

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW072222\
 Data File : VW024020.D
 Acq On : 22 Jul 2022 21:45
 Operator : SY/VA
 Sample : N3741-06
 Misc : 9.03g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 H0B14

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: VW024020.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.148	35	40	47	rBV	79794	162778	16.21%	2.123%
2	2.337	68	71	85	rVB	117850	208890	20.80%	2.724%
3	2.635	116	120	129	rBV	151268	263749	26.27%	3.440%
4	2.873	154	159	170	rVB	72878	164412	16.37%	2.144%
5	4.007	335	345	358	rBV2	69555	227058	22.61%	2.961%
6	4.196	369	376	394	rVB	105435	282772	28.16%	3.688%
7	4.909	479	493	499	rBV5	34141	120503	12.00%	1.572%
8	5.275	551	553	556	rVB3	1059	790	0.08%	0.010%
9	5.488	585	588	589	rBV3	964	917	0.09%	0.012%
10	5.513	589	592	593	rBV2	856	838	0.08%	0.011%
11	5.726	624	627	628	rBV3	792	1044	0.10%	0.014%
12	5.842	645	646	649	rVB3	1055	926	0.09%	0.012%
13	5.872	649	651	652	rBV2	925	712	0.07%	0.009%
14	5.921	653	659	661	rBV5	5324	9307	0.93%	0.121%
15	6.068	682	683	686	rBV3	833	806	0.08%	0.011%
16	6.171	698	700	702	rBV3	957	927	0.09%	0.012%
17	6.250	711	713	714	rBV2	1131	1016	0.10%	0.013%
18	6.275	714	717	718	rBV3	1820	1570	0.16%	0.020%
19	6.470	747	749	755	rBV5	1408	2593	0.26%	0.034%
20	6.519	755	757	758	rBV	785	671	0.07%	0.009%
21	6.714	788	789	794	rVB5	962	1405	0.14%	0.018%
22	6.763	794	797	799	rBV3	1360	1548	0.15%	0.020%
23	6.854	809	812	814	rBV4	1062	1006	0.10%	0.013%
24	6.885	814	817	818	rVB3	897	649	0.06%	0.008%
25	6.909	818	821	822	rBV2	1453	963	0.10%	0.013%
26	7.086	844	850	851	rBV	6823	11713	1.17%	0.153%
27	7.360	894	895	897	rBV	1167	854	0.09%	0.011%
28	7.647	929	942	954	rBV2	151898	390828	38.92%	5.097%
29	7.756	958	960	961	rBV2	913	596	0.06%	0.008%
30	7.866	976	978	979	rBV2	1057	918	0.09%	0.012%
31	8.104	1014	1017	1018	rBV3	613	725	0.07%	0.009%
32	8.165	1025	1027	1031	rBV5	814	1014	0.10%	0.013%
33	8.268	1035	1044	1061	rBV2	315894	1004160	100.00%	13.096%
34	8.689	1109	1113	1115	rBV5	2059	2962	0.29%	0.039%
35	8.841	1129	1138	1151	rVV	375707	719686	71.67%	9.386%
36	9.183	1191	1194	1196	rBV3	964	1202	0.12%	0.016%

