1040	rBV2	2099	1876	0.48%	0.068%
38	8.276	1040	1048	1062	rVB2	124391	389500	100.00%	14.222%
39	8.508	1084	1086	1088	rBV3	1608	1327	0.34%	0.048%
40	8.721	1119	1121	1124	rVB3	1878	1340	0.34%	0.049%
41	8.843	1133	1141	1149	rBV	106256	215573	55.35%	7.871%
42	9.032	1170	1172	1174	rBV3	1973	2191	0.56%	0.080%
43	9.276	1203	1212	1223	rVB	97770	206092	52.91%	7.525%
44	9.367	1223	1227	1229	rBV5	1947	3086	0.79%	0.113%
45	9.453	1238	1241	1245	rBV5	1836	2869	0.74%	0.105%
46	9.520	1250	1252	1256	rVB5	2496	2232	0.57%	0.081%
47	9.690	1276	1280	1283	rBV6	1974	2477	0.64%	0.090%
48	9.788	1294	1296	1298	rVB3	2416	1569	0.40%	0.057%
49	9.855	1304	1307	1311	rVB6	1836	3052	0.78%	0.111%
50	9.892	1311	1313	1314	rBV2	1233	1225	0.31%	0.045%
51	10.032	1330	1336	1343	rBV	42471	78734	20.21%	2.875%
52	10.105	1347	1348	1351	rBV3	1534	1713	0.44%	0.063%
53	10.324	1373	1384	1391	rBV	143385	262812	67.47%	9.596%
54	10.532	1416	1418	1420	rBV3	1152	1221	0.31%	0.045%
55	10.581	1420	1426	1435	rVB2	28090	52098	13.38%	1.902%
56	10.654	1435	1438	1441	rBV5	2810	2160	0.55%	0.079%
57	10.696	1441	1445	1451	rBV	9716	18146	4.66%	0.663%
58	10.837	1466	1468	1472	rVB5	1286	1533	0.39%	0.056%
59	10.928	1477	1483	1491	rBV	30764	61046	15.67%	2.229%
60	11.062	1502	1505	1511	rVB7	3601	5527	1.42%	0.202%
61	11.257	1535	1537	1538	rBV2	1788	1284	0.33%	0.047%
62	11.276	1538	1540	1542	rVB3	2515	2156	0.55%	0.079%
63	11.300	1542	1544	1546	rBV3	2904	3004	0.77%	0.110%
64	11.343	1549	1551	1553	rBV3	1740	1695	0.44%	0.062%
65	11.428	1561	1565	1566	rBV4	4021	3476	0.89%	0.127%
66	11.629	1590	1598	1607	rVV	155017	266457	68.41%	9.729%
67	11.751	1617	1618	1620	rVB2	2051	1096	0.28%	0.040%
68	11.995	1655	1658	1659	rBV3	1557	1646	0.42%	0.060%
69	12.099	1673	1675	1676	rBV2	1570	1382	0.35%	0.050%
70	12.269	1701	1703	1706	rBV4	1244	1293	0.33%	0.047%
71	12.330	1711	1713	1717	rVB5	838	1089	0.28%	0.040%
72	12.403	1724	1725	1728	rBV3	1279	1409	0.36%	0.051%
73	12.568	1749	1752	1753	rBV3	963	1082	0.28%	0.040%
74	12.605	1753	1758	1765	rVB3	12109	23494	6.03%	0.858%
75	12.690	1765	1772	1780	rBV	74887	130514	33.51%	4.765%
76	12.812	1791	1792	1798	rVV6	1737	1974	0.51%	0.072%

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM050123SMA.M
 Title : SFAM01.0

