

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW040122\
 Data File : VW022377.D
 Acq On : 01 Apr 2022 19:31
 Operator : SY/VA
 Sample : N2179-04
 Misc : 3.75g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 C0R43

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\SFAMWLM040122SMA.M
 Title : SFAM01.0

Signal : TIC: VW022377.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.355	70	74	80	rVB	134000	207612	18.69%	2.903%
2	3.452	252	254	257	rBV4	989	984	0.09%	0.014%
3	3.647	283	286	287	rBV3	1721	1392	0.13%	0.019%
4	3.690	291	293	294	rBV	1705	1322	0.12%	0.018%
5	3.824	312	315	316	rBV3	828	839	0.08%	0.012%
6	3.867	320	322	323	rVV2	1309	910	0.08%	0.013%
7	3.879	323	324	327	rVB3	2281	1364	0.12%	0.019%
8	3.922	329	331	333	rBV3	1328	857	0.08%	0.012%
9	4.019	335	347	358	rBV2	114522	357730	32.21%	5.002%
10	4.123	358	364	373	rVB	26600	67092	6.04%	0.938%
11	4.342	398	400	401	rBV2	1562	1320	0.12%	0.018%
12	4.629	445	447	450	rVB4	1393	1631	0.15%	0.023%
13	4.672	452	454	456	rVB2	1370	1193	0.11%	0.017%
14	4.696	456	458	460	rBV3	2262	2235	0.20%	0.031%
15	4.824	478	479	481	rBV2	1181	979	0.09%	0.014%
16	4.922	486	495	497	rBV8	5309	14280	1.29%	0.200%
17	5.037	512	514	515	rBV2	1179	826	0.07%	0.012%
18	5.068	517	519	524	rBV6	1178	1913	0.17%	0.027%
19	5.239	546	547	550	rBV3	1034	1011	0.09%	0.014%
20	5.293	555	556	560	rBV4	1567	1789	0.16%	0.025%
21	5.440	577	580	582	rBV4	1904	1902	0.17%	0.027%
22	5.726	625	627	630	rBV4	1053	1564	0.14%	0.022%
23	6.062	679	682	683	rBV3	1031	940	0.08%	0.013%
24	6.104	686	689	690	rVV3	1177	1015	0.09%	0.014%
25	6.159	697	698	701	rVV3	1101	932	0.08%	0.013%
26	6.214	706	707	711	rVB4	1810	1431	0.13%	0.020%
27	6.245	711	712	715	rBV3	1059	918	0.08%	0.013%
28	6.421	739	741	744	rVB4	1039	949	0.09%	0.013%
29	6.531	757	759	763	rBV5	1062	1262	0.11%	0.018%
30	6.562	763	764	767	rBV2	904	1009	0.09%	0.014%
31	6.842	808	810	812	rBV3	1011	1108	0.10%	0.015%
32	6.872	812	815	817	rVB4	1091	977	0.09%	0.014%
33	6.897	817	819	823	rBV5	1374	1803	0.16%	0.025%
34	6.927	823	824	827	rBV2	953	872	0.08%	0.012%
35	7.007	835	837	840	rBV4	1456	2239	0.20%	0.031%
36	7.080	840	849	857	rVV	40124	111920	10.08%	1.565%

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM040122SMA.M
 Title : SFAM01.0

