

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW040422\
 Data File : VW022388.D
 Acq On : 04 Apr 2022 15:52
 Operator : SY/VA
 Sample : N2179-01RE
 Misc : 3.32g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 C0R21RE

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: VW022388.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	82	rVB	111856	179678	20.56%	3.013%
2	2.892	157	162	170	rVB	58468	124659	14.26%	2.090%
3	3.660	286	288	289	rVB3	1271	757	0.09%	0.013%
4	3.715	295	297	298	rBV2	1634	1099	0.13%	0.018%
5	3.812	311	313	314	rBV2	1559	1046	0.12%	0.018%
6	3.861	317	321	322	rBV4	1220	1484	0.17%	0.025%
7	4.026	337	348	357	rBV2	92245	279161	31.94%	4.681%
8	4.123	358	364	374	rVB	55163	138056	15.79%	2.315%
9	4.489	422	424	425	rBV2	859	787	0.09%	0.013%
10	4.586	438	440	441	rBV2	795	566	0.06%	0.009%
11	4.629	445	447	450	rVB4	1146	1198	0.14%	0.020%
12	4.708	458	460	462	rVB3	1049	657	0.08%	0.011%
13	4.916	484	494	506	rBV4	8574	33268	3.81%	0.558%
14	5.397	570	573	578	rBV6	974	1948	0.22%	0.033%
15	5.537	593	596	598	rBV4	605	707	0.08%	0.012%
16	5.580	602	603	604	rBV	1045	441	0.05%	0.007%
17	5.611	604	608	609	rVB3	1002	979	0.11%	0.016%
18	5.629	609	611	614	rBV3	1019	1382	0.16%	0.023%
19	5.726	624	627	630	rBV5	710	1006	0.12%	0.017%
20	5.775	632	635	637	rBV3	1618	2050	0.23%	0.034%
21	5.922	657	659	661	rBV3	1057	1038	0.12%	0.017%
22	6.098	685	688	690	rVB4	1061	1232	0.14%	0.021%
23	6.123	690	692	693	rBV2	772	543	0.06%	0.009%
24	6.178	699	701	702	rBV2	1034	845	0.10%	0.014%
25	6.257	712	714	715	rBV3	799	513	0.06%	0.009%
26	6.470	748	749	751	rBV2	878	428	0.05%	0.007%
27	6.489	751	752	755	rVV3	888	929	0.11%	0.016%
28	6.543	759	761	763	rVV4	706	362	0.04%	0.006%
29	6.696	784	786	788	rBV3	1239	918	0.11%	0.015%
30	6.714	788	789	791	rVV2	1012	499	0.06%	0.008%
31	6.732	791	792	794	rVB2	626	359	0.04%	0.006%
32	6.751	794	795	797	rVB	708	360	0.04%	0.006%
33	6.775	797	799	800	rBV2	578	344	0.04%	0.006%
34	6.940	825	826	827	rBV	657	336	0.04%	0.006%
35	7.080	842	849	857	rBV	22458	57960	6.63%	0.972%
36	7.171	859	864	874	rVB	28611	69604	7.96%	1.167%

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Integration Parameters: LSCINT.P

