

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW040122\
 Data File : VW022378.D
 Acq On : 01 Apr 2022 19:55
 Operator : SY/VA
 Sample : N2179-01
 Misc : 3.72g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 C0R21

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: VW022378.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	81	rVB	141455	220689	18.26%	2.844%
2	3.434	249	251	252	rBV2	1327	891	0.07%	0.011%
3	3.623	280	282	284	rVB3	1188	1065	0.09%	0.014%
4	3.647	284	286	289	rBV3	1112	1582	0.13%	0.020%
5	4.025	338	348	359	rBV3	114708	358147	29.63%	4.615%
6	4.348	399	401	403	rBV2	2024	2151	0.18%	0.028%
7	4.537	430	432	434	rBV3	1087	1008	0.08%	0.013%
8	4.629	443	447	448	rBV4	1189	1215	0.10%	0.016%
9	4.793	472	474	478	rBV4	1547	2453	0.20%	0.032%
10	4.915	486	494	495	rBV7	5646	11234	0.93%	0.145%
11	5.043	512	515	516	rBV3	1009	785	0.06%	0.010%
12	5.397	572	573	577	rBV4	813	783	0.06%	0.010%
13	5.458	582	583	587	rBV4	1645	1386	0.11%	0.018%
14	5.525	592	594	595	rBV2	1456	868	0.07%	0.011%
15	5.568	599	601	602	rBV2	839	783	0.06%	0.010%
16	6.123	690	692	694	rBV3	1377	1176	0.10%	0.015%
17	6.311	722	723	726	rBV3	1167	821	0.07%	0.011%
18	6.403	735	738	740	rBV3	1002	1102	0.09%	0.014%
19	6.476	747	750	751	rBV3	1461	1429	0.12%	0.018%
20	6.519	754	757	759	rBV4	1522	1871	0.15%	0.024%
21	6.574	763	766	767	rBV3	1090	1013	0.08%	0.013%
22	6.616	771	773	775	rBV3	1623	1798	0.15%	0.023%
23	6.671	778	782	785	rBV5	1009	1434	0.12%	0.018%
24	6.793	800	802	804	rBV3	866	775	0.06%	0.010%
25	6.897	817	819	820	rBV2	1323	1310	0.11%	0.017%
26	6.982	832	833	835	rBV2	1619	1180	0.10%	0.015%
27	7.080	841	849	858	rBV2	36641	100336	8.30%	1.293%
28	7.421	903	905	909	rVB5	1864	2301	0.19%	0.030%
29	7.458	909	911	913	rBV3	1302	1157	0.10%	0.015%
30	7.488	913	916	917	rBV3	827	995	0.08%	0.013%
31	7.573	929	930	933	rBV3	1066	1271	0.11%	0.016%
32	7.647	933	942	957	rVB	192555	475450	39.34%	6.126%
33	7.823	969	971	973	rBV3	1066	758	0.06%	0.010%
34	7.890	981	982	986	rVB4	976	844	0.07%	0.011%
35	7.939	986	990	992	rBV4	1723	2278	0.19%	0.029%
36	8.116	1016	1019	1022	rBV5	1526	2128	0.18%	0.027%

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Integrator: RTE

Smoothing : OFF

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Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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