37	7.250	876	877	879	rBV2	1582	964	0.09%	0.013%
38	7.543	923	925	926	rBV2	1181	830	0.07%	0.012%
39	7.647	932	942	953	rBV	183690	445988	40.15%	6.237%
40	7.830	971	972	976	rVB4	1696	1857	0.17%	0.026%
41	7.891	979	982	983	rVV2	1405	1291	0.12%	0.018%
42	7.927	986	988	992	rVB4	1130	1337	0.12%	0.019%
43	7.970	992	995	996	rBV3	1445	1525	0.14%	0.021%
44	8.080	1010	1013	1014	rBV3	1346	1602	0.14%	0.022%
45	8.275	1035	1045	1060	rBV2	363452	1110764	100.00%	15.533%
46	8.842	1130	1138	1149	rVB	278079	556778	50.13%	7.786%
47	9.079	1171	1177	1181	rBV8	2159	4266	0.38%	0.060%
48	9.183	1192	1194	1195	rBV2	1454	1009	0.09%	0.014%
49	9.274	1201	1209	1223	rVB	255901	515989	46.45%	7.216%
50	9.378	1225	1226	1229	rVV3	1594	1009	0.09%	0.014%
51	9.409	1229	1231	1234	rVB3	1279	1119	0.10%	0.016%
52	9.506	1245	1247	1249	rBV3	1105	1168	0.11%	0.016%
53	9.543	1251	1253	1255	rVV3	1016	878	0.08%	0.012%
54	9.616	1263	1265	1267	rVB3	1207	858	0.08%	0.012%
55	9.646	1267	1270	1273	rBV5	1369	2134	0.19%	0.030%
56	9.695	1276	1278	1281	rVB3	1151	1007	0.09%	0.014%
57	9.738	1281	1285	1286	rBV3	1030	1167	0.11%	0.016%
58	9.762	1287	1289	1295	rVB6	1623	3065	0.28%	0.043%
59	10.030	1327	1333	1343	rBV	118865	220269	19.83%	3.080%
60	10.323	1373	1381	1388	rBV	496711	866751	78.03%	12.121%
61	10.494	1404	1409	1413	rVB4	8934	14746	1.33%	0.206%
62	10.579	1417	1423	1429	rVB	78972	140390	12.64%	1.963%
63	10.701	1439	1443	1448	rBV5	4658	7434	0.67%	0.104%
64	10.823	1461	1463	1465	rBV3	1298	1527	0.14%	0.021%
65	10.847	1465	1467	1469	rVV3	1583	1326	0.12%	0.019%
66	10.921	1472	1479	1488	rBV	175545	296462	26.69%	4.146%
67	11.189	1521	1523	1527	rBV5	803	861	0.08%	0.012%
68	11.256	1533	1534	1537	rVB3	1445	1113	0.10%	0.016%
69	11.311	1540	1543	1545	rBV4	1215	1341	0.12%	0.019%
70	11.378	1551	1554	1555	rBV2	1546	1276	0.11%	0.018%
71	11.628	1586	1595	1608	rBV	360898	603978	54.38%	8.446%
72	11.805	1619	1624	1626	rBV6	1640	3349	0.30%	0.047%
73	11.981	1650	1653	1654	rBV3	1575	1988	0.18%	0.028%
74	12.030	1659	1661	1665	rVV4	1040	1237	0.11%	0.017%
75	12.164	1681	1683	1684	rBV2	1258	910	0.08%	0.013%
76	12.341	1708	1712	1714	rBV5	2020	2453	0.22%	0.034%

