

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW082523\
 Data File : VW026921.D
 Acq On : 26 Aug 2023 02:40
 Operator : SY/MD
 Sample : 04175-09
 Misc : 5.76g/10mL/MSVOA_W/SOIL
 ALS Vial : 42 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 EZYK3

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\SFAMWLM081023SMA.M
 Title : SFAM01.0

Signal : TIC: VW026921.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.967	11	13	18	rVB6	2423	3271	0.20%	0.025%
2	2.156	41	44	45	rBV3	2695	2397	0.15%	0.019%
3	2.235	50	57	58	rBV7	7127	14705	0.89%	0.114%
4	2.314	66	70	72	rBV4	6705	10227	0.62%	0.080%
5	2.363	72	78	92	rVB	37982	118331	7.16%	0.921%
6	2.619	118	120	121	rBV2	4065	3574	0.22%	0.028%
7	2.668	124	128	133	rVB8	4183	8847	0.54%	0.069%
8	2.893	159	165	178	rBV	47619	130869	7.92%	1.018%
9	3.113	197	201	202	rBV4	2945	4109	0.25%	0.032%
10	3.387	241	246	254	rVB7	4019	8995	0.54%	0.070%
11	3.771	307	309	312	rVB4	2274	2130	0.13%	0.017%
12	4.021	340	350	363	rBV2	98987	374219	22.65%	2.912%
13	4.161	372	373	378	rVB5	2356	3026	0.18%	0.024%
14	4.314	394	398	400	rBV5	1783	2594	0.16%	0.020%
15	4.399	400	412	426	rVV	68752	237841	14.39%	1.851%
16	4.923	487	498	518	rBV3	24454	120790	7.31%	0.940%
17	5.100	522	527	531	rBV7	1601	2702	0.16%	0.021%
18	5.387	570	574	576	rBV5	2281	3474	0.21%	0.027%
19	5.429	576	581	583	rBV5	5379	9427	0.57%	0.073%
20	5.576	601	605	608	rBV6	2410	4200	0.25%	0.033%
21	5.941	656	665	673	rVV7	8366	24980	1.51%	0.194%
22	6.386	734	738	742	rBV7	1352	2701	0.16%	0.021%
23	6.722	788	793	795	rBV5	2124	3533	0.21%	0.027%
24	6.801	802	806	807	rBV4	1937	2222	0.13%	0.017%
25	6.868	814	817	823	rVB8	1726	2697	0.16%	0.021%
26	6.978	829	835	838	rBV8	2754	5441	0.33%	0.042%
27	7.088	843	853	870	rVV5	46064	196024	11.86%	1.525%
28	7.374	896	900	903	rBV6	2154	3639	0.22%	0.028%
29	7.557	927	930	933	rVB5	1714	2210	0.13%	0.017%
30	7.587	933	935	938	rBV4	1650	2272	0.14%	0.018%
31	7.673	938	949	960	rVB	300323	751406	45.47%	5.847%
32	7.911	985	988	989	rBV3	5449	5261	0.32%	0.041%
33	8.026	1002	1007	1009	rBV5	3086	5410	0.33%	0.042%
34	8.161	1023	1029	1034	rVV4	12315	27079	1.64%	0.211%
35	8.276	1037	1048	1062	rVV2	526599	1652443	100.00%	12.857%
36	8.423	1069	1072	1081	rVB2	4068	9990	0.60%	0.078%

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM081023SMA.M
 Title : SFAM01.0