37	8.275	1034	1045	1059	rBV2	405163	1208611	100.00%	15.573%
38	8.842	1130	1138	1147	rVB	290985	573371	47.44%	7.388%
39	9.031	1166	1169	1170	rBV3	1569	1366	0.11%	0.018%
40	9.152	1188	1189	1193	rVB4	1327	1238	0.10%	0.016%
41	9.274	1199	1209	1220	rBV	283677	565956	46.83%	7.292%
42	9.591	1258	1261	1264	rBV5	1076	1437	0.12%	0.019%
43	9.780	1289	1292	1293	rBV3	857	899	0.07%	0.012%
44	9.908	1312	1313	1315	rBV2	1447	1072	0.09%	0.014%
45	9.945	1315	1319	1322	rVB6	2205	2933	0.24%	0.038%
46	10.036	1326	1334	1344	rVB	140798	264860	21.91%	3.413%
47	10.207	1360	1362	1365	rVB4	1453	1759	0.15%	0.023%
48	10.323	1373	1381	1388	rBV	531593	943432	78.06%	12.156%
49	10.384	1388	1391	1398	rVB2	14511	25304	2.09%	0.326%
50	10.494	1405	1409	1414	rVB3	7798	14101	1.17%	0.182%
51	10.579	1416	1423	1430	rBV	96715	167900	13.89%	2.163%
52	10.701	1439	1443	1449	rVB5	5145	8677	0.72%	0.112%
53	10.792	1456	1458	1462	rVB5	1591	1529	0.13%	0.020%
54	10.829	1462	1464	1465	rBV2	984	917	0.08%	0.012%
55	10.920	1472	1479	1487	rBV	166935	279695	23.14%	3.604%
56	11.176	1517	1521	1523	rBV4	1365	1749	0.14%	0.023%
57	11.347	1547	1549	1553	rBV5	1237	1745	0.14%	0.022%
58	11.439	1562	1564	1568	rBV5	1080	1482	0.12%	0.019%
59	11.530	1576	1579	1580	rBV3	912	873	0.07%	0.011%
60	11.561	1583	1584	1588	rBV4	1133	1212	0.10%	0.016%
61	11.628	1588	1595	1603	rBV	390168	660728	54.67%	8.514%
62	11.817	1622	1626	1628	rBV4	2093	3185	0.26%	0.041%
63	11.890	1636	1638	1640	rVB3	1511	1191	0.10%	0.015%
64	12.128	1675	1677	1680	rBV2	1152	1390	0.12%	0.018%
65	12.335	1709	1711	1713	rBV3	1282	1235	0.10%	0.016%
66	12.469	1730	1733	1737	rBV5	1853	2934	0.24%	0.038%
67	12.499	1737	1738	1741	rVB3	1396	926	0.08%	0.012%
68	12.530	1741	1743	1747	rBV5	1375	1697	0.14%	0.022%
69	12.597	1747	1754	1762	rBV4	9752	22319	1.85%	0.288%
70	12.688	1762	1769	1779	rBV	206933	338283	27.99%	4.359%
71	12.792	1784	1786	1790	rVV5	947	755	0.06%	0.010%
72	12.993	1817	1819	1822	rBV3	1736	1853	0.15%	0.024%
73	13.402	1883	1886	1891	rVB6	3198	4764	0.39%	0.061%
74	13.463	1891	1896	1904	rBV4	14563	25108	2.08%	0.324%
75	13.554	1904	1911	1922	rBV	317912	508170	42.05%	6.548%
76	13.853	1953	1960	1973	rVB	298035	510252	42.22%	6.575%