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 Title : SFAM01.0

77	12.536	1742	1744	1747	rBV4	1286	1021	0.09%	0.014%
78	12.591	1747	1753	1761	rBV5	9171	20942	1.89%	0.293%
79	12.689	1763	1769	1776	rVB	187768	305614	27.51%	4.274%
80	13.469	1892	1897	1902	rBV7	6597	11021	0.99%	0.154%
81	13.554	1904	1911	1922	rBV	261002	418181	37.65%	5.848%
82	13.694	1932	1934	1937	rBV4	1251	863	0.08%	0.012%
83	13.847	1953	1959	1966	rBV	253389	410589	36.96%	5.742%
84	14.066	1990	1995	2003	rVB2	12978	21752	1.96%	0.304%
85	14.286	2029	2031	2034	rBV4	1621	2461	0.22%	0.034%
86	14.408	2050	2051	2052	rBV	1957	1147	0.10%	0.016%
87	14.426	2052	2054	2061	rVB8	2838	4631	0.42%	0.065%
88	14.676	2091	2095	2096	rBV4	1289	1703	0.15%	0.024%
89	14.780	2109	2112	2116	rVB5	2263	2928	0.26%	0.041%
90	14.950	2136	2140	2141	rBV4	1835	1956	0.18%	0.027%
91	15.005	2147	2149	2151	rVB3	1323	979	0.09%	0.014%
92	15.389	2207	2212	2217	rVB	16825	29224	2.63%	0.409%
93	15.456	2218	2223	2231	rVV4	25779	51672	4.65%	0.723%
94	15.548	2231	2238	2249	rVB2	125880	235189	21.17%	3.289%
95	16.072	2322	2324	2326	rVB3	1975	1106	0.10%	0.015%
96	16.096	2326	2328	2329	rBV2	1477	1120	0.10%	0.016%
97	16.310	2362	2363	2364	rBV	1885	1191	0.11%	0.017%
98	16.438	2382	2384	2386	rBV2	1263	1117	0.10%	0.016%
99	16.462	2386	2388	2390	rVB3	1747	1503	0.14%	0.021%
100	16.541	2399	2401	2403	rBV2	1296	997	0.09%	0.014%