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

37	9.274	1200	1209	1217	rBV	243391	496367	49.43%	6.473%
38	9.427	1231	1234	1235	rBV3	1483	1533	0.15%	0.020%
39	9.500	1243	1246	1247	rBV3	863	822	0.08%	0.011%
40	9.604	1259	1263	1264	rBV3	1192	1351	0.13%	0.018%
41	9.914	1310	1314	1316	rBV5	834	1258	0.13%	0.016%
42	9.939	1316	1318	1321	rVV4	800	1003	0.10%	0.013%
43	9.982	1324	1325	1327	rBV2	918	633	0.06%	0.008%
44	10.030	1327	1333	1341	rBV	42009	79896	7.96%	1.042%
45	10.134	1343	1350	1359	rVB	70442	140395	13.98%	1.831%
46	10.323	1373	1381	1388	rBV	439112	755596	75.25%	9.854%
47	10.579	1416	1423	1432	rVB	34012	60159	5.99%	0.785%
48	10.762	1446	1453	1459	rVB3	12821	26660	2.65%	0.348%
49	10.926	1474	1480	1492	rBV4	32355	95258	9.49%	1.242%
50	11.256	1532	1534	1535	rBV	1450	1127	0.11%	0.015%
51	11.304	1540	1542	1545	rBV3	1185	1734	0.17%	0.023%
52	11.445	1560	1565	1573	rVB5	9937	18708	1.86%	0.244%
53	11.628	1587	1595	1605	rBV	482607	826790	82.34%	10.783%
54	11.938	1645	1646	1648	rBV	1053	915	0.09%	0.012%
55	11.987	1651	1654	1656	rBV4	1253	1122	0.11%	0.015%
56	12.036	1660	1662	1664	rBV3	946	649	0.06%	0.008%
57	12.097	1669	1672	1673	rVB3	981	807	0.08%	0.011%
58	12.115	1673	1675	1676	rBV2	788	780	0.08%	0.010%
59	12.170	1681	1684	1691	rVB7	1569	3186	0.32%	0.042%
60	12.359	1713	1715	1716	rBV	1718	1274	0.13%	0.017%
61	12.554	1745	1747	1748	rBV2	883	664	0.07%	0.009%
62	12.603	1749	1755	1762	rVV2	16234	28872	2.88%	0.377%
63	12.688	1762	1769	1777	rVV	215186	358015	35.65%	4.669%
64	12.768	1781	1782	1785	rBV3	875	983	0.10%	0.013%
65	12.847	1791	1795	1797	rBV4	875	1329	0.13%	0.017%
66	12.883	1799	1801	1804	rVB4	1092	854	0.09%	0.011%
67	13.042	1825	1827	1830	rVB4	744	582	0.06%	0.008%
68	13.109	1835	1838	1840	rBV3	1272	1844	0.18%	0.024%
69	13.207	1849	1854	1858	rBV5	8567	14874	1.48%	0.194%
70	13.396	1881	1885	1886	rBV3	1882	2055	0.20%	0.027%
71	13.463	1893	1896	1898	rBV3	1723	2364	0.24%	0.031%
72	13.554	1904	1911	1923	rVB	356179	582798	58.04%	7.601%
73	13.761	1944	1945	1948	rVB3	1519	1268	0.13%	0.017%
74	13.847	1951	1959	1972	rBV	280954	497626	49.56%	6.490%
75	13.981	1979	1981	1984	rBV3	1221	1227	0.12%	0.016%
76	14.066	1989	1995	1999	rBV	15337	25267	2.52%	0.330%

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 Title : SFAM01.0

77	14.158	2008	2010	2013	rVB3	1081	931	0.09%	0.012%
78	14.206	2016	2018	2019	rBV2	841	732	0.07%	0.010%
79	14.231	2019	2022	2028	rVB8	1785	3207	0.32%	0.042%
80	14.310	2028	2035	2038	rBV9	1725	3704	0.37%	0.048%
81	14.408	2049	2051	2052	rBV2	1111	664	0.07%	0.009%
82	14.450	2052	2058	2059	rBV5	3319	5015	0.50%	0.065%
83	14.615	2082	2085	2086	rBV3	1144	1371	0.14%	0.018%
84	14.883	2127	2129	2132	rBV4	867	1206	0.12%	0.016%
85	14.981	2143	2145	2149	rBV3	1152	1334	0.13%	0.017%
86	15.109	2163	2166	2167	rBV3	1484	1390	0.14%	0.018%
87	15.462	2222	2224	2225	rBV2	1256	957	0.10%	0.012%
88	15.657	2254	2256	2257	rVV2	811	571	0.06%	0.007%
89	15.712	2263	2265	2268	rBV3	731	977	0.10%	0.013%
90	15.791	2276	2278	2283	rVV6	1443	1823	0.18%	0.024%
91	15.834	2283	2285	2289	rVB5	1235	1380	0.14%	0.018%
92	15.962	2301	2306	2310	rBV7	993	2304	0.23%	0.030%
93	16.078	2323	2325	2326	rBV2	1196	806	0.08%	0.011%
94	16.139	2333	2335	2337	rBV2	916	771	0.08%	0.010%
95	16.310	2357	2363	2364	rBV5	1782	2406	0.24%	0.031%
96	16.432	2382	2383	2385	rBV2	1521	1055	0.11%	0.014%
97	16.456	2385	2387	2389	rBV3	1173	1111	0.11%	0.014%
98	16.541	2399	2401	2403	rBV2	700	679	0.07%	0.009%
99	16.614	2411	2413	2415	rBV2	1267	1032	0.10%	0.013%
100	16.724	2429	2431	2433	rBV2	1304	1186	0.12%	0.015%

