

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW040422\
 Data File : VW022390.D
 Acq On : 04 Apr 2022 16:40
 Operator : SY/VA
 Sample : N2179-04
 Misc : 4.43g/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: VW022390.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	69	74	83	rVB	116687	184151	18.73%	2.748%
2	2.885	157	161	175	rVB	73395	147875	15.04%	2.207%
3	3.757	302	304	308	rVB5	886	1052	0.11%	0.016%
4	3.927	330	332	335	rBV3	688	871	0.09%	0.013%
5	4.019	336	347	358	rBV2	97523	298517	30.37%	4.454%
6	4.336	396	399	400	rBV3	1154	1277	0.13%	0.019%
7	4.476	421	422	428	rVB6	1287	1652	0.17%	0.025%
8	4.531	428	431	434	rBV5	1087	1206	0.12%	0.018%
9	4.629	446	447	452	rVB5	979	763	0.08%	0.011%
10	4.805	474	476	480	rVB5	1392	1119	0.11%	0.017%
11	4.879	485	488	489	rBV3	1788	1854	0.19%	0.028%
12	5.049	513	516	517	rBV2	616	724	0.07%	0.011%
13	5.147	529	532	534	rBV3	1254	1767	0.18%	0.026%
14	5.214	540	543	545	rBV4	1277	1618	0.16%	0.024%
15	5.299	555	557	558	rBV2	870	548	0.06%	0.008%
16	5.372	567	569	570	rBV2	1019	604	0.06%	0.009%
17	5.476	584	586	587	rVB2	942	520	0.05%	0.008%
18	5.726	625	627	630	rBV4	783	790	0.08%	0.012%
19	6.110	688	690	691	rVV2	740	654	0.07%	0.010%
20	6.147	694	696	697	rBV2	850	645	0.07%	0.010%
21	6.323	721	725	726	rBV3	1168	1235	0.13%	0.018%
22	6.451	743	746	749	rBV4	1123	1665	0.17%	0.025%
23	6.476	749	750	753	rBV3	1133	854	0.09%	0.013%
24	6.671	779	782	783	rBV3	937	1039	0.11%	0.016%
25	6.720	789	790	795	rVB4	941	719	0.07%	0.011%
26	6.762	795	797	802	rVB6	755	1047	0.11%	0.016%
27	6.829	806	808	809	rBV	968	720	0.07%	0.011%
28	6.872	813	815	820	rBV5	1312	1956	0.20%	0.029%
29	7.079	841	849	859	rBV	29520	81177	8.26%	1.211%
30	7.378	895	898	899	rBV3	1494	1587	0.16%	0.024%
31	7.470	911	913	916	rBV4	924	911	0.09%	0.014%
32	7.646	933	942	952	rBV	156467	382072	38.86%	5.701%
33	7.805	965	968	969	rBV3	1013	804	0.08%	0.012%
34	7.860	976	977	979	rBV	1106	877	0.09%	0.013%
35	7.939	989	990	995	rVB5	2029	1731	0.18%	0.026%
36	7.982	995	997	999	rBV2	563	628	0.06%	0.009%