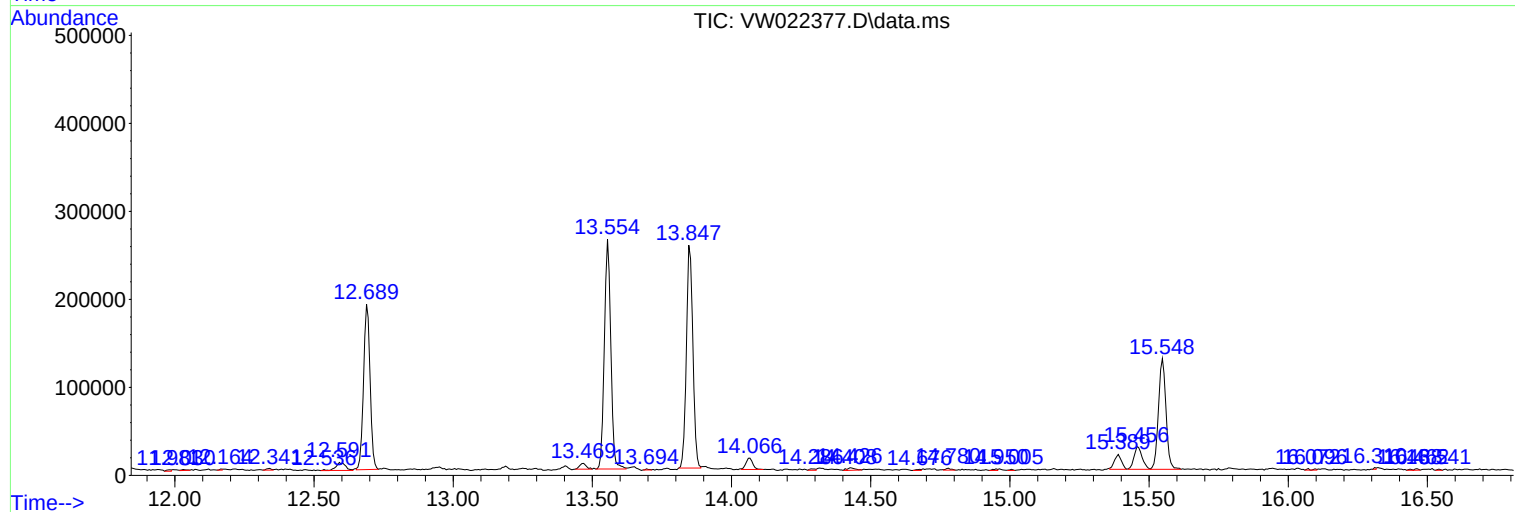
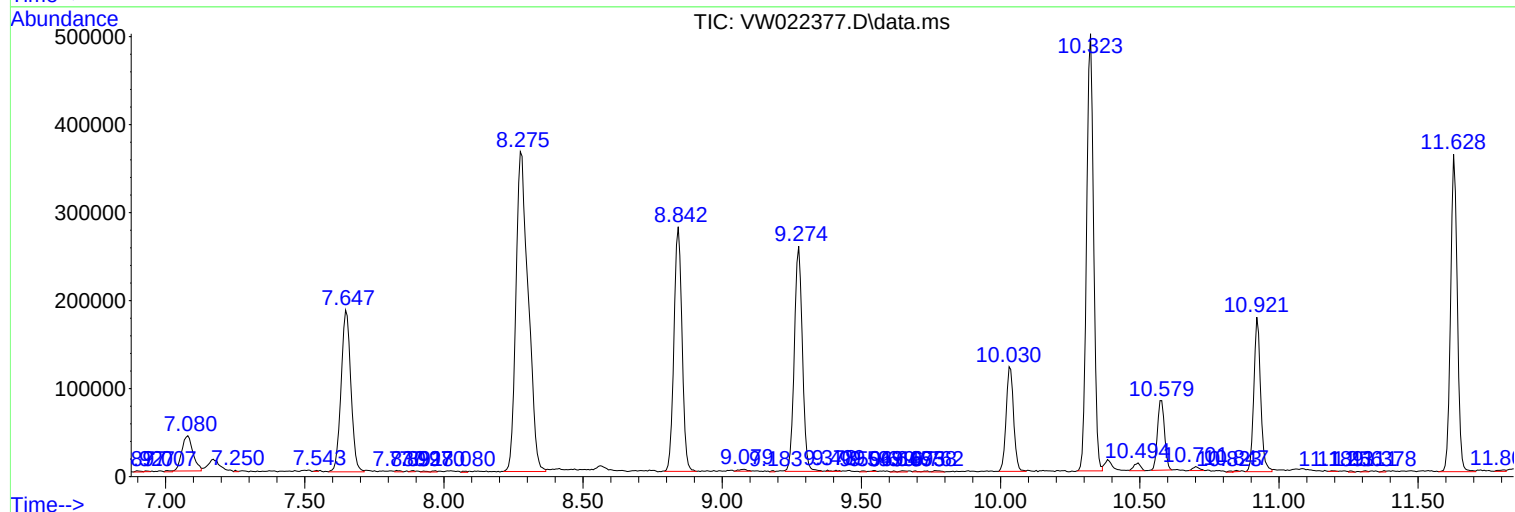