Integrator: RTE

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

37	7.397	899	901	902	rBV2	1212	613	0.07%	0.010%
38	7.653	933	943	956	rVB	142293	352078	40.28%	5.904%
39	7.744	956	958	960	rBV3	1220	947	0.11%	0.016%
40	7.799	966	967	970	rVB3	1328	628	0.07%	0.011%
41	7.836	972	973	975	rVB2	1072	442	0.05%	0.007%
42	7.872	975	979	980	rBV3	929	850	0.10%	0.014%
43	8.007	999	1001	1004	rBV4	1401	1921	0.22%	0.032%
44	8.281	1036	1046	1063	rBV2	290705	874118	100.00%	14.658%
45	8.842	1130	1138	1147	rBV	242034	477499	54.63%	8.007%
46	8.994	1159	1163	1164	rBV4	785	1218	0.14%	0.020%
47	9.019	1164	1167	1168	rBV3	789	744	0.09%	0.012%
48	9.147	1185	1188	1190	rBV4	1044	1171	0.13%	0.020%
49	9.201	1196	1197	1198	rBV	509	187	0.02%	0.003%
50	9.275	1200	1209	1218	rVV	199198	398433	45.58%	6.681%
51	9.799	1292	1295	1296	rBV2	569	492	0.06%	0.008%
52	9.896	1309	1311	1314	rBV3	767	877	0.10%	0.015%
53	10.037	1327	1334	1343	rVB	81059	150605	17.23%	2.525%
54	10.183	1357	1358	1360	rBV2	837	883	0.10%	0.015%
55	10.323	1370	1381	1388	rBV	409397	718649	82.21%	12.051%
56	10.390	1388	1392	1402	rVB3	11159	23695	2.71%	0.397%
57	10.488	1404	1408	1414	rVV3	9447	17475	2.00%	0.293%
58	10.579	1417	1423	1429	rVB	54349	90476	10.35%	1.517%
59	10.707	1438	1444	1448	rBV2	2465	5120	0.59%	0.086%
60	10.744	1448	1450	1452	rBV3	1110	712	0.08%	0.012%
61	10.921	1473	1479	1493	rVB	93920	164301	18.80%	2.755%
62	11.256	1532	1534	1537	rBV4	1141	1374	0.16%	0.023%
63	11.353	1548	1550	1553	rBV4	1374	1695	0.19%	0.028%
64	11.628	1588	1595	1607	rVV	305107	513424	58.74%	8.609%
65	11.731	1610	1612	1616	rVB5	1198	1017	0.12%	0.017%
66	12.061	1662	1666	1667	rBV3	892	1299	0.15%	0.022%
67	12.097	1670	1672	1673	rBV2	763	502	0.06%	0.008%
68	12.122	1673	1676	1677	rBV3	779	613	0.07%	0.010%
69	12.146	1677	1680	1681	rBV3	1111	1025	0.12%	0.017%
70	12.463	1730	1732	1733	rBV2	826	674	0.08%	0.011%
71	12.603	1748	1755	1760	rBV4	10281	18606	2.13%	0.312%
72	12.689	1763	1769	1778	rVB	119014	200721	22.96%	3.366%
73	13.073	1830	1832	1834	rBV2	1012	1105	0.13%	0.019%
74	13.402	1879	1886	1893	rBV2	3149	8008	0.92%	0.134%
75	13.554	1905	1911	1919	rBV	224963	357238	40.87%	5.990%
76	13.847	1953	1959	1966	rBV	191909	329496	37.69%	5.525%

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 ClientSampleId :
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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

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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

77	14.066	1991	1995	2000	rVB2	9052	13830	1.58%	0.232%
78	14.103	2000	2001	2005	rVB4	1152	1101	0.13%	0.018%
79	14.152	2007	2009	2011	rVB2	1069	888	0.10%	0.015%
80	14.188	2011	2015	2016	rBV4	1097	1141	0.13%	0.019%
81	14.249	2024	2025	2028	rBV3	822	580	0.07%	0.010%
82	14.579	2077	2079	2081	rBV3	906	919	0.11%	0.015%
83	14.676	2093	2095	2097	rBV3	1492	1624	0.19%	0.027%
84	14.780	2106	2112	2113	rBV6	1979	3154	0.36%	0.053%
85	15.066	2155	2159	2160	rBV3	1408	1900	0.22%	0.032%
86	15.176	2176	2177	2179	rBV2	1101	871	0.10%	0.015%
87	15.389	2204	2212	2218	rBV2	19444	39157	4.48%	0.657%
88	15.456	2218	2223	2231	rVV3	24277	48302	5.53%	0.810%
89	15.548	2231	2238	2249	rVV2	113355	213277	24.40%	3.576%
90	15.932	2299	2301	2304	rBV3	1325	1866	0.21%	0.031%
91	16.188	2341	2343	2346	rBV4	1437	2005	0.23%	0.034%
92	16.255	2353	2354	2355	rBV	1069	552	0.06%	0.009%
93	16.304	2360	2362	2363	rBV2	1796	1429	0.16%	0.024%
94	16.450	2384	2386	2387	rVB2	1184	732	0.08%	0.012%
95	16.474	2387	2390	2391	rBV3	1188	1173	0.13%	0.020%
96	16.621	2412	2414	2416	rBV3	917	926	0.11%	0.016%