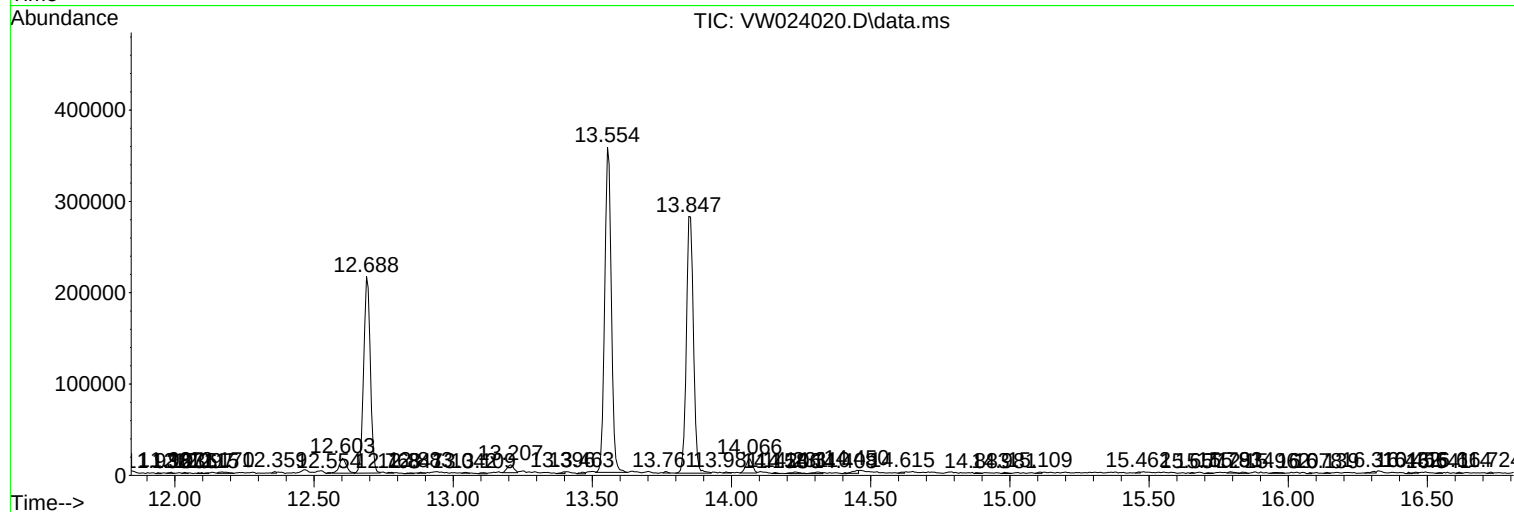
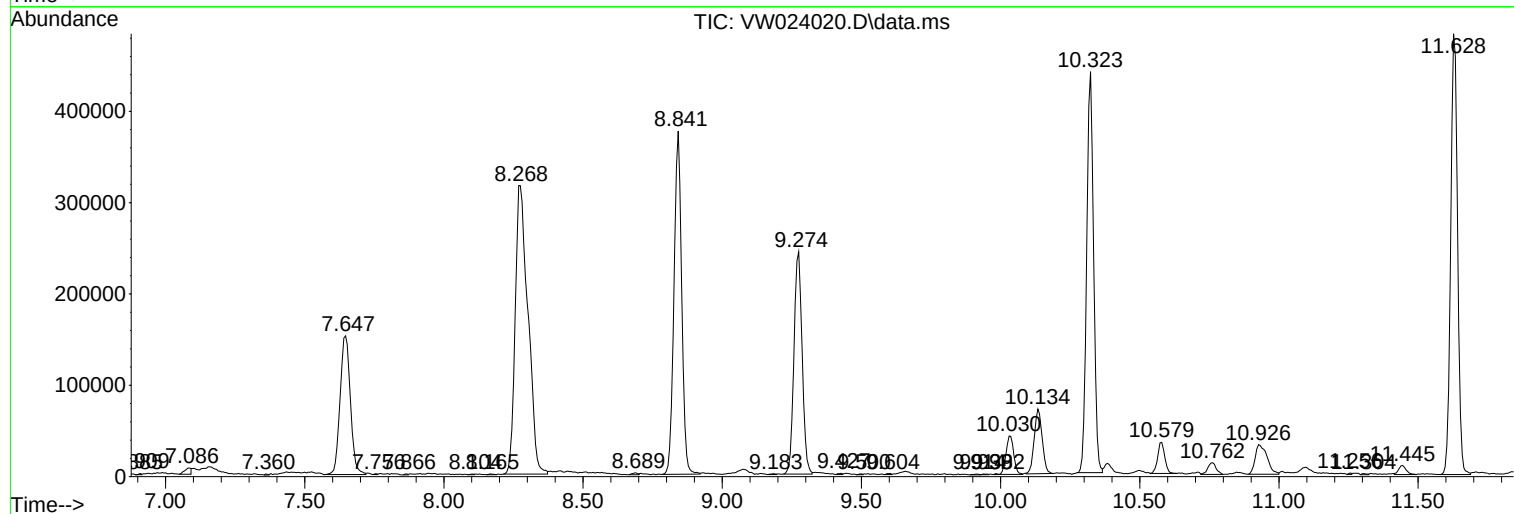