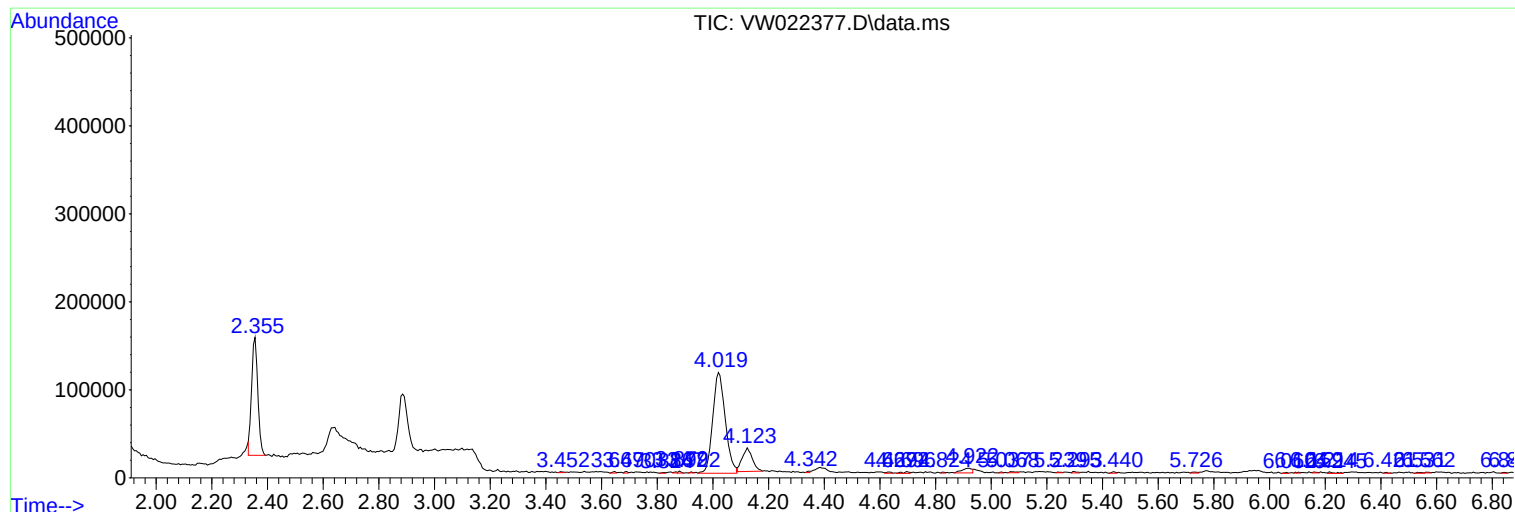
Sum of corrected areas: 7151043