37	8.508	1081	1086	1089	rBV7	3002	4216	0.26%	0.033%
38	8.569	1089	1096	1098	rBV8	4710	6962	0.42%	0.054%
39	8.697	1110	1117	1118	rBV6	5372	8219	0.50%	0.064%
40	8.746	1120	1125	1133	rVB2	27220	56508	3.42%	0.440%
41	8.843	1133	1141	1151	rBV	522672	1030195	62.34%	8.016%
42	9.081	1170	1180	1190	rBV3	339358	797982	48.29%	6.209%
43	9.276	1202	1212	1219	rBV	408528	863076	52.23%	6.715%
44	9.337	1219	1222	1228	rVB3	22858	36148	2.19%	0.281%
45	9.496	1246	1248	1249	rBV2	2197	2134	0.13%	0.017%
46	9.605	1263	1266	1271	rVB7	5722	9534	0.58%	0.074%
47	9.654	1271	1274	1277	rBV5	3115	4779	0.29%	0.037%
48	9.752	1285	1290	1295	rVB9	6564	13820	0.84%	0.108%
49	9.800	1295	1298	1303	rVB7	1117	2198	0.13%	0.017%
50	9.855	1305	1307	1309	rBV3	1825	2210	0.13%	0.017%
51	9.892	1310	1313	1318	rVB6	4167	5393	0.33%	0.042%
52	9.959	1318	1324	1327	rBV7	7986	15238	0.92%	0.119%
53	10.032	1331	1336	1343	rBV	98548	176455	10.68%	1.373%
54	10.215	1364	1366	1369	rVB4	2337	2394	0.14%	0.019%
55	10.325	1376	1384	1393	rBV	676596	1214000	73.47%	9.446%
56	10.502	1407	1413	1419	rBV8	7766	16499	1.00%	0.128%
57	10.575	1419	1425	1432	rVV	96855	170783	10.34%	1.329%
58	10.666	1435	1440	1443	rVV6	7474	14265	0.86%	0.111%
59	10.697	1443	1445	1451	rVB3	6920	11057	0.67%	0.086%
60	10.758	1451	1455	1460	rBV6	3948	8388	0.51%	0.065%
61	10.843	1466	1469	1476	rBV9	2252	4007	0.24%	0.031%
62	10.928	1476	1483	1494	rBV4	139592	306166	18.53%	2.382%
63	11.172	1521	1523	1528	rVB6	5181	7205	0.44%	0.056%
64	11.227	1528	1532	1538	rBV7	9592	18285	1.11%	0.142%
65	11.629	1590	1598	1607	rBV	747930	1248265	75.54%	9.712%
66	11.800	1623	1626	1628	rBV4	2949	4647	0.28%	0.036%
67	11.837	1628	1632	1635	rVV5	6058	11403	0.69%	0.089%
68	12.099	1673	1675	1677	rBV3	2677	3033	0.18%	0.024%
69	12.166	1683	1686	1691	rVB5	7183	11355	0.69%	0.088%
70	12.288	1704	1706	1708	rBV3	2754	3027	0.18%	0.024%
71	12.459	1732	1734	1740	rVB6	4277	6896	0.42%	0.054%
72	12.568	1750	1752	1753	rBV2	3858	3196	0.19%	0.025%
73	12.599	1753	1757	1765	rVB5	18849	41599	2.52%	0.324%
74	12.702	1770	1774	1775	rBV4	2345	3739	0.23%	0.029%
75	12.751	1778	1782	1785	rBV6	4496	8674	0.52%	0.067%
76	12.861	1797	1800	1803	rBV2	7946	8436	0.51%	0.066%

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 Title : SFAM01.0

77	12.940	1809	1813	1818	rVB	15577	22609	1.37%	0.176%
78	13.099	1836	1839	1842	rVB2	7417	9350	0.57%	0.073%
79	13.245	1858	1863	1871	rBV2	24461	48042	2.91%	0.374%
80	13.397	1886	1888	1889	rBV2	3716	2809	0.17%	0.022%
81	13.556	1907	1914	1925	rBV	694442	1144641	69.27%	8.906%
82	13.647	1927	1929	1931	rVV3	3984	4047	0.24%	0.031%
83	13.745	1943	1945	1949	rBV5	5360	4528	0.27%	0.035%
84	13.849	1956	1962	1971	rVB	578673	939294	56.84%	7.308%
85	14.001	1985	1987	1988	rBV2	4655	3476	0.21%	0.027%
86	14.196	2016	2019	2026	rVB7	10023	17682	1.07%	0.138%
87	14.324	2036	2040	2044	rBV7	13449	24765	1.50%	0.193%
88	14.422	2052	2056	2058	rBV5	5313	6397	0.39%	0.050%
89	14.458	2058	2062	2065	rVB3	6333	10698	0.65%	0.083%
90	14.678	2096	2098	2099	rBV2	3943	2589	0.16%	0.020%
91	14.787	2109	2116	2125	rBV3	17349	48318	2.92%	0.376%
92	14.952	2141	2143	2150	rVB8	7929	11760	0.71%	0.092%
93	15.171	2174	2179	2183	rBV8	5374	12321	0.75%	0.096%
94	15.385	2207	2214	2220	rBV4	26161	62703	3.79%	0.488%
95	15.458	2220	2226	2234	rVB3	82653	159325	9.64%	1.240%
96	15.549	2234	2241	2249	rBV2	164561	309479	18.73%	2.408%
97	16.031	2316	2320	2324	rVB7	7205	12479	0.76%	0.097%
98	16.379	2369	2377	2381	rBV10	12261	34701	2.10%	0.270%
99	16.580	2408	2410	2412	rBV3	2547	2797	0.17%	0.022%
100	16.635	2414	2419	2426	rVV3	13207	31971	1.93%	0.249%