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

77	14.066	1989	1995	2000	rBV2	15099	25347	2.10%	0.327%
78	14.328	2033	2038	2041	rBV5	2510	3698	0.31%	0.048%
79	14.426	2052	2054	2062	rVB9	2623	4188	0.35%	0.054%
80	14.609	2080	2084	2085	rBV3	3189	4293	0.36%	0.055%
81	14.877	2126	2128	2130	rBV3	1659	1522	0.13%	0.020%
82	14.926	2134	2136	2139	rVV4	854	811	0.07%	0.010%
83	14.956	2139	2141	2145	rVB5	1871	1738	0.14%	0.022%
84	14.999	2145	2148	2149	rBV3	1247	1206	0.10%	0.016%
85	15.188	2177	2179	2183	rBV4	1298	1417	0.12%	0.018%
86	15.237	2183	2187	2190	rBV6	1751	2222	0.18%	0.029%
87	15.340	2202	2204	2205	rBV2	1787	1727	0.14%	0.022%
88	15.389	2207	2212	2217	rVV	21638	37485	3.10%	0.483%
89	15.456	2218	2223	2232	rVV3	26954	56935	4.71%	0.734%
90	15.548	2232	2238	2248	rVB	129207	235884	19.52%	3.039%
91	15.688	2259	2261	2265	rVB4	1466	1369	0.11%	0.018%
92	15.761	2272	2273	2274	rBV	1104	783	0.06%	0.010%
93	16.029	2314	2317	2322	rVB6	2027	3121	0.26%	0.040%
94	16.163	2337	2339	2341	rBV2	1673	1885	0.16%	0.024%
95	16.310	2358	2363	2364	rBV5	2087	3407	0.28%	0.044%
96	16.328	2364	2366	2368	rVB3	2045	1379	0.11%	0.018%
97	16.438	2380	2384	2387	rBV6	2144	2843	0.24%	0.037%
98	16.486	2390	2392	2398	rBV6	1229	2078	0.17%	0.027%
99	16.615	2411	2413	2416	rBV4	1429	1240	0.10%	0.016%
100	16.724	2428	2431	2432	rBV3	1037	954	0.08%	0.012%