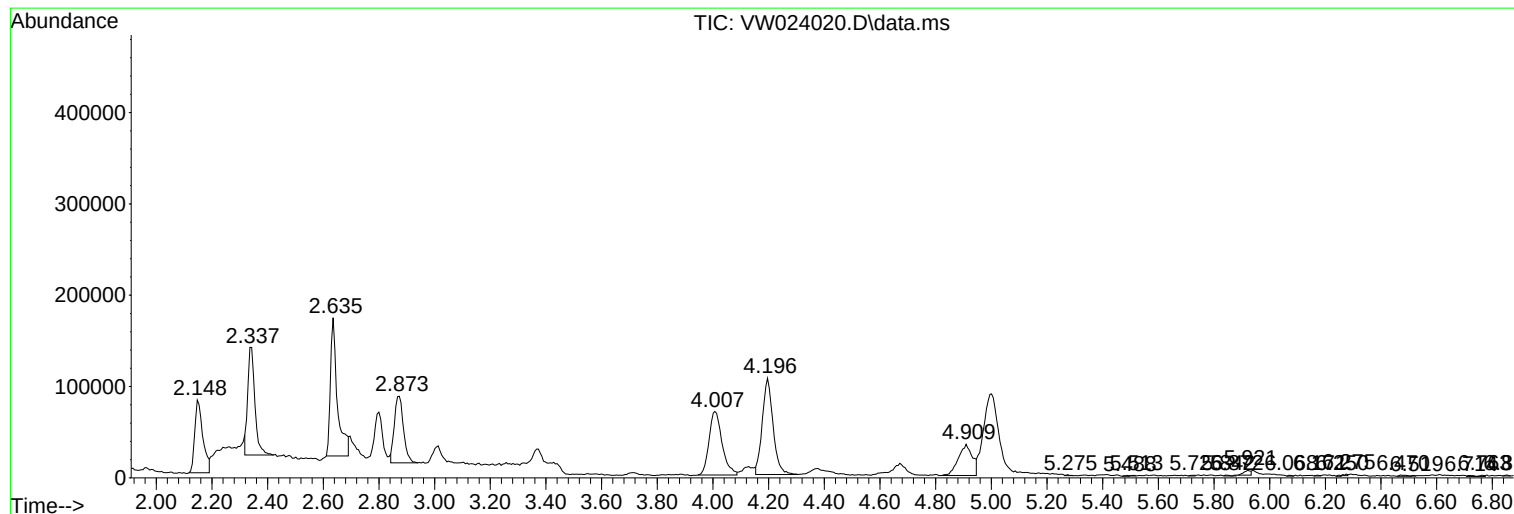
Sum of corrected areas: 7667765