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

37	8.000	999	1000	1003	rVB3	1164	986	0.10%	0.015%
38	8.061	1008	1010	1011	rBV2	778	668	0.07%	0.010%
39	8.134	1020	1022	1027	rBV4	633	731	0.07%	0.011%
40	8.177	1027	1029	1031	rVB3	941	753	0.08%	0.011%
41	8.195	1031	1032	1035	rBV3	754	973	0.10%	0.015%
42	8.274	1035	1045	1059	rBV2	318080	983089	100.00%	14.670%
43	8.671	1108	1110	1111	rBV	1081	731	0.07%	0.011%
44	8.841	1128	1138	1147	rBV	265845	514581	52.34%	7.679%
45	8.957	1156	1157	1162	rBV5	926	906	0.09%	0.014%
46	9.012	1162	1166	1168	rBV5	911	1143	0.12%	0.017%
47	9.036	1168	1170	1172	rBV3	962	709	0.07%	0.011%
48	9.073	1172	1176	1178	rBV4	2092	2996	0.30%	0.045%
49	9.170	1189	1192	1193	rBV3	1282	1002	0.10%	0.015%
50	9.219	1198	1200	1201	rBV2	972	770	0.08%	0.011%
51	9.274	1201	1209	1217	rBV	230655	453415	46.12%	6.766%
52	9.542	1251	1253	1256	rVB3	759	593	0.06%	0.009%
53	9.585	1256	1260	1261	rBV4	1134	1291	0.13%	0.019%
54	9.670	1268	1274	1275	rBV5	1322	1993	0.20%	0.030%
55	9.798	1294	1295	1299	rVB3	1056	888	0.09%	0.013%
56	9.975	1320	1324	1326	rBV4	1398	1340	0.14%	0.020%
57	10.036	1326	1334	1343	rVV	122086	222267	22.61%	3.317%
58	10.128	1348	1349	1353	rBV4	993	930	0.09%	0.014%
59	10.195	1358	1360	1365	rVB5	765	1140	0.12%	0.017%
60	10.323	1373	1381	1388	rBV	482762	825700	83.99%	12.321%
61	10.493	1404	1409	1415	rBV5	4059	8719	0.89%	0.130%
62	10.573	1416	1422	1431	rVB	82968	144869	14.74%	2.162%
63	10.701	1439	1443	1448	rBV4	3763	7905	0.80%	0.118%
64	10.786	1455	1457	1463	rVB6	984	1171	0.12%	0.017%
65	10.920	1473	1479	1489	rVV	130938	224081	22.79%	3.344%
66	11.182	1520	1522	1525	rVB3	950	969	0.10%	0.014%
67	11.292	1538	1540	1543	rVB4	937	1124	0.11%	0.017%
68	11.579	1585	1587	1588	rBV2	836	732	0.07%	0.011%
69	11.627	1588	1595	1606	rVV	368863	630849	64.17%	9.414%
70	11.792	1619	1622	1623	rBV3	1319	1153	0.12%	0.017%
71	11.841	1626	1630	1633	rVV6	2279	3653	0.37%	0.055%
72	11.889	1636	1638	1639	rBV2	892	861	0.09%	0.013%
73	11.944	1646	1647	1649	rVB2	1699	1004	0.10%	0.015%
74	11.963	1649	1650	1651	rBV	884	593	0.06%	0.009%
75	12.048	1662	1664	1670	rBV7	957	2268	0.23%	0.034%
76	12.237	1691	1695	1699	rVB5	1205	2030	0.21%	0.030%

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

77	12.280	1699	1702	1703	rBV2	1079	1238	0.13%	0.018%
78	12.389	1718	1720	1721	rBV2	605	581	0.06%	0.009%
79	12.597	1750	1754	1761	rVV3	8357	15744	1.60%	0.235%
80	12.688	1762	1769	1776	rVV	177283	292431	29.75%	4.364%
81	13.164	1843	1847	1848	rBV4	1179	1707	0.17%	0.025%
82	13.182	1848	1850	1854	rVB5	1819	2017	0.21%	0.030%
83	13.401	1880	1886	1889	rBV8	2548	4995	0.51%	0.075%
84	13.554	1903	1911	1918	rBV	324552	512902	52.17%	7.654%
85	13.853	1953	1960	1968	rVB	303644	501749	51.04%	7.487%
86	14.060	1990	1994	2001	rVB	8952	14500	1.47%	0.216%
87	14.426	2052	2054	2056	rBV3	1341	1471	0.15%	0.022%
88	14.706	2098	2100	2102	rBV3	808	617	0.06%	0.009%
89	14.779	2109	2112	2116	rBV4	1354	2078	0.21%	0.031%
90	14.907	2131	2133	2135	rBV4	773	733	0.07%	0.011%
91	14.986	2144	2146	2149	rBV4	760	818	0.08%	0.012%
92	15.096	2162	2164	2167	rVB4	1042	560	0.06%	0.008%
93	15.224	2183	2185	2187	rBV3	636	814	0.08%	0.012%
94	15.249	2187	2189	2191	rVV3	1427	1185	0.12%	0.018%
95	15.389	2208	2212	2217	rVB2	9691	16824	1.71%	0.251%
96	15.462	2217	2224	2232	rBV4	13831	28663	2.92%	0.428%
97	15.547	2232	2238	2246	rBV2	61381	117580	11.96%	1.755%
98	15.852	2286	2288	2293	rBV5	1092	1166	0.12%	0.017%
99	16.322	2362	2365	2367	rBV4	1100	1319	0.13%	0.020%
100	16.541	2400	2401	2404	rBV3	857	988	0.10%	0.015%