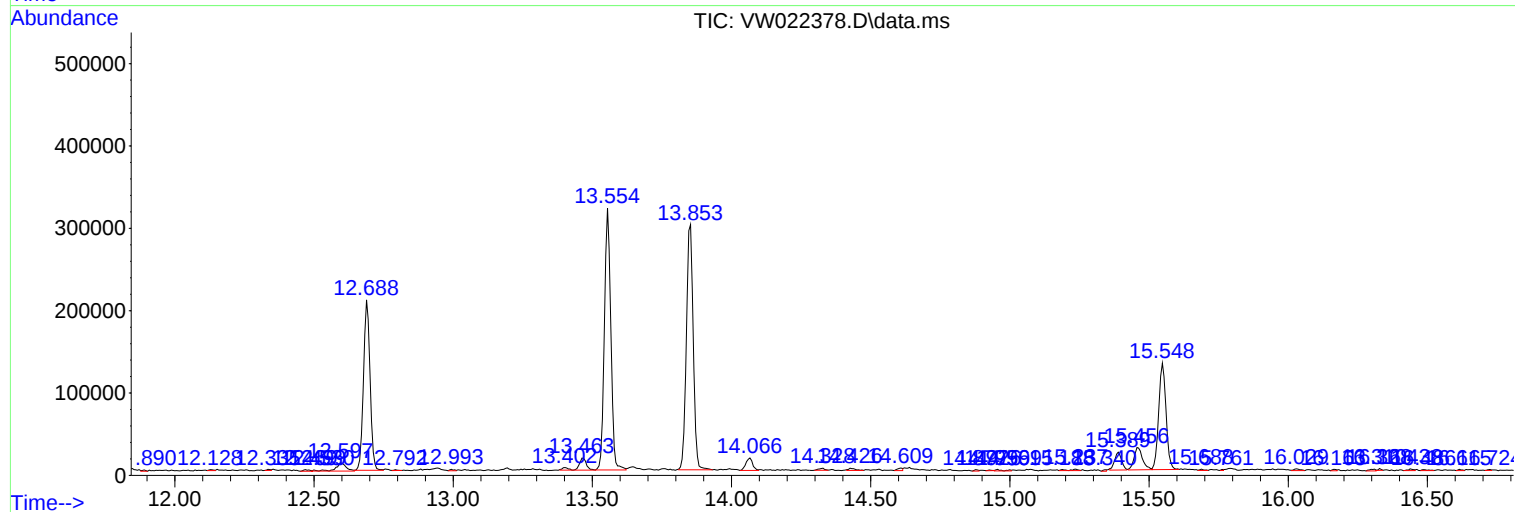
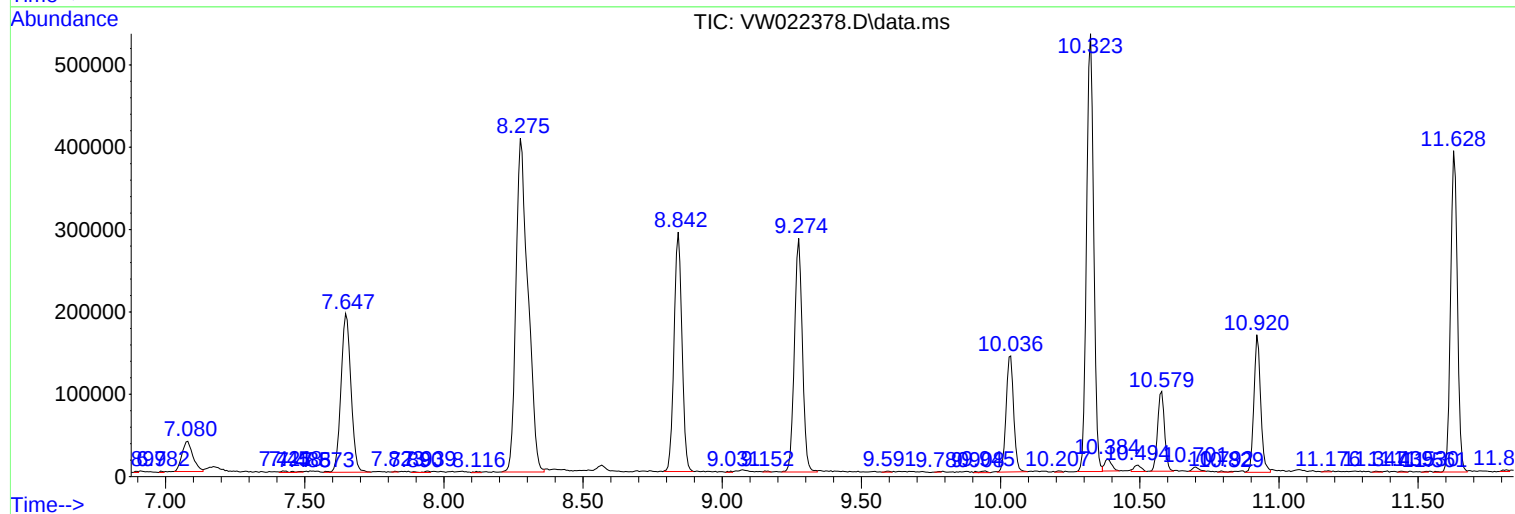