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM040122SMA.M
Quant Title : SFAM01.0

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



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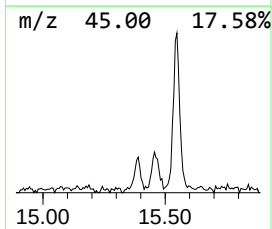
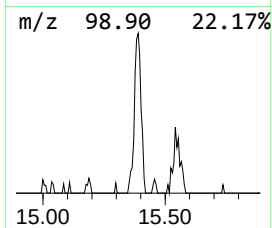
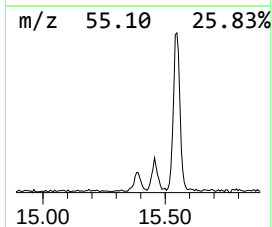
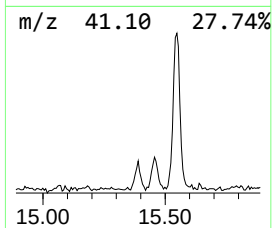
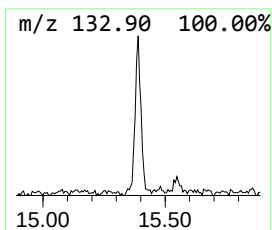
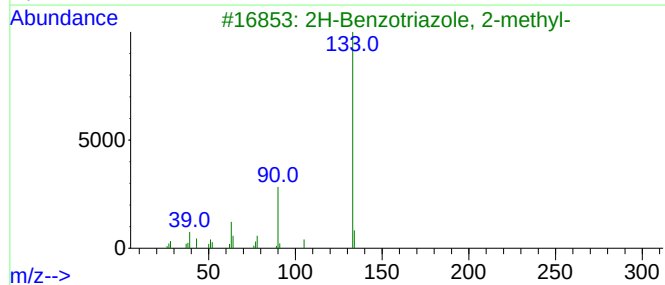
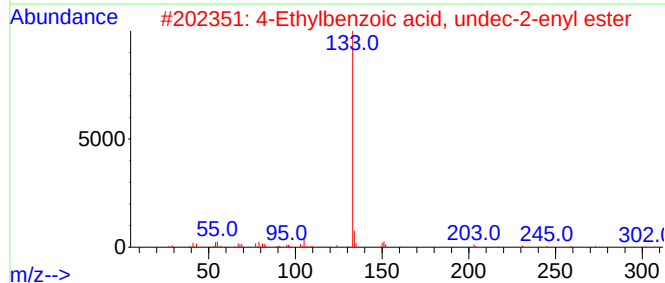
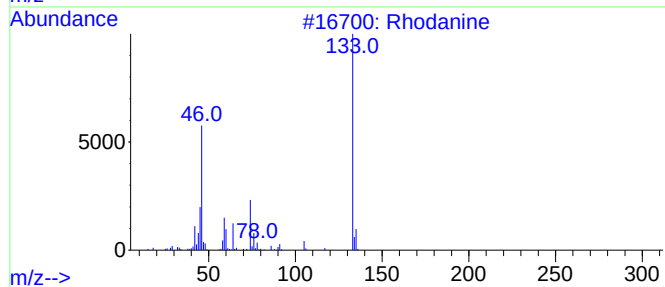
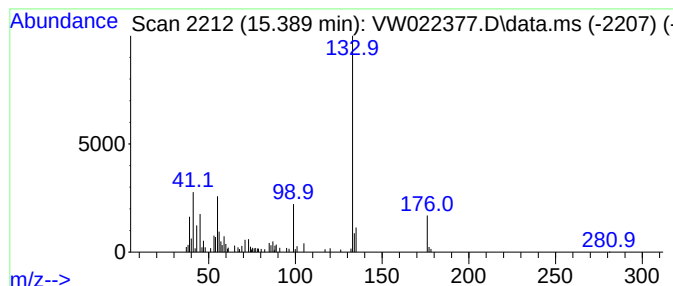
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM040122SMA.M
Quant Title : SFAM01.0