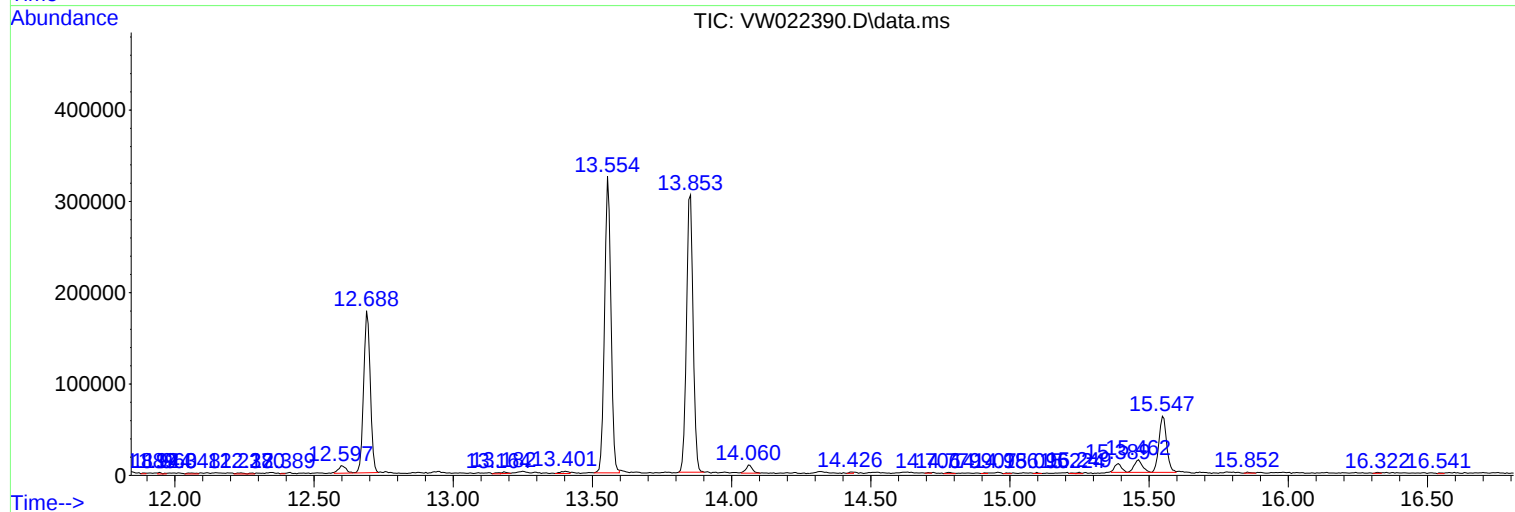
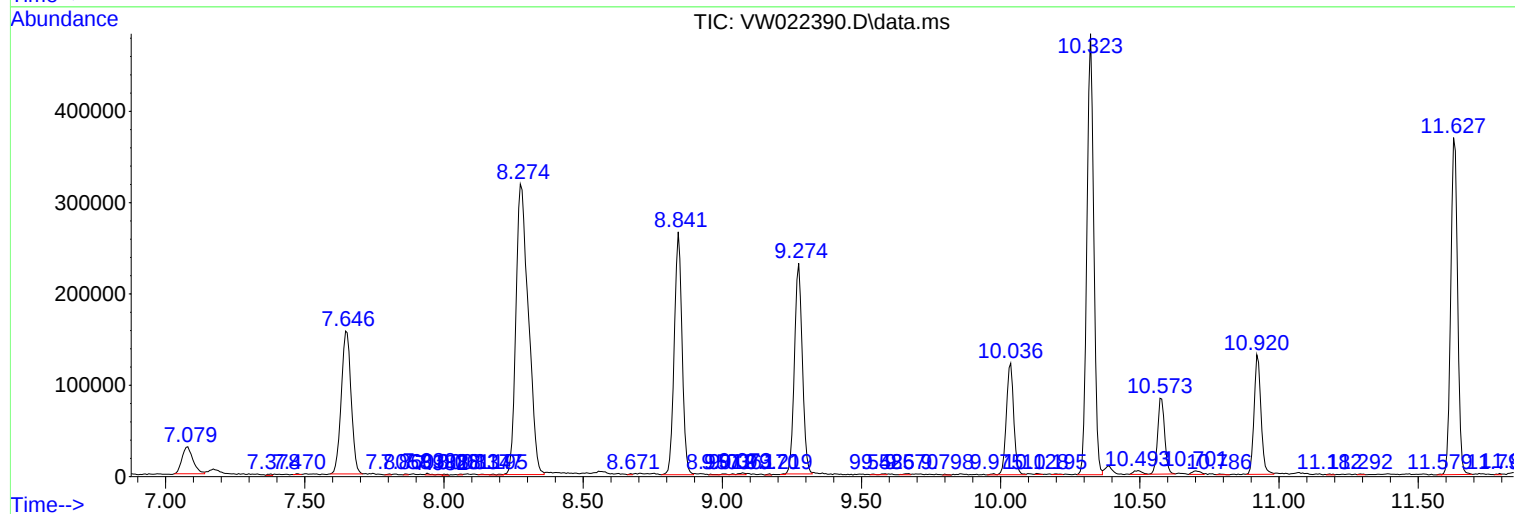