77	12.855	1798	1799	1802	rVB3	2194	1700	0.44%	0.062%
78	12.964	1816	1817	1820	rBV3	1938	1637	0.42%	0.060%
79	13.056	1828	1832	1834	rVB5	1656	1640	0.42%	0.060%
80	13.111	1838	1841	1847	rVB7	4362	8120	2.08%	0.296%
81	13.281	1866	1869	1870	rBV3	2094	2171	0.56%	0.079%
82	13.336	1875	1878	1880	rBV4	1314	1326	0.34%	0.048%
83	13.556	1907	1914	1923	rBV	129661	218932	56.21%	7.994%
84	13.647	1926	1929	1934	rVB7	2459	4066	1.04%	0.148%
85	13.684	1934	1935	1937	rBV2	1749	1447	0.37%	0.053%
86	13.751	1944	1946	1948	rBV2	1871	1806	0.46%	0.066%
87	13.848	1953	1962	1970	rBV	125483	214286	55.02%	7.824%
88	14.062	1991	1997	2000	rBV3	6791	10019	2.57%	0.366%
89	14.305	2032	2037	2038	rBV5	2381	3266	0.84%	0.119%
90	14.415	2051	2055	2061	rBV9	3865	6812	1.75%	0.249%
91	14.562	2078	2079	2081	rBV2	1125	1080	0.28%	0.039%
92	14.647	2087	2093	2097	rBV8	3300	6782	1.74%	0.248%
93	14.714	2103	2104	2106	rVB2	2074	1424	0.37%	0.052%
94	14.909	2135	2136	2138	rBV2	1970	1562	0.40%	0.057%
95	15.269	2193	2195	2197	rBV3	1426	1663	0.43%	0.061%
96	15.336	2204	2206	2208	rBV3	2802	3021	0.78%	0.110%
97	15.671	2256	2261	2262	rBV5	1901	2727	0.70%	0.100%
98	16.012	2315	2317	2319	rBV3	2423	2485	0.64%	0.091%
99	16.073	2325	2327	2328	rBV2	1799	1741	0.45%	0.064%
100	16.195	2345	2347	2350	rBV4	2086	2449	0.63%	0.089%