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

Peak Number 3 Rhodanine Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.389	1.75 ug/L	29224	1,4-Dichlorobenzene-d4	13.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Rhodanine	133	C3H3NOS2	000141-84-4	58
2			4-Ethylbenzoic acid, undec-2-eny...	302	C20H30O2	1000292-54-8	47
3			2H-Benzotriazole, 2-methyl-	133	C7H7N3	016584-00-2	47
4			5-Aminoindazole	133	C7H7N3	019335-11-6	43
5			(2-Methyl[1,3]dithian-2-yl)methanol	164	C6H12OS2	1000191-37-4	40



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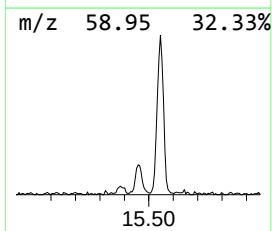
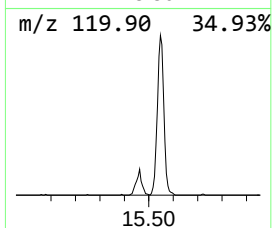
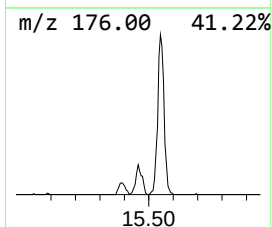
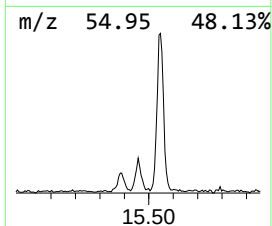
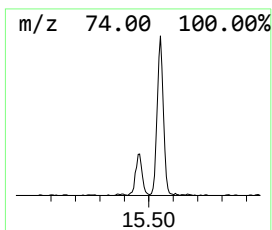
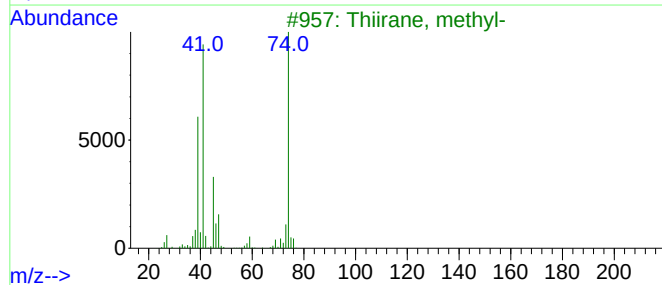
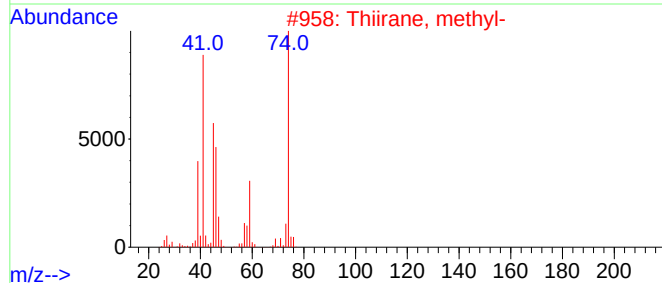
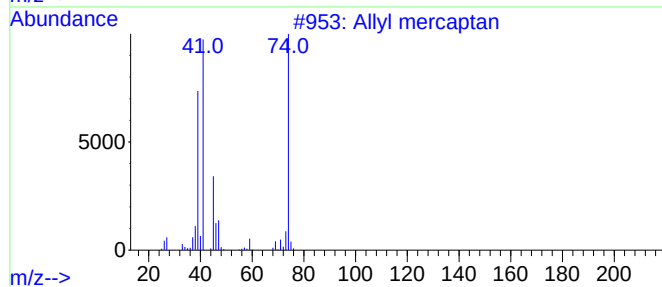
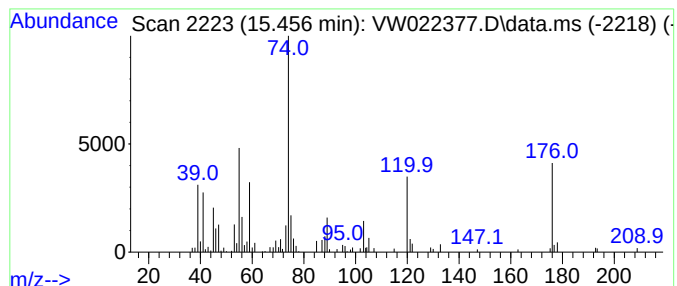
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM040122SMA.M
Quant Title : SFAM01.0

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

Peak Number 4 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.456	3.09 ug/L	51672	1,4-Dichlorobenzene-d4	13.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Allyl mercaptan	74	C3H6S	000870-23-5	46
2			Thiirane, methyl-	74	C3H6S	001072-43-1	46
3			Thiirane, methyl-	74	C3H6S	001072-43-1	43
4			Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	25
5			Methyl 3-O-methyl-.beta.-D-xylop...	178	C7H14O5	007381-10-4	23