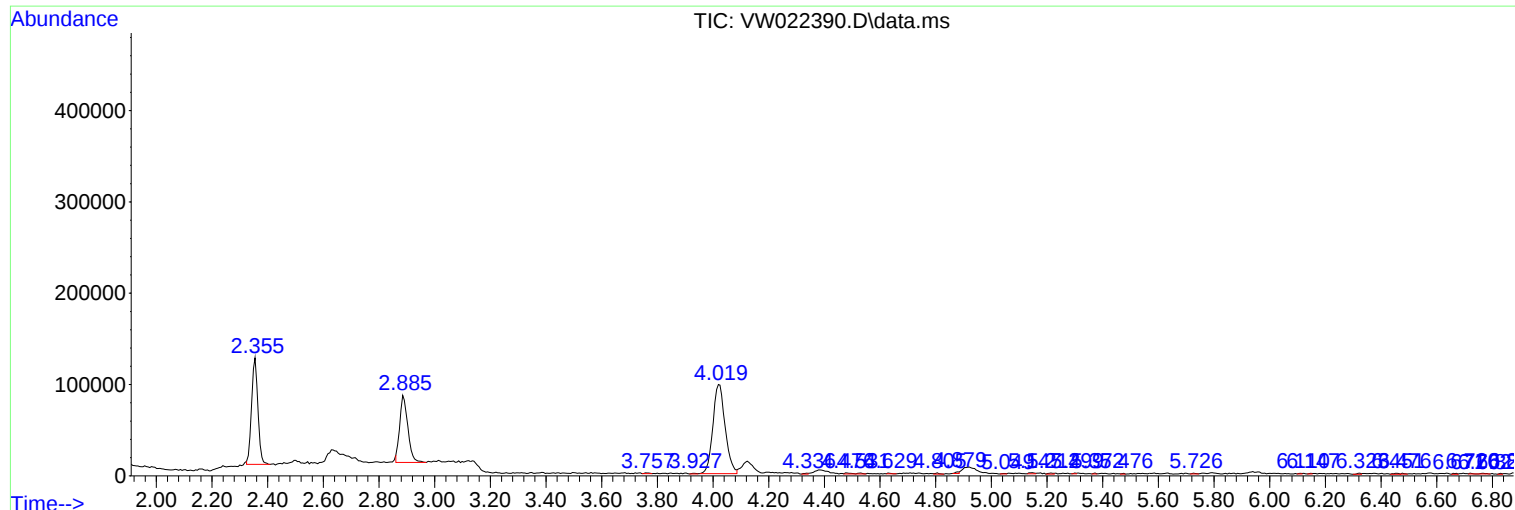
Sum of corrected areas: 6701485