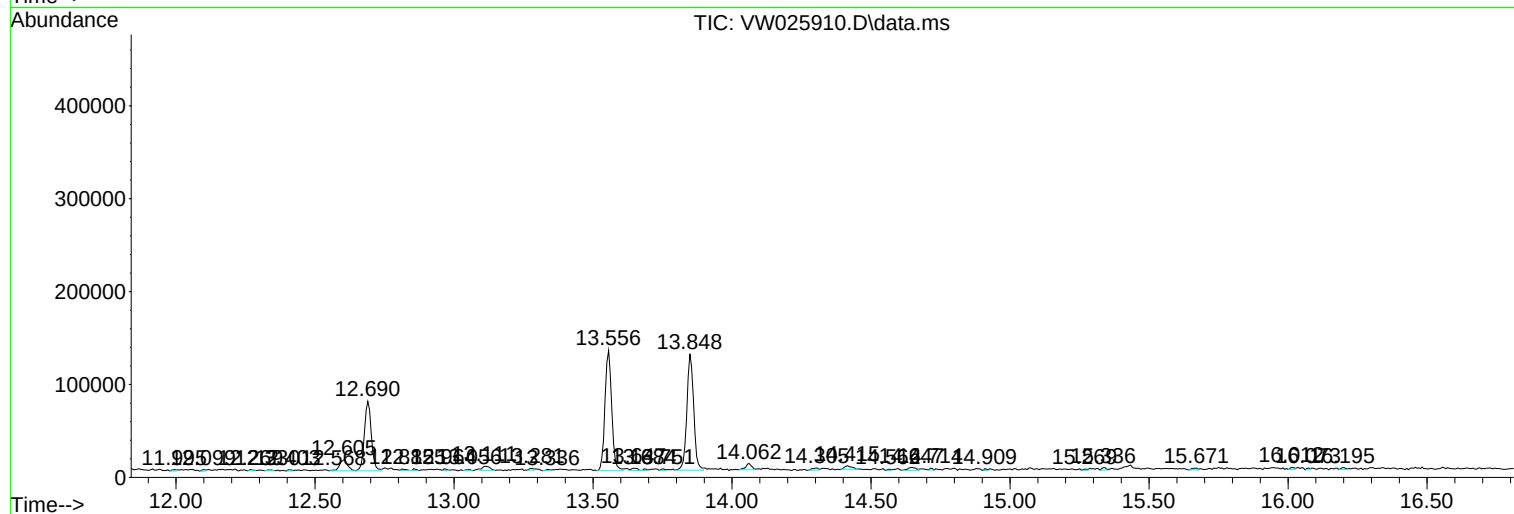
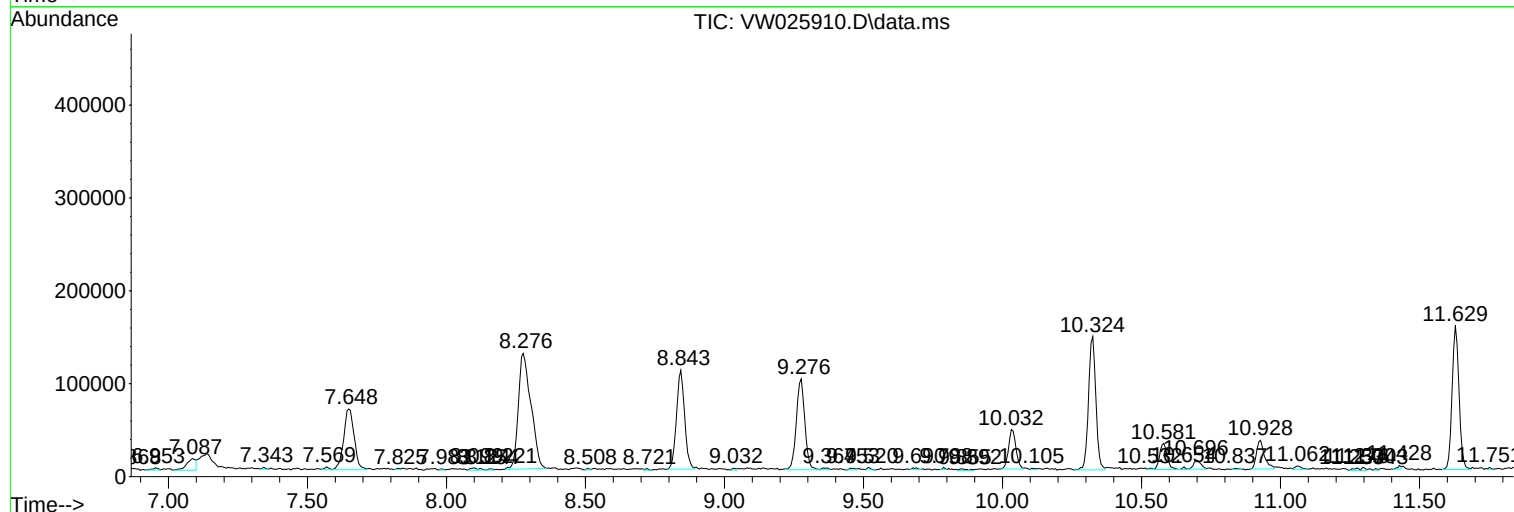
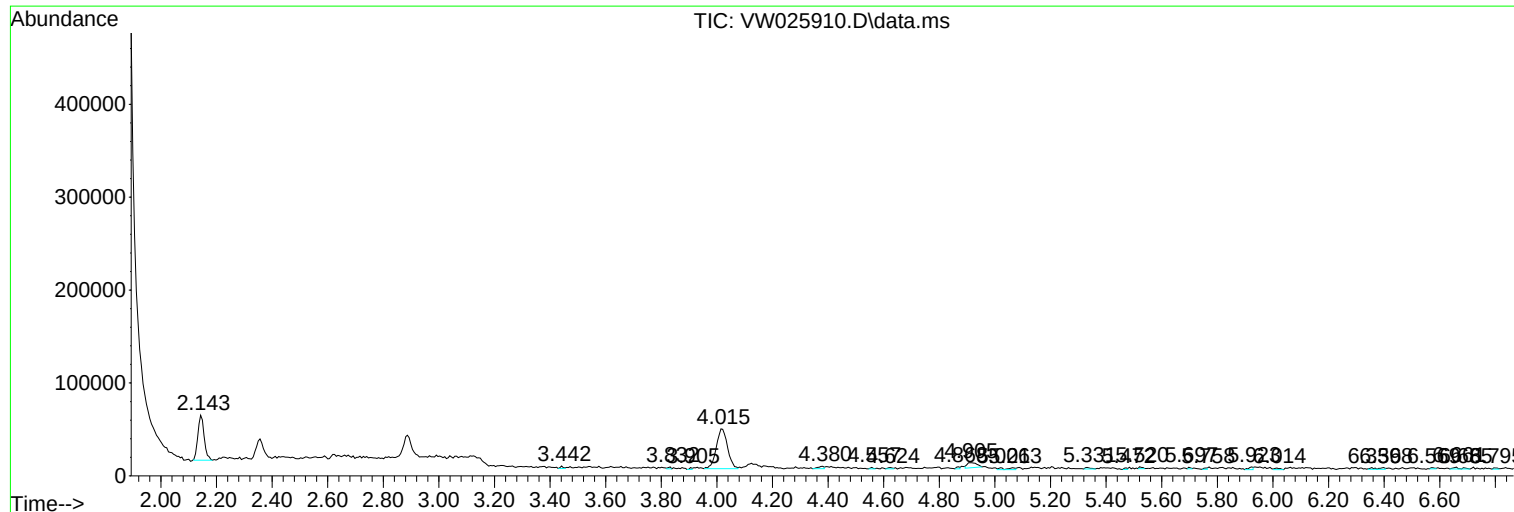
Sum of corrected areas: 2738758

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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM050123SMA.M
Quant Title : SFAM01.0