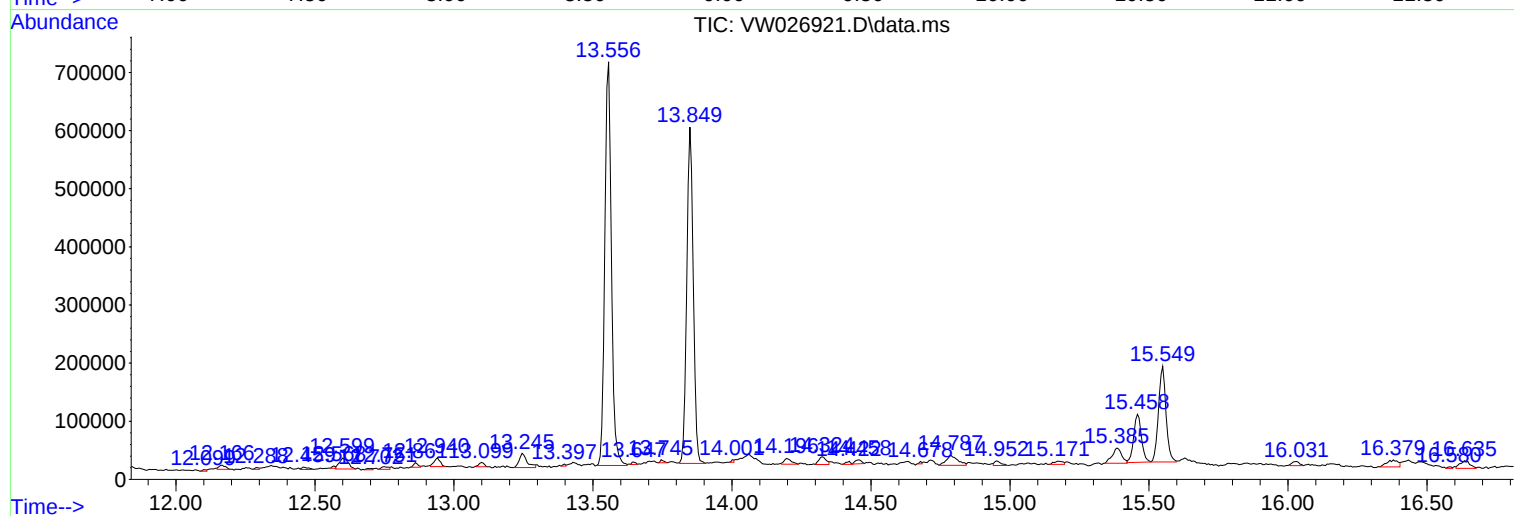
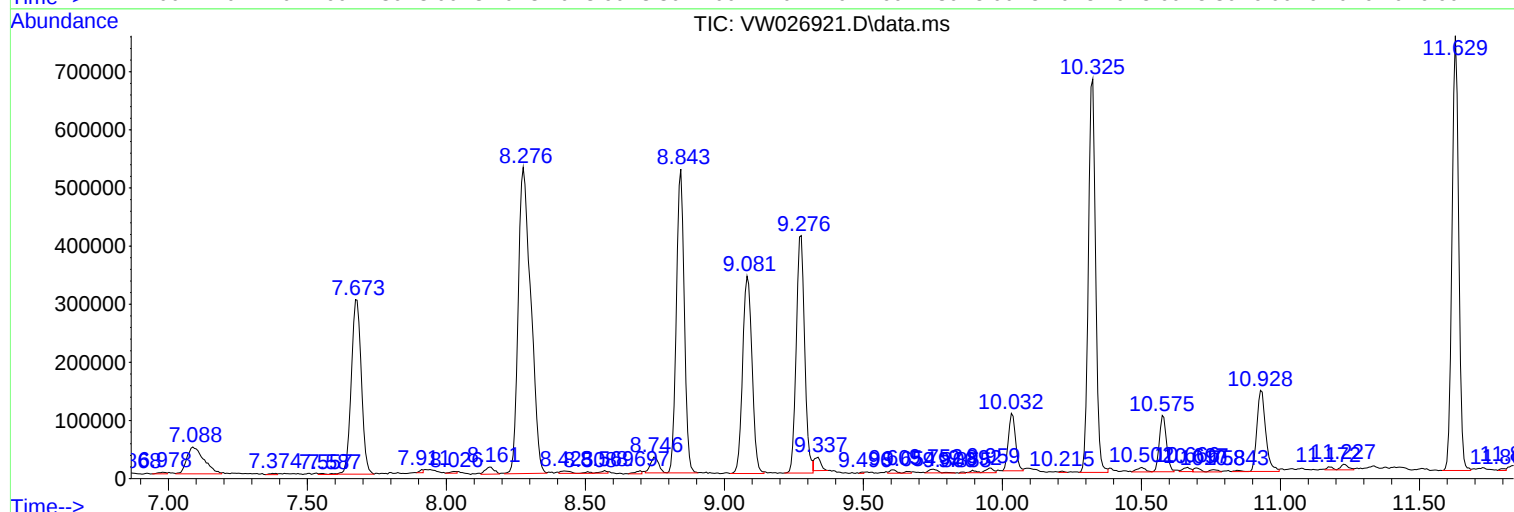
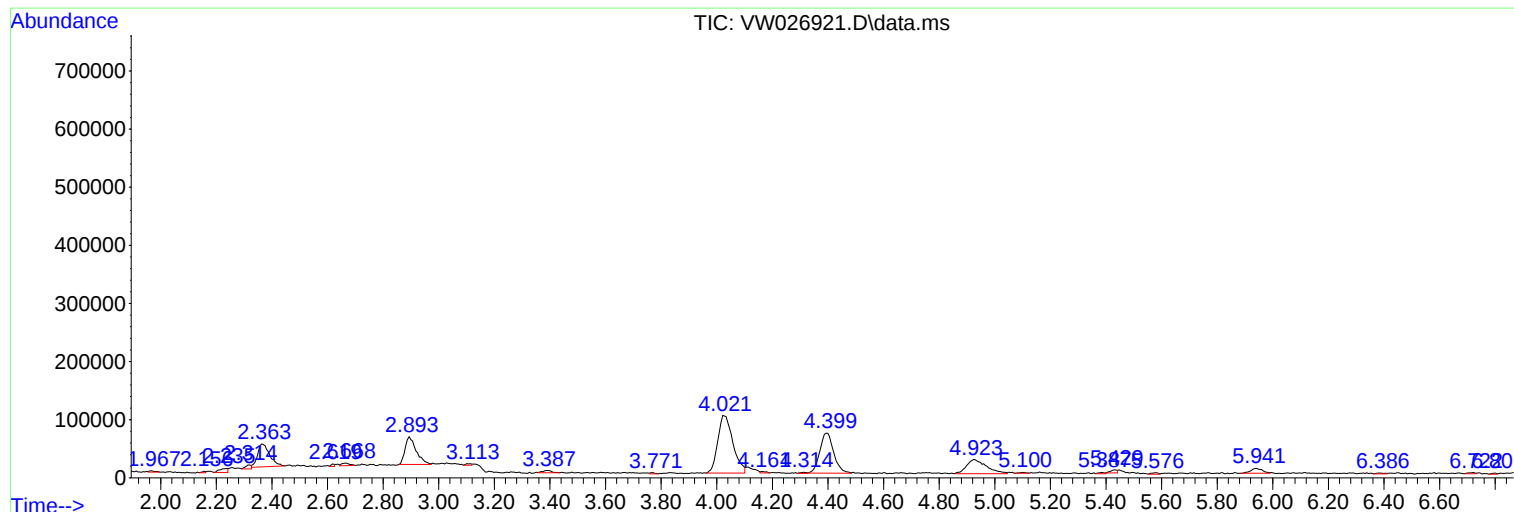
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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM081023SMA.M
Quant Title : SFAM01.0