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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



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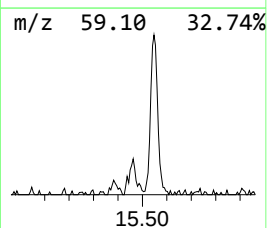
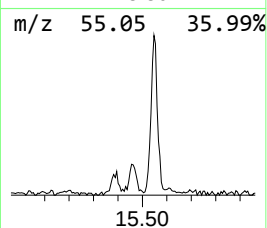
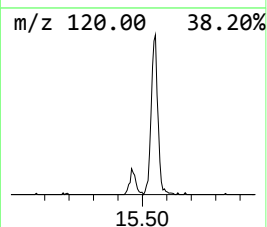
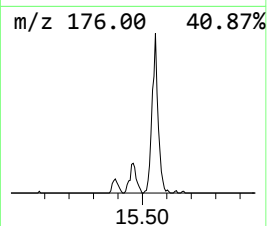
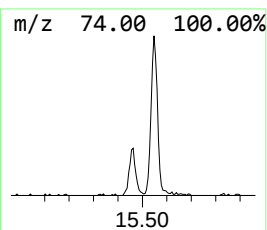
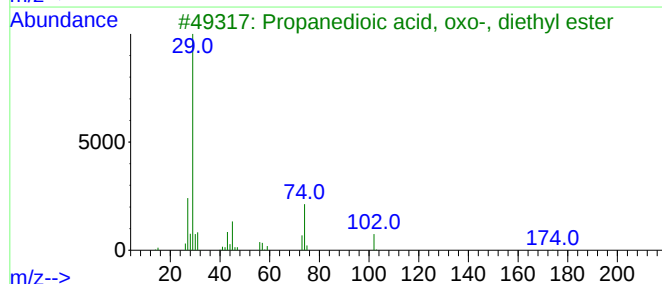
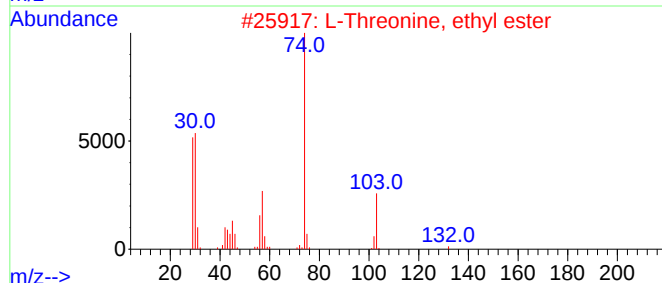
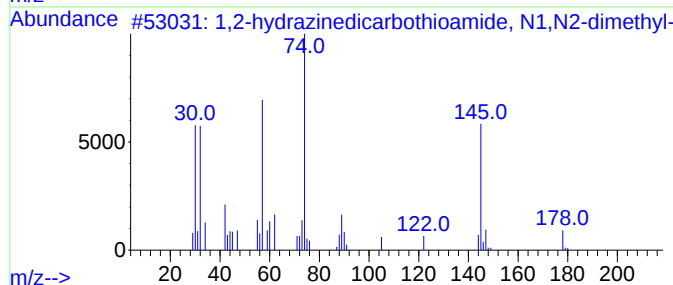
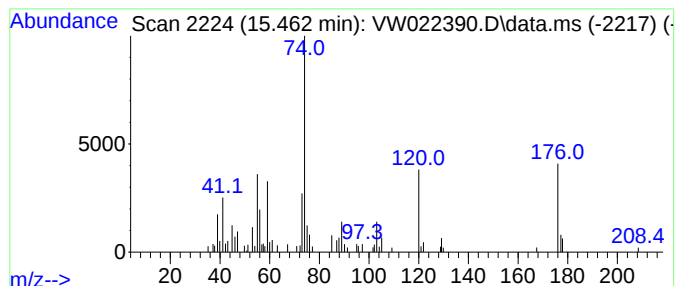
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM040122SMA.M
Quant Title : SFAM01.0

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

Peak Number 2 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.462	1.40 ug/L	28663	1,4-Dichlorobenzene-d4	13.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-hydrazinedicarbothioamide, N...	178	C4H10N4S2	1000404-79-0	35
2			L-Threonine, ethyl ester	147	C6H13NO3	023926-51-4	27
3			Propanedioic acid, oxo-, diethyl...	174	C7H10O5	000609-09-6	23
4			Pentanoic acid, 3-methyl-, methy...	130	C7H14O2	002177-78-8	22
5			Pentanoic acid, 3-hydroxy-2-meth...	174	C9H18O3	1000151-17-3	17