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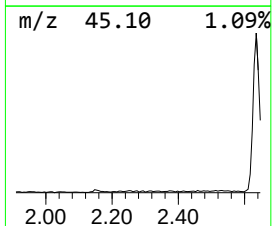
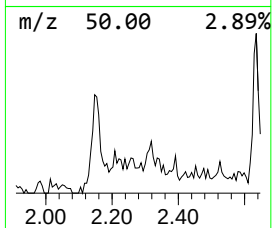
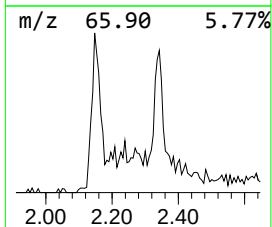
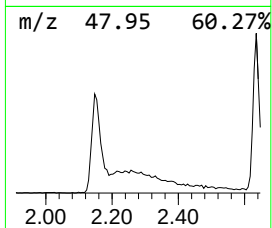
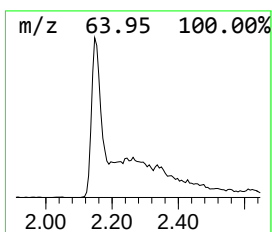
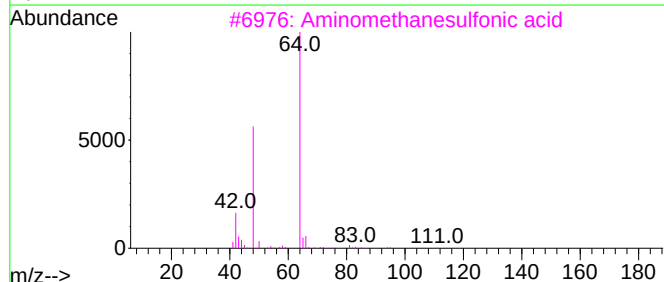
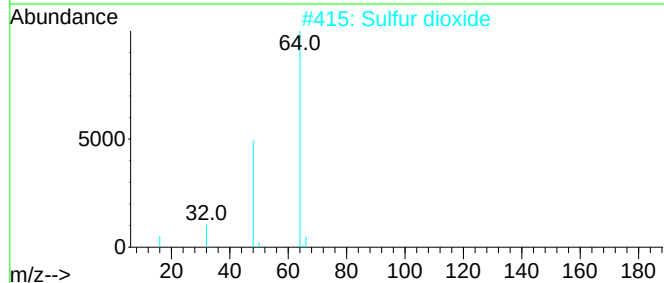
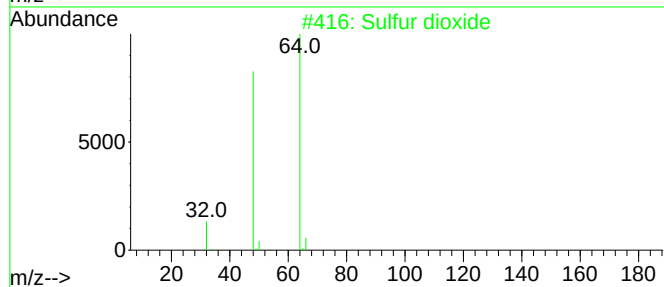
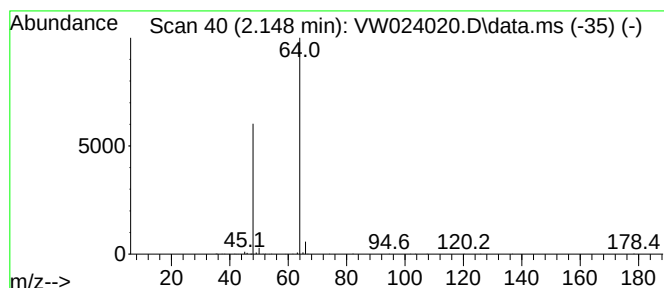
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM071322SMA.M
Quant Title : SFAM01.0