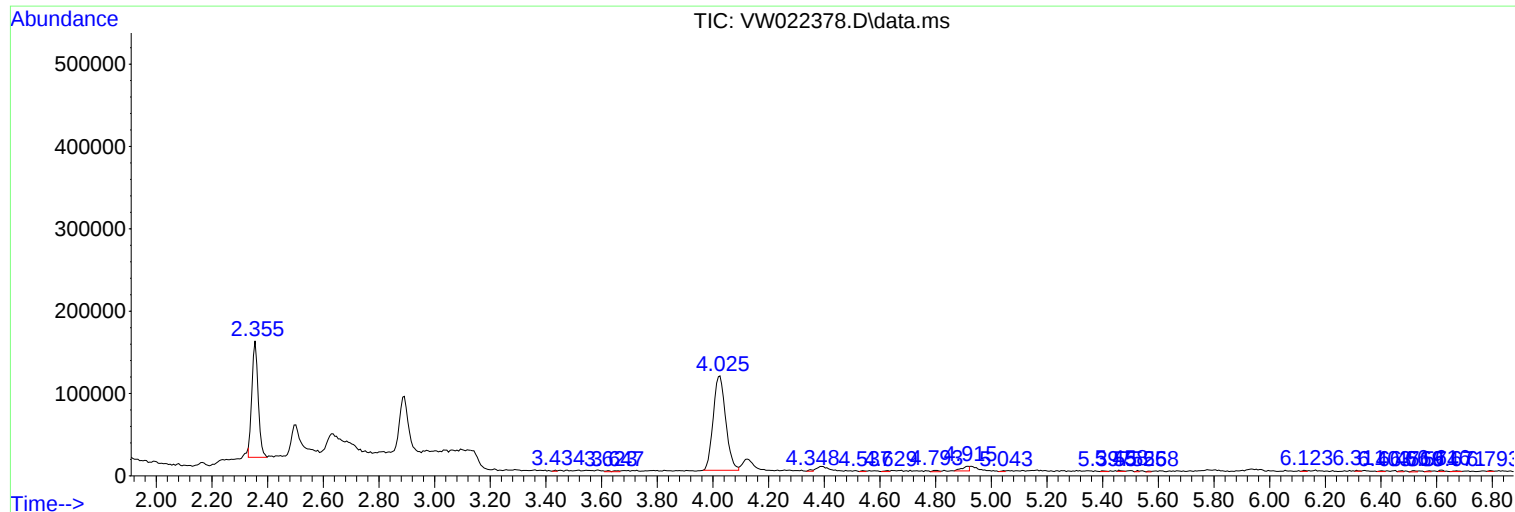
Sum of corrected areas: 7760907