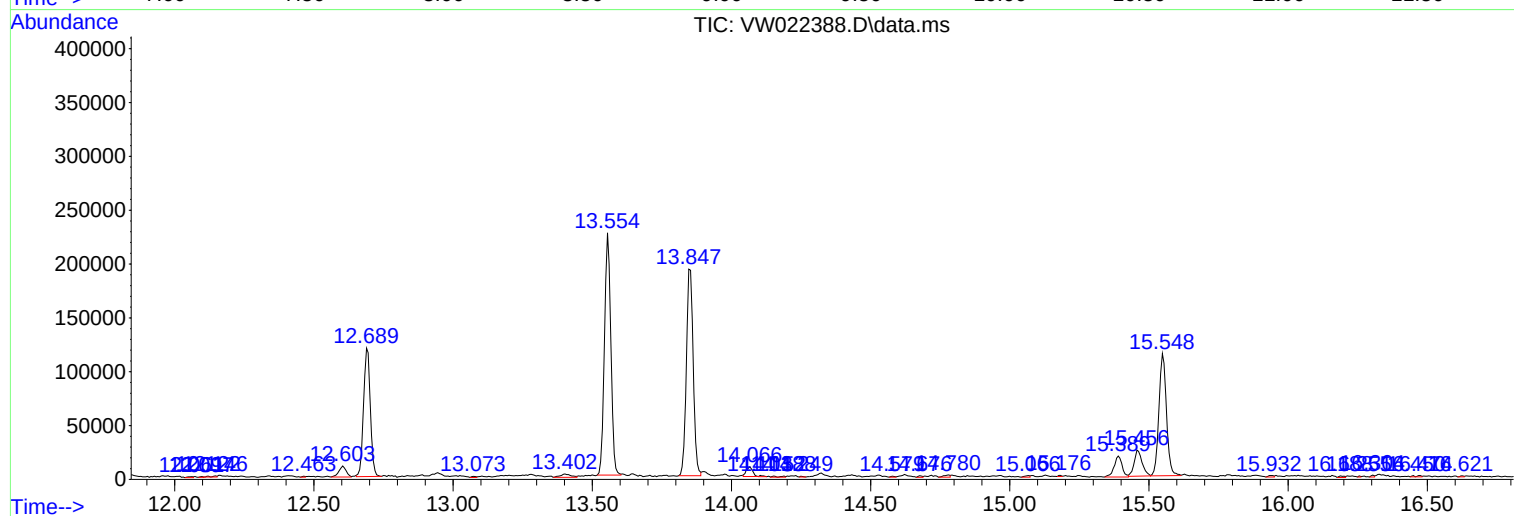
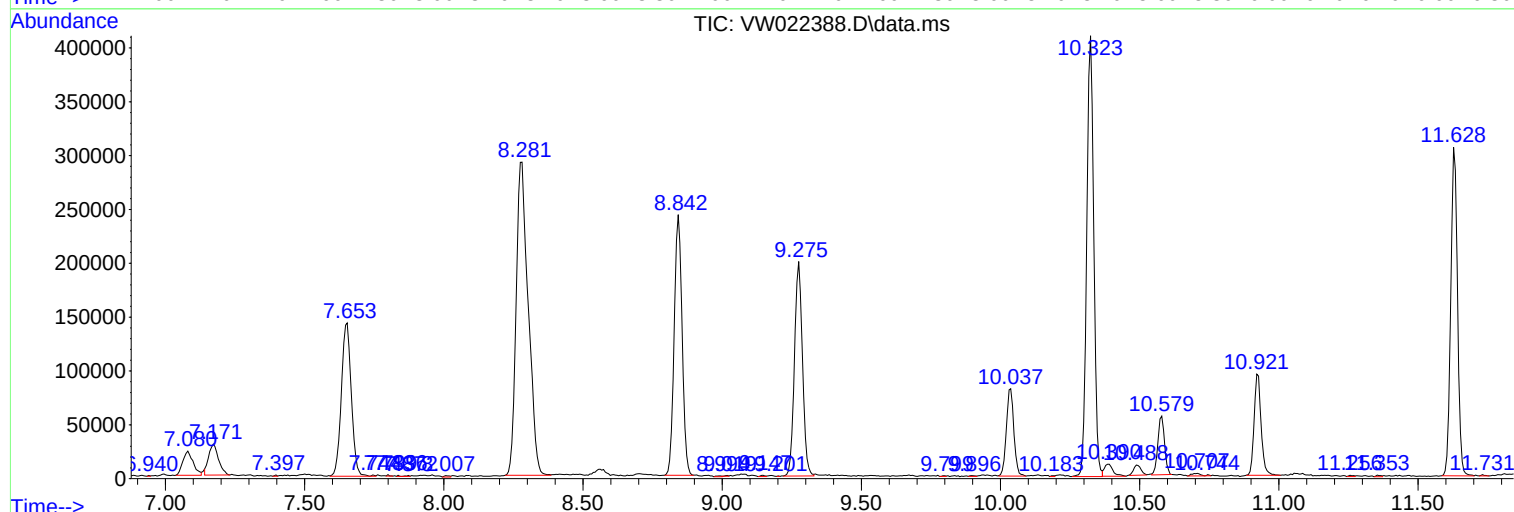