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

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.148	5.65 ug/L	162778	1,4-Difluorobenzene	8.841

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Sulfur dioxide	64	O2S	007446-09-5	83
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
5			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9



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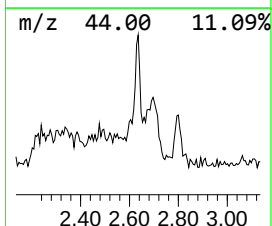
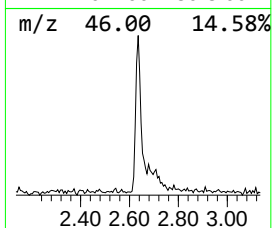
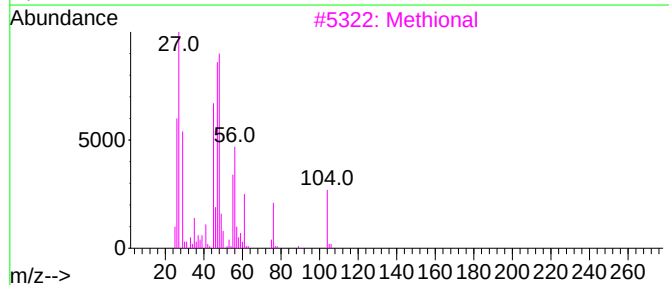
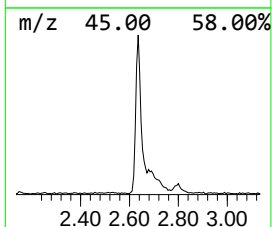
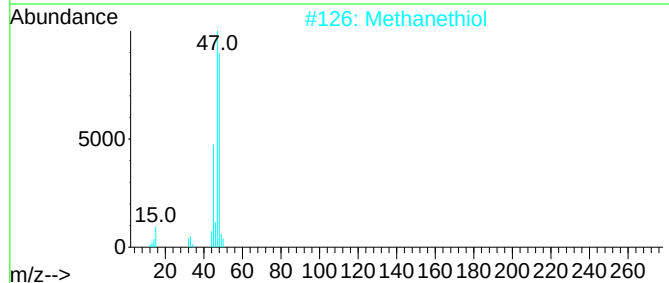
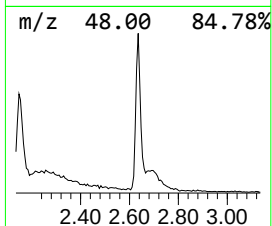
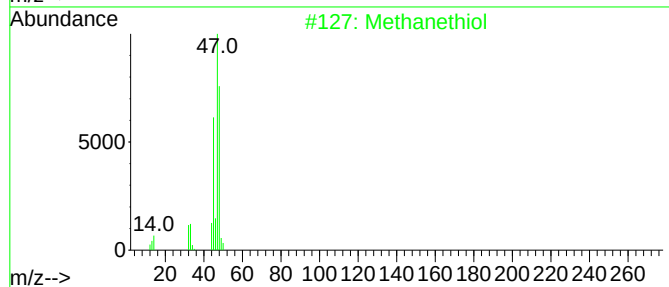
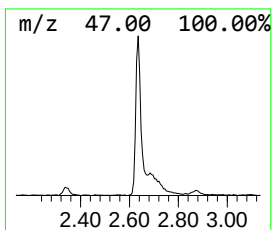
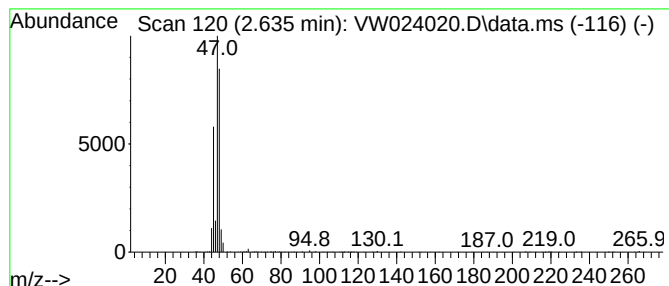
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM071322SMA.M
Quant Title : SFAM01.0

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

Peak Number 2 Methanethiol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.635	9.16 ug/L	263749	1,4-Difluorobenzene	8.841

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanethiol	48	CH4S	000074-93-1	91
2			Methanethiol	48	CH4S	000074-93-1	90
3			Methional	104	C4H8OS	003268-49-3	45
4			Acetic acid, mercapto-	92	C2H4O2S	000068-11-1	9
5			Methional	104	C4H8OS	003268-49-3	9