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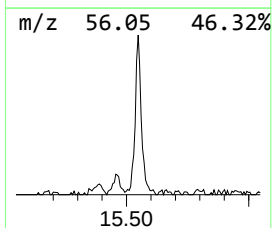
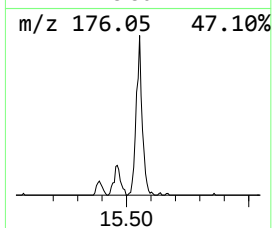
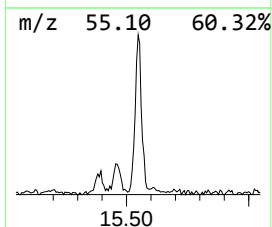
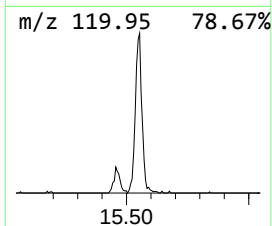
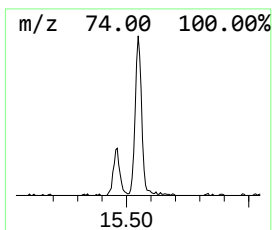
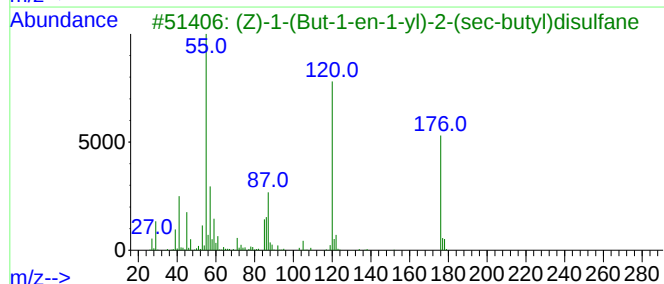
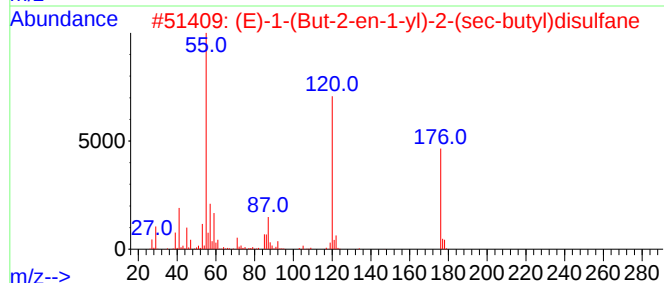
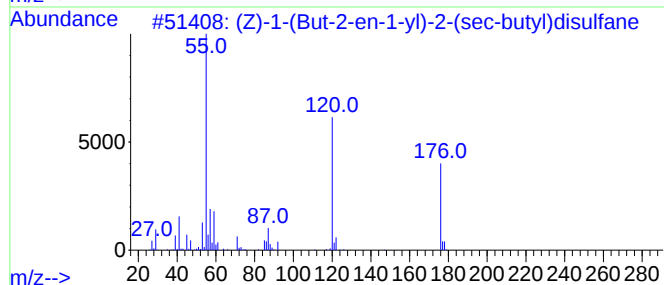
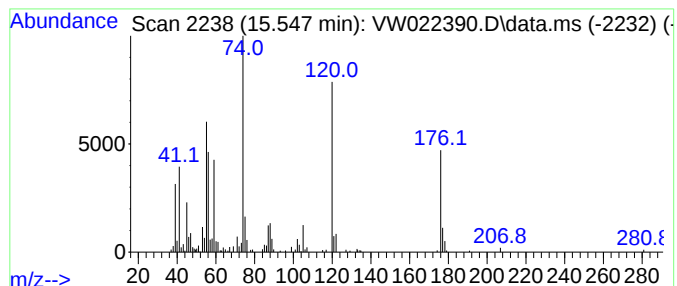
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM040122SMA.M
Quant Title : SFAM01.0

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

Peak Number 3 unknown-02 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.547	5.73 ug/L	117580	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	43		
2	(E)-1-(But-2-en-1-yl)-2-(sec-but...	176	C8H16S2	110690-24-9	38		
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	1,3,5-Trithiane, 2,2,4,4,6-hex...	222	C9H18S3	000828-26-2	27		



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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
unknown-01	15.462	1.4	ug/L	28663	3	13.554	512902	25.0
unknown-02	15.547	5.7	ug/L	117580	3	13.554	512902	25.0