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



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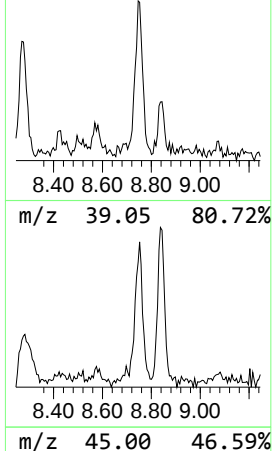
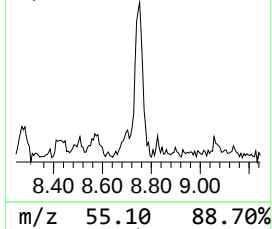
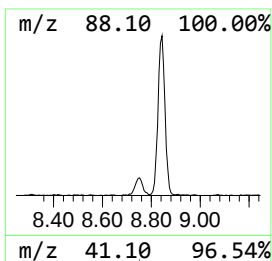
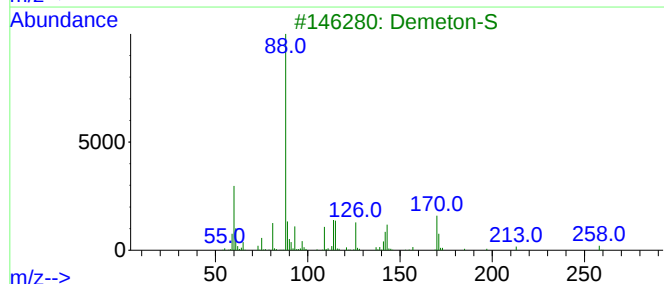
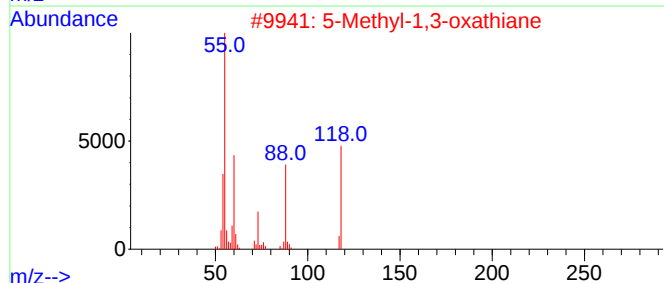
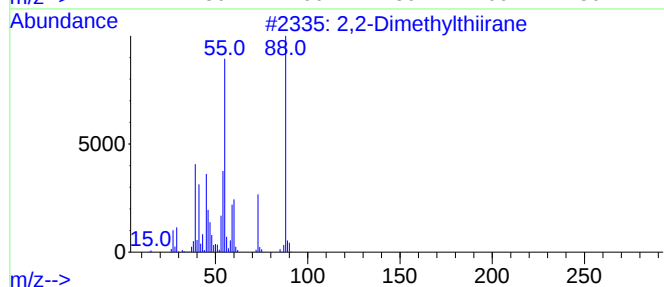
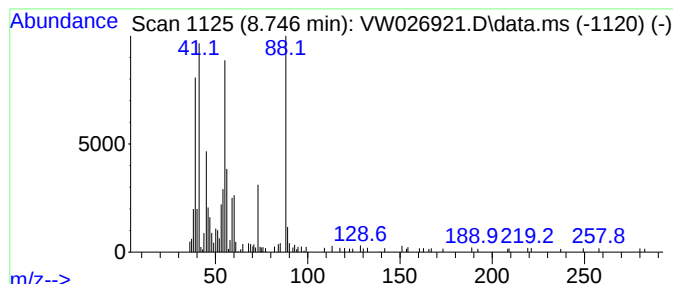
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM081023SMA.M
Quant Title : SFAM01.0

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

Peak Number 1 2,2-Dimethylthiirane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.746	1.37 ug/L	56508	1,4-Difluorobenzene	8.843

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,2-Dimethylthiirane	88	C4H8S	003772-13-2	60
2			5-Methyl-1,3-oxathiane	118	C5H10OS	058175-24-9	47
3			Demeton-S	258	C8H19O3PS2	000126-75-0	43
4			Methyl 6-O-acetyl-2,3,4-tri-O-me...	278	C12H22O7	072922-16-8	35
5			1,2,5-Oxadiazol-3-amine, N-methy...	160	C3H4N4O4	337311-85-0	33