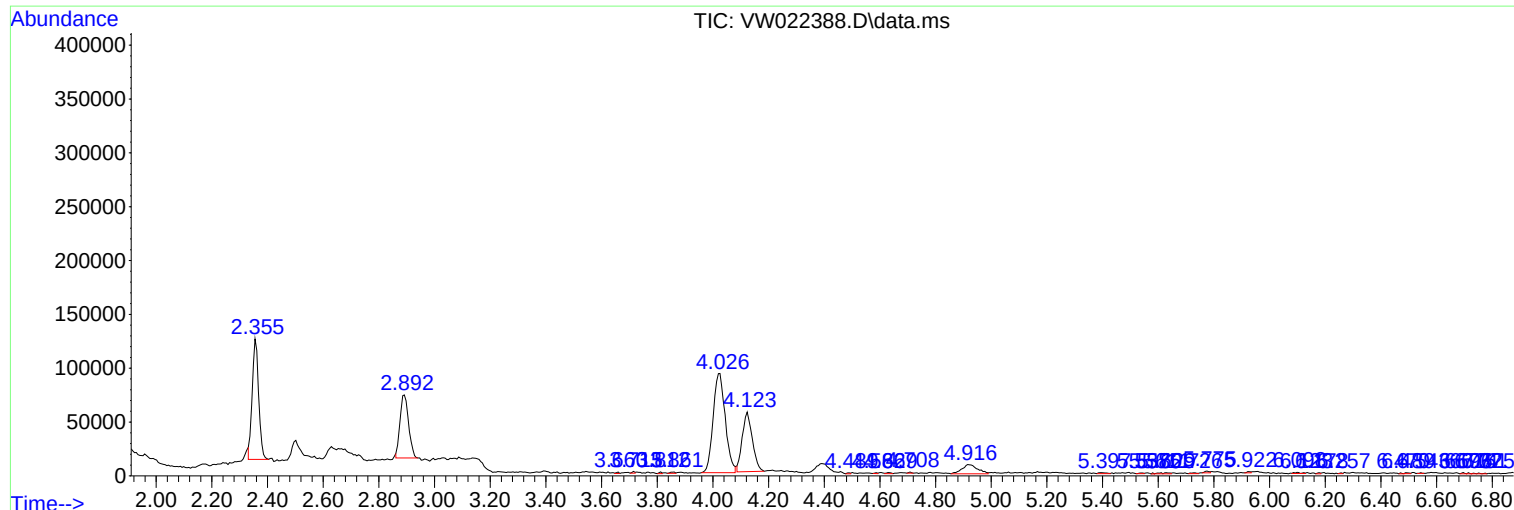
Sum of corrected areas: 5963557