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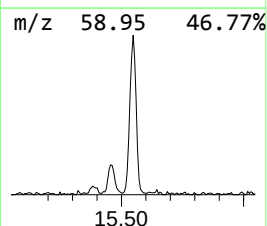
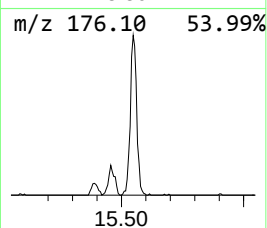
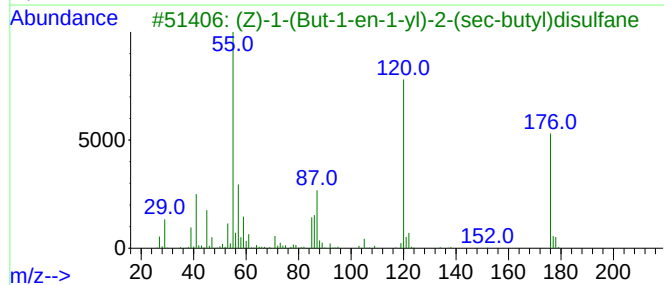
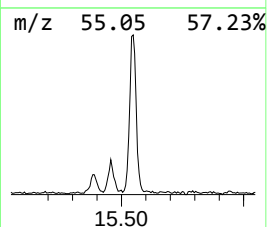
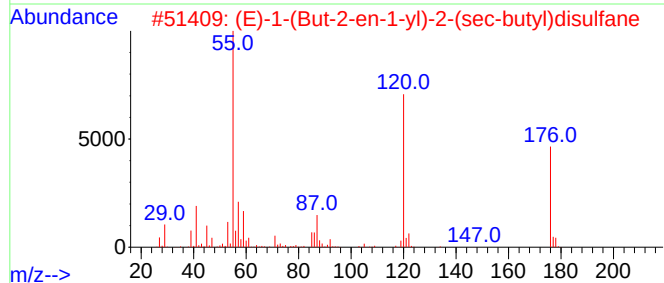
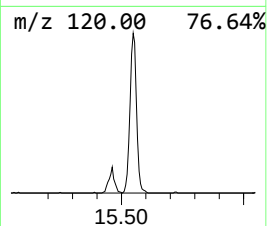
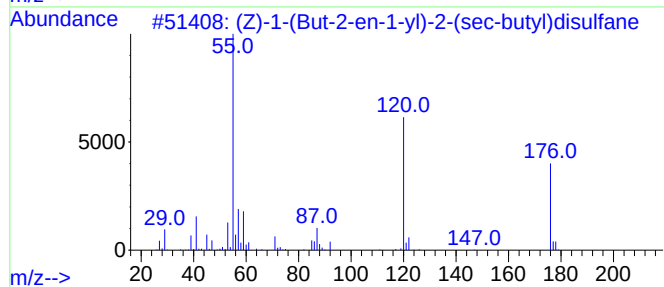
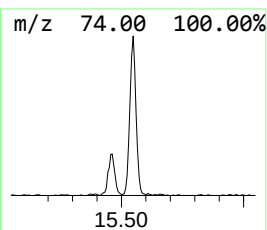
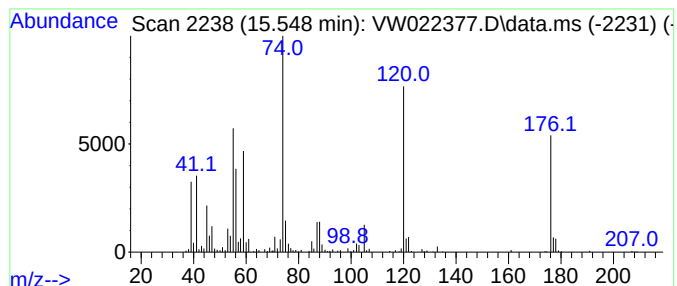
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM040122SMA.M
Quant Title : SFAM01.0

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

Peak Number 5 unknown-02 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.548	14.06 ug/L	235189	1,4-Dichlorobenzene-d4	13.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(Z)-1-(But-2-en-1-yl)-2-(sec-but...	176	C8H16S2	110690-23-8	41		
2	(E)-1-(But-2-en-1-yl)-2-(sec-but...	176	C8H16S2	110690-24-9	41		
3	(Z)-1-(But-1-en-1-yl)-2-(sec-but...	176	C8H16S2	110690-21-6	38		
4	(E)-1-(But-1-en-1-yl)-2-(sec-but...	176	C8H16S2	110690-22-7	38		
5	dl-Homoserine	119	C4H9NO3	001927-25-9	30		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW040122\
Data File : VW022377.D
Acq On : 01 Apr 2022 19:31
Operator : SY/VA
Sample : N2179-04
Misc : 3.75g/10mL/MSVOA_W/SOIL
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
C0R43

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM040122SMA.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
Rhodanine	15.389	1.8	ug/L	29224	3	13.554	418181	25.0
unknown-01	15.456	3.1	ug/L	51672	3	13.554	418181	25.0
unknown-02	15.548	14.1	ug/L	235189	3	13.554	418181	25.0