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Instrument :
MSVOA_W
ClientSampleId :
C0R21

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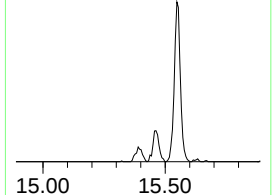
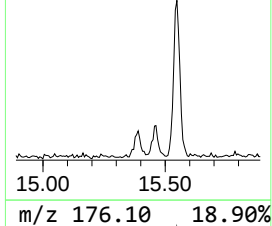
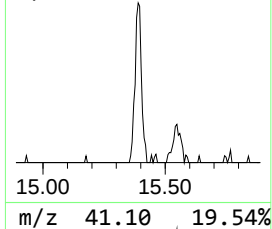
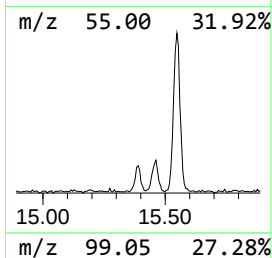
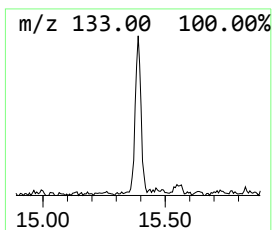
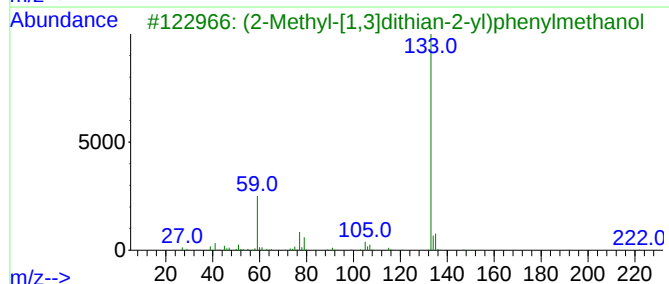
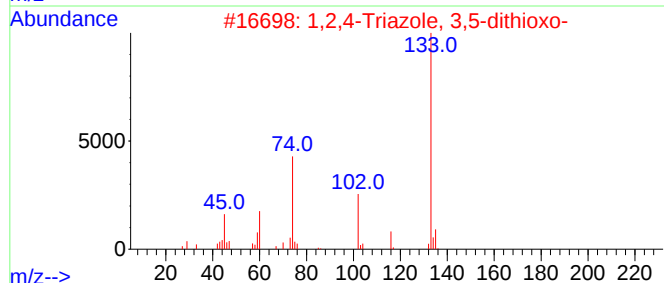
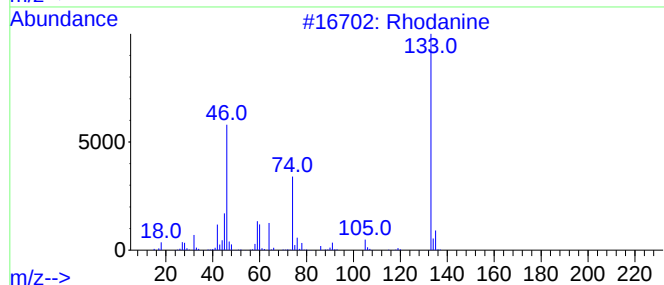
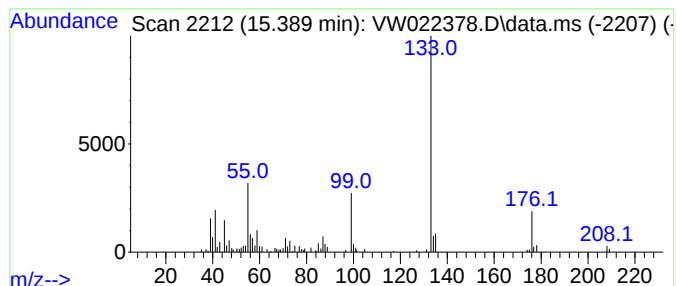
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM040122SMA.M
Quant Title : SFAM01.0