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ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
C0R21RE

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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Instrument :
MSVOA_W
ClientSampleId :
C0R21RE

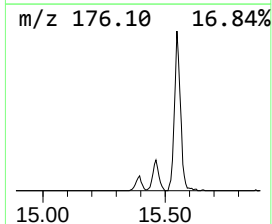
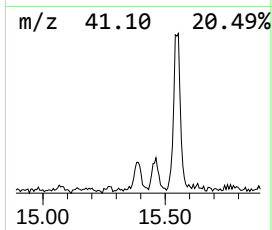
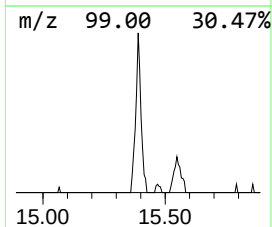
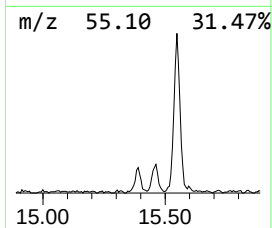
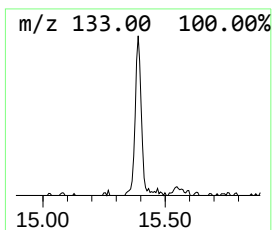
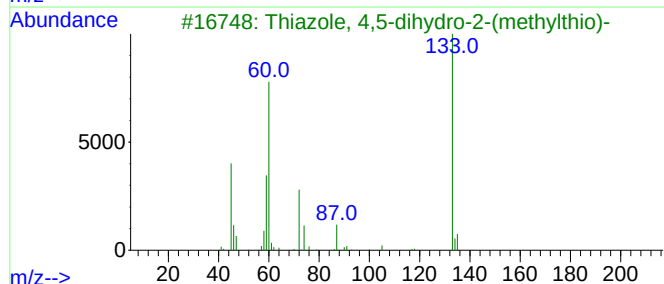
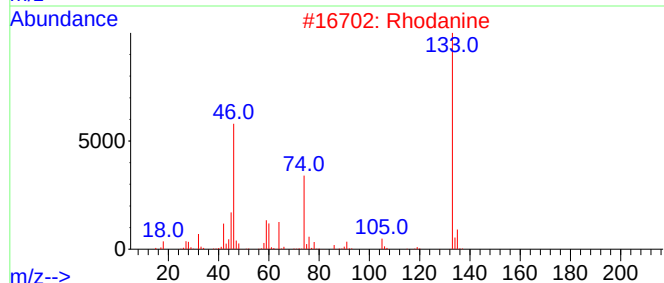
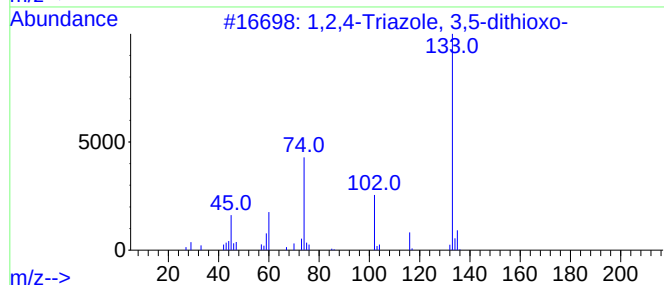
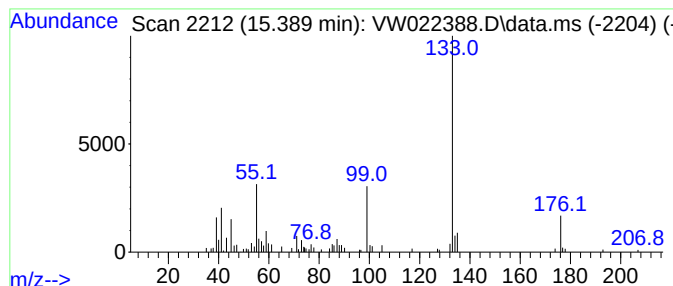
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM040122SMA.M
Quant Title : SFAM01.0

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

Peak Number 4 1,2,4-Triazole, 3,5-dithio- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.389	2.74 ug/L	39157	1,4-Dichlorobenzene-d4	13.560

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4-Triazole, 3,5-dithio-	133	C2H3N3S2	005650-03-3	68		
2	Rhodanine	133	C3H3NOS2	000141-84-4	53		
3	Thiazole, 4,5-dihydro-2-(methylt...	133	C4H7NS2	019975-56-5	50		
4	3-Methylthiazolidine-2-thione	133	C4H7NS2	001908-87-8	50		
5	3-(Difluoromethyl)-1H-pyrazol-5-...	133	C4H5F2N3	1284220-49-0	49		