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



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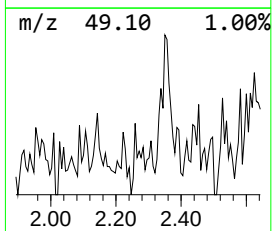
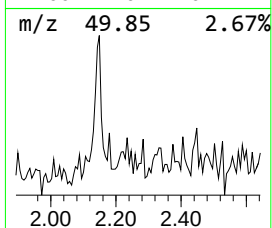
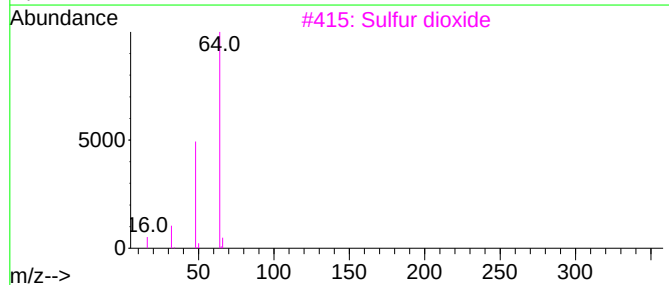
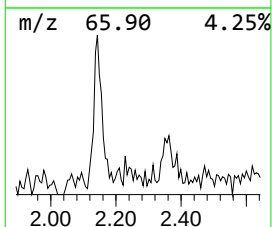
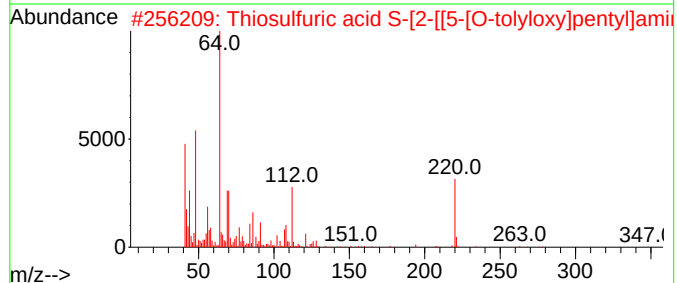
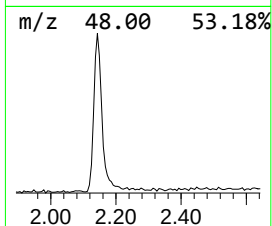
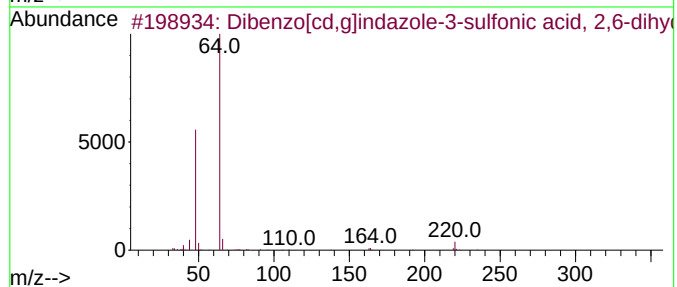
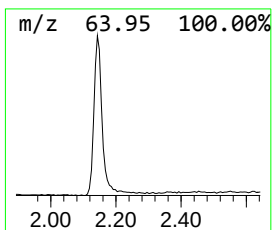
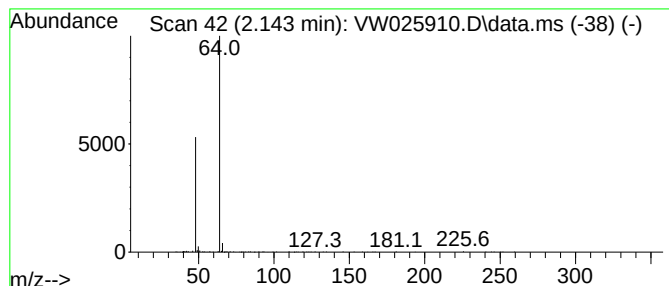
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM050123SMA.M
Quant Title : SFAM01.0

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

Peak Number 1 Dibenzo[cd,g]indazole-3-sul... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.143	8.78 ug/L	75680	1,4-Difluorobenzene	8.843

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dibenzo[cd,g]indazole-3-sulfonic...	300	C14H8N2O4S	293765-87-4	64
2			Thiosulfuric acid S-[2-[[5-[O-to...	347	C15H25NO4S2	038920-47-7	64
3			Sulfur dioxide	64	O2S	007446-09-5	9
4			2-Benzimidazolyl methane thiosul...	244	C8H8N2O3S2	1010256-39-2	9
5			Methanethiol, (N-cycloheptylmeth...	280	C10H20N2O3S2	040283-61-2	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Dibenzo[cd,g]in...	2.143	8.8	ug/L	75680	1	8.843	215573	25.0