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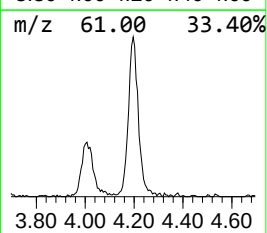
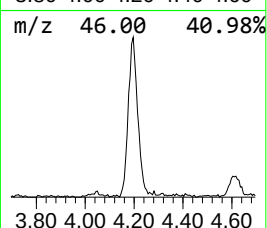
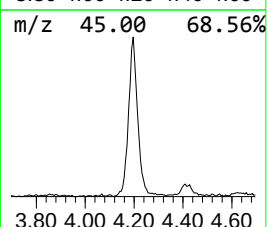
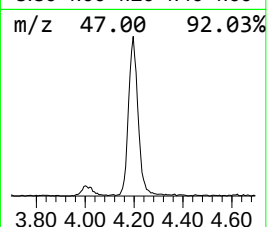
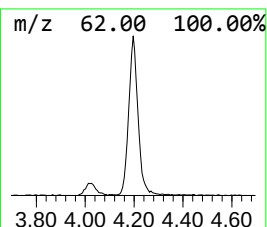
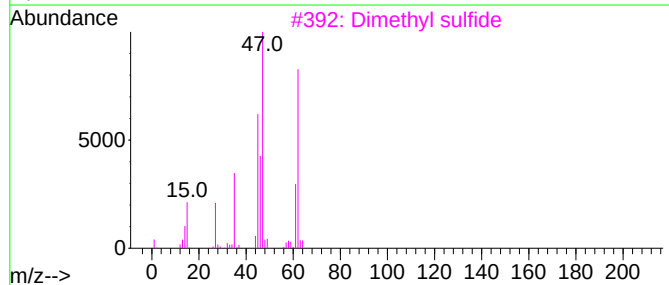
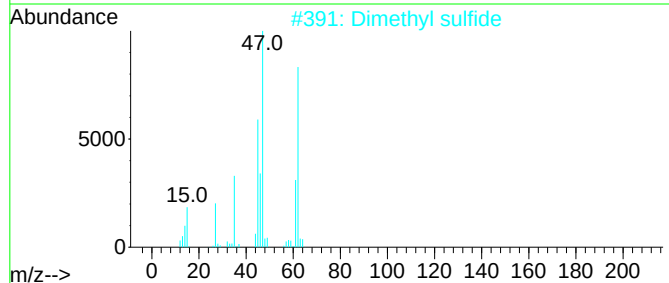
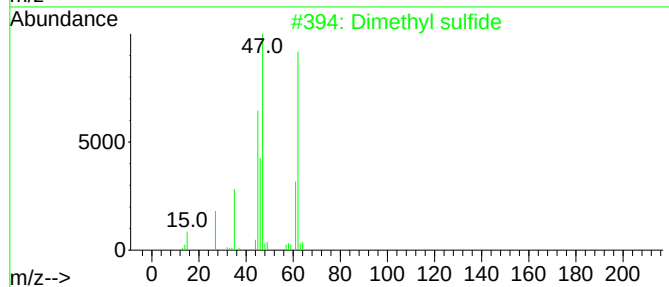
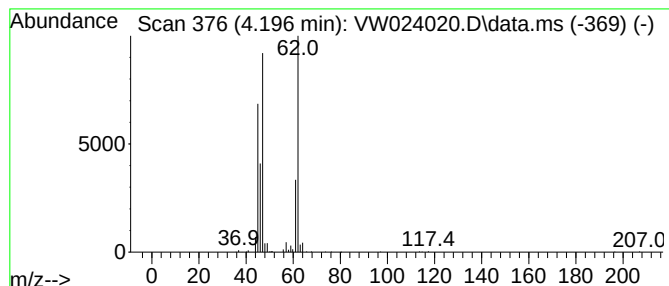
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM071322SMA.M
Quant Title : SFAM01.0

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

Peak Number 3 Dimethyl sulfide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.196	9.82 ug/L	282772	1,4-Difluorobenzene	8.841

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl sulfide	62	C2H6S	000075-18-3	94
2			Dimethyl sulfide	62	C2H6S	000075-18-3	94
3			Dimethyl sulfide	62	C2H6S	000075-18-3	91
4			Dimethyl sulfide	62	C2H6S	000075-18-3	91
5			Dimethyl sulfide	62	C2H6S	000075-18-3	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW072222\
Data File : VW024020.D
Acq On : 22 Jul 2022 21:45
Operator : SY/VA
Sample : N3741-06
Misc : 9.03g/10mL/MSVOA_W/SOIL
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
H0B14