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

Peak Number 2 Rhodanine Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.389	1.84 ug/L	37485	1,4-Dichlorobenzene-d4	13.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Rhodanine	133	C3H3NOS2	000141-84-4	64
2			1,2,4-Triazole, 3,5-dithioxo-	133	C2H3N3S2	005650-03-3	58
3			(2-Methyl-[1,3]dithian-2-yl)phen...	240	C12H16OS2	078349-00-5	53
4			3-Methylthiazolidine-2-thione	133	C4H7NS2	001908-87-8	50
5			l-Alanine, N-(4-ethylbenzoyl)-, ...	263	C15H21NO3	1000314-15-9	50



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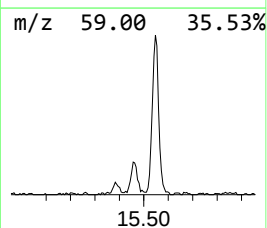
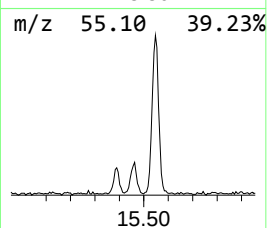
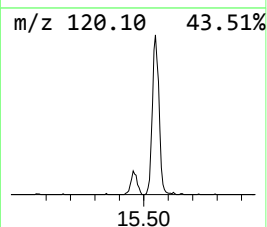
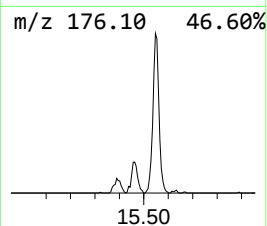
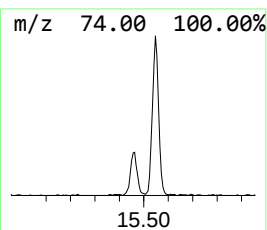
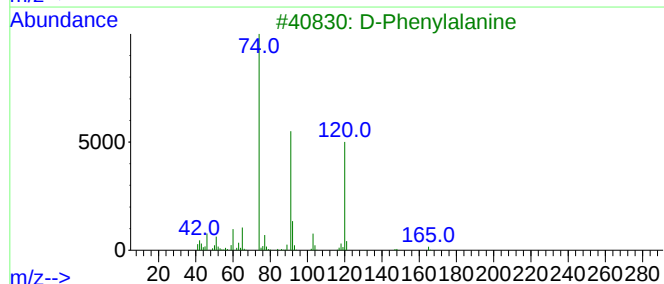
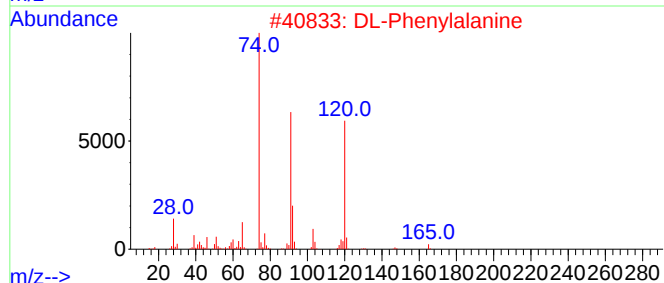
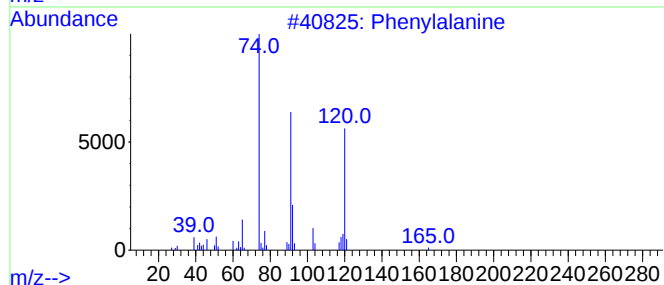
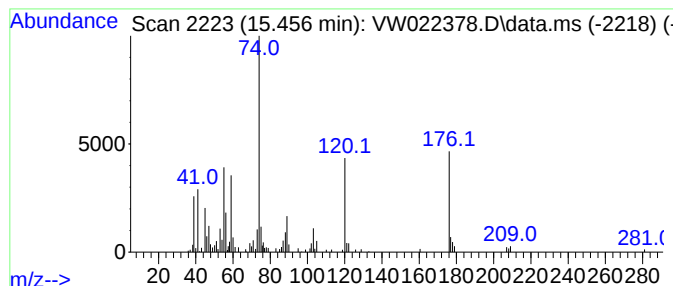
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM040122SMA.M
Quant Title : SFAM01.0

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

Peak Number 3 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.456	2.80 ug/L	56935	1,4-Dichlorobenzene-d4	13.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenylalanine	165	C9H11NO2	000063-91-2	43
2			DL-Phenylalanine	165	C9H11NO2	000150-30-1	43
3			D-Phenylalanine	165	C9H11NO2	000673-06-3	43
4			Thiirane, methyl-	74	C3H6S	001072-43-1	38
5			Phenylalanine	165	C9H11NO2	000063-91-2	37