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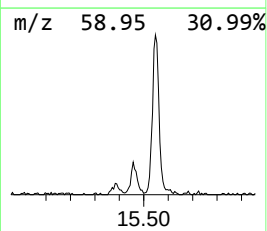
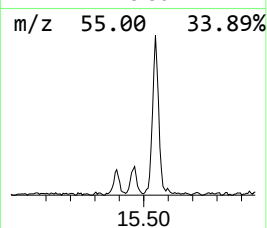
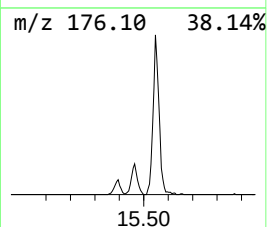
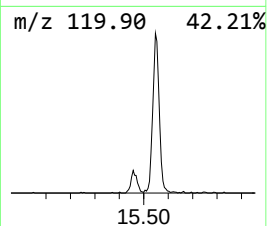
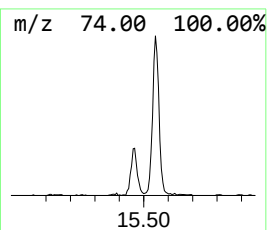
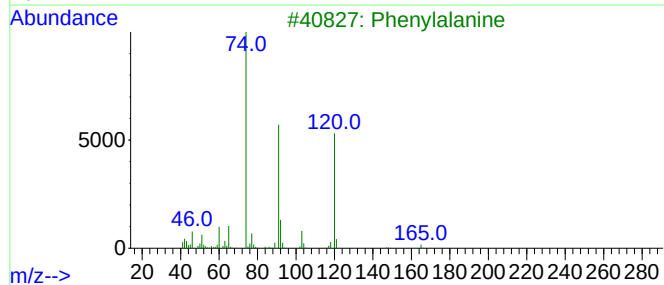
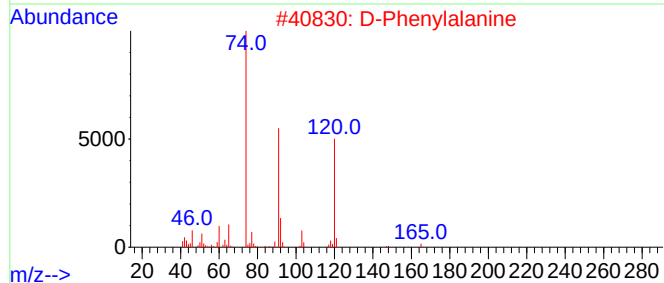
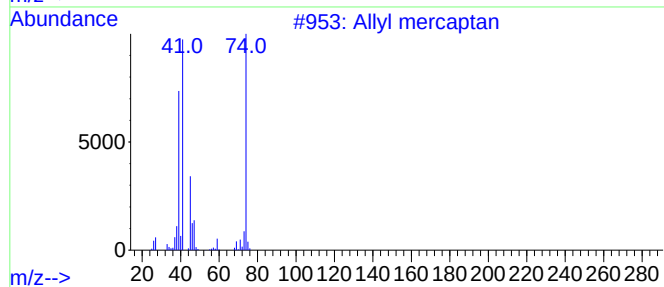
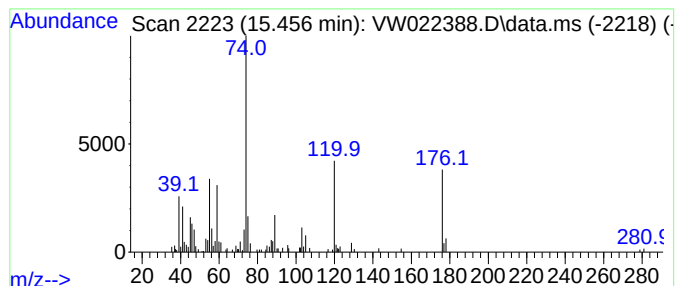
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM040122SMA.M
Quant Title : SFAM01.0

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

Peak Number 5 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.456	3.38 ug/L	48302	1,4-Dichlorobenzene-d4	13.560

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Allyl mercaptan	74	C3H6S	000870-23-5	43
2			D-Phenylalanine	165	C9H11NO2	000673-06-3	38
3			Phenylalanine	165	C9H11NO2	000063-91-2	38
4			Thiirane, methyl-	74	C3H6S	001072-43-1	38
5			Thiirane, methyl-	74	C3H6S	001072-43-1	38