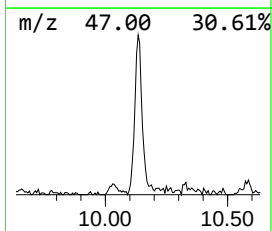
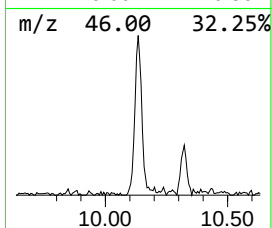
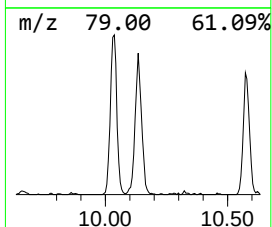
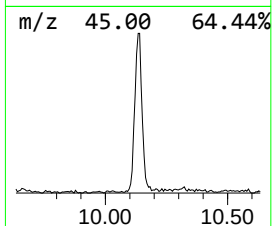
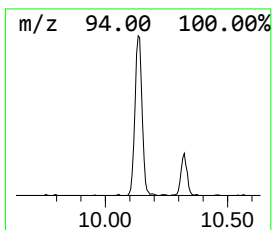
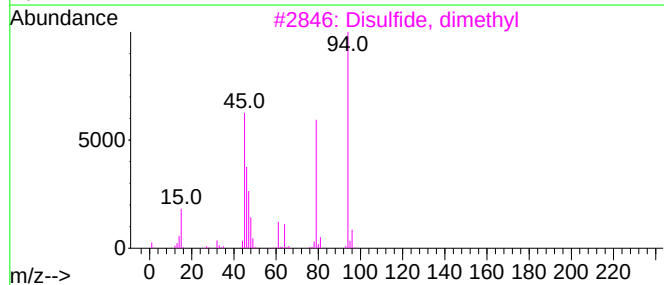
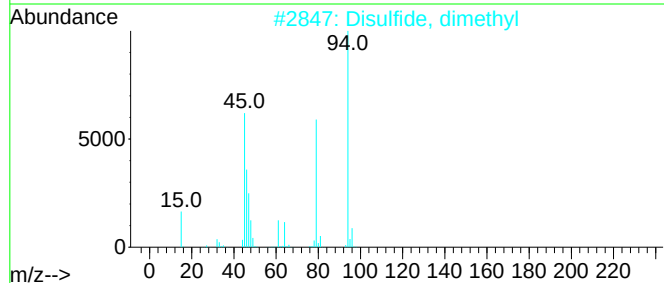
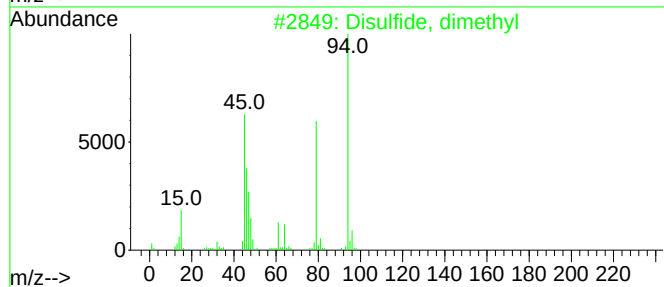
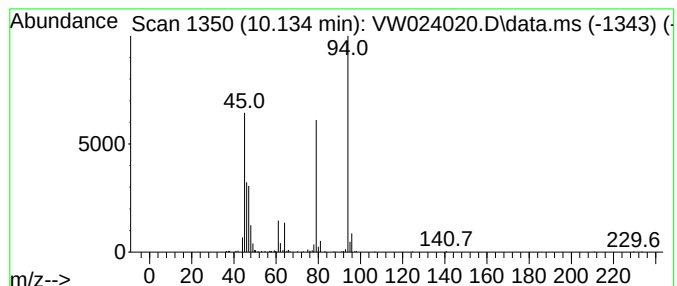
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Quant Title : SFAM01.0

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

Peak Number 5 Disulfide, dimethyl Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.134	4.88 ug/L	140395	1,4-Difluorobenzene	8.841

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Disulfide, dimethyl	94	C2H6S2	000624-92-0	97
2			Disulfide, dimethyl	94	C2H6S2	000624-92-0	97
3			Disulfide, dimethyl	94	C2H6S2	000624-92-0	97
4			Disulfide, dimethyl	94	C2H6S2	000624-92-0	96
5			Disulfide, dimethyl	94	C2H6S2	000624-92-0	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW072222\
Data File : VW024020.D
Acq On : 22 Jul 2022 21:45
Operator : SY/VA
Sample : N3741-06
Misc : 9.03g/10mL/MSVOA_W/SOIL
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
H0B14

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.148	5.7	ug/L	162778	1	8.841	719686	25.0
Methanethiol	2.635	9.2	ug/L	263749	1	8.841	719686	25.0
Dimethyl sulfide	4.196	9.8	ug/L	282772	1	8.841	719686	25.0
Disulfide, dime...	10.134	4.9	ug/L	140395	1	8.841	719686	25.0