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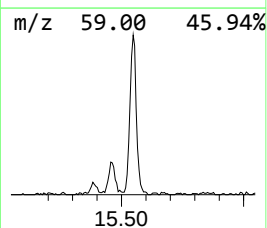
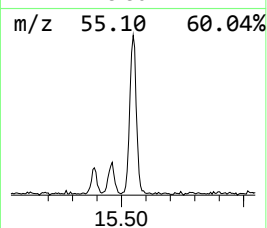
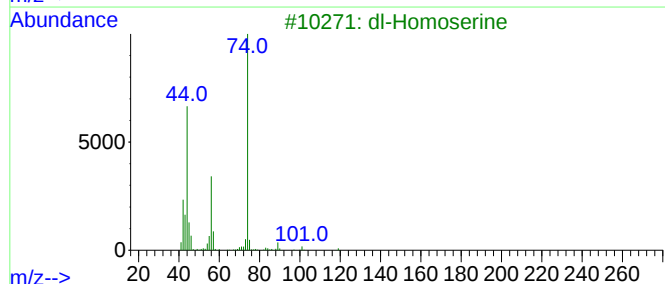
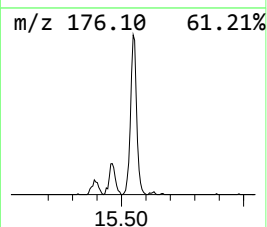
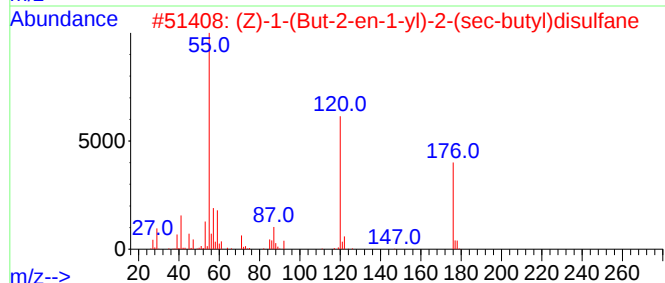
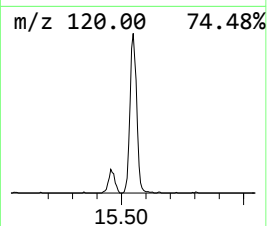
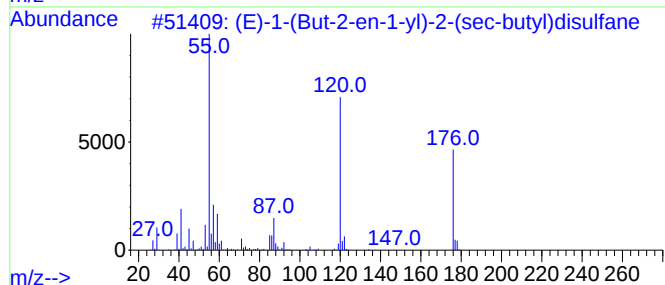
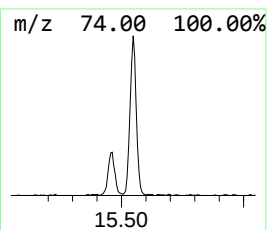
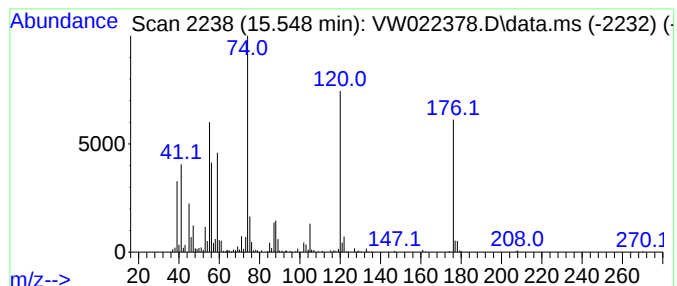
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM040122SMA.M
Quant Title : SFAM01.0

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

Peak Number 4 unknown-02 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.548	11.60 ug/L	235884	1,4-Dichlorobenzene-d4	13.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-1-(But-2-en-1-yl)-2-(sec-but...	176	C8H16S2	110690-24-9	41		
2	(Z)-1-(But-2-en-1-yl)-2-(sec-but...	176	C8H16S2	110690-23-8	41		
3	dl-Homoserine	119	C4H9NO3	001927-25-9	30		
4	(Z)-1-(But-1-en-1-yl)-2-(sec-but...	176	C8H16S2	110690-21-6	27		
5	(E)-1-(But-1-en-1-yl)-2-(sec-but...	176	C8H16S2	110690-22-7	27		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW040122\
Data File : VW022378.D
Acq On : 01 Apr 2022 19:55
Operator : SY/VA
Sample : N2179-01
Misc : 3.72g/10mL/MSVOA_W/SOIL
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
C0R21

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	37485	3	13.554	508170	25.0
unknown-01	15.456	2.8	ug/L	56935	3	13.554	508170	25.0
unknown-02	15.548	11.6	ug/L	235884	3	13.554	508170	25.0