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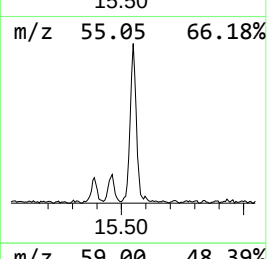
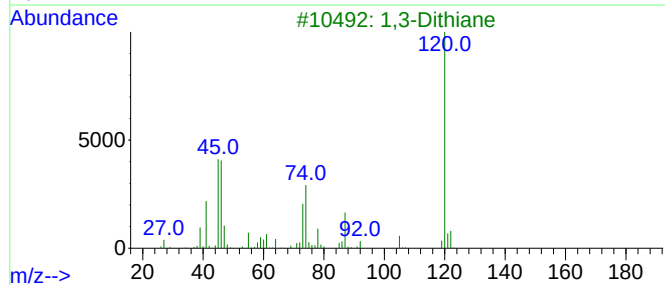
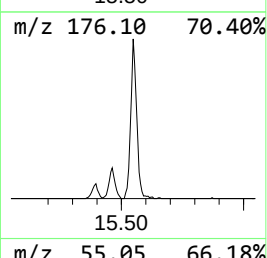
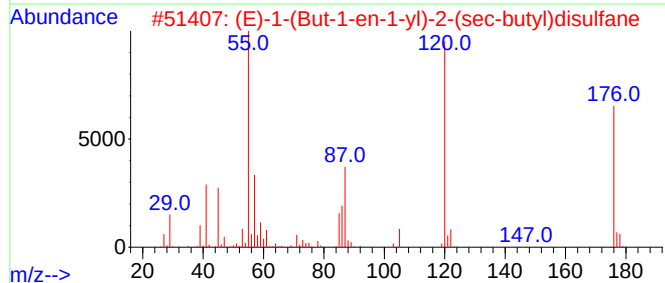
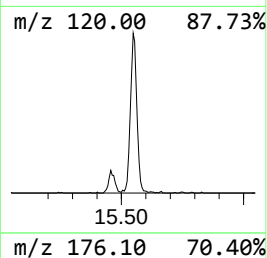
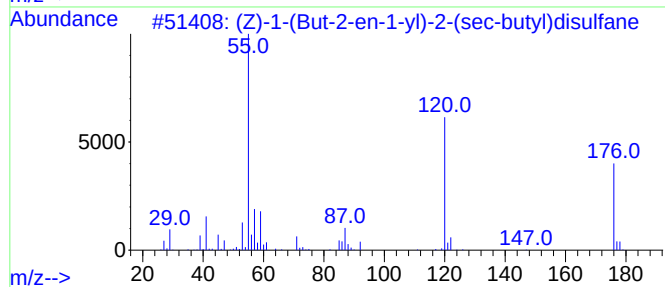
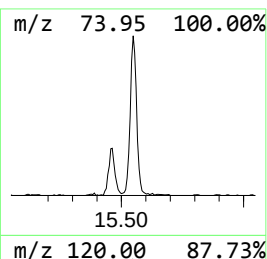
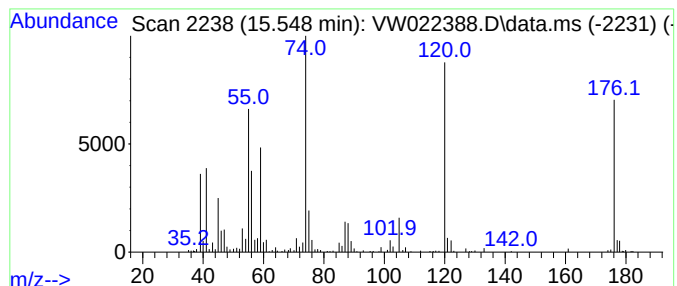
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM040122SMA.M
Quant Title : SFAM01.0

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

Peak Number 6 unknown-02 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.548	14.93 ug/L	213277	1,4-Dichlorobenzene-d4	13.560

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	38		
2	(E)-1-(But-1-en-1-yl)-2-(sec-but...	176	C8H16S2	110690-22-7	27		
3	1,3-Dithiane	120	C4H8S2	000505-23-7	25		
4	(E)-1-Methyl-2-(prop-1-en-1-yl)d...	120	C4H8S2	023838-19-9	16		
5	Allyl mercaptan	74	C3H6S	000870-23-5	14		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW040422\
Data File : VW022388.D
Acq On : 04 Apr 2022 15:52
Operator : SY/VA
Sample : N2179-01RE
Misc : 3.32g/10mL/MSVOA_W/SOIL
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
C0R21RE

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
1,2,4-Triazole,...	15.389	2.7	ug/L	39157	3	13.560	357238	25.0
unknown-01	15.456	3.4	ug/L	48302	3	13.560	357238	25.0
unknown-02	15.548	14.9	ug/L	213277	3	13.560	357238	25.0