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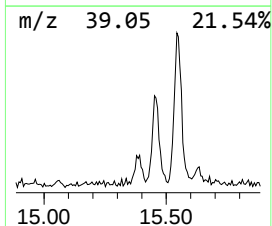
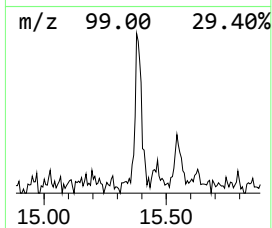
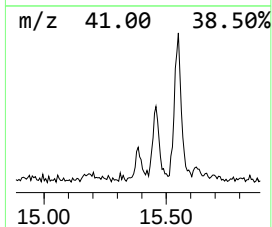
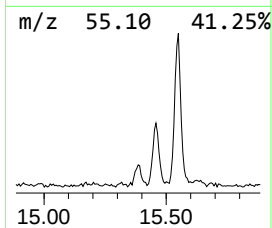
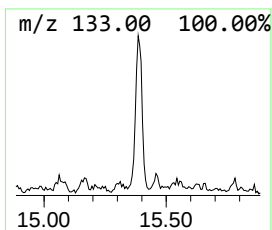
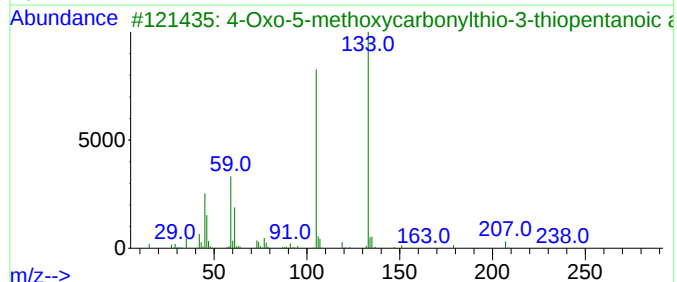
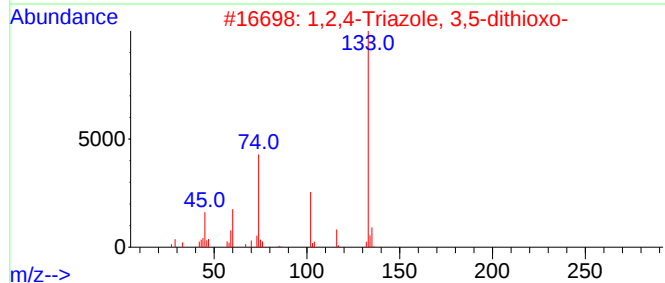
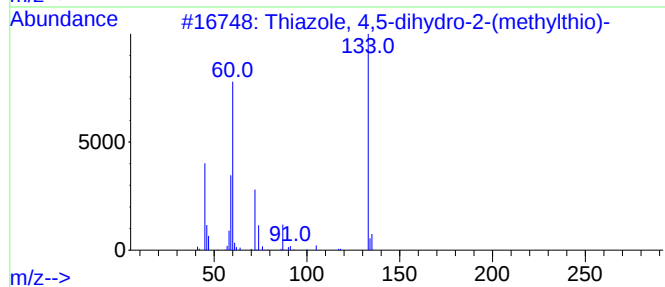
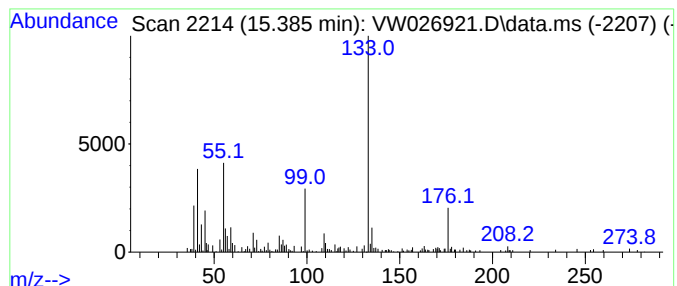
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM081023SMA.M
Quant Title : SFAM01.0

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

Peak Number 3 Thiazole, 4,5-dihydro-2-(me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.385	1.37 ug/L	62703	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiazole, 4,5-dihydro-2-(methylt...	133	C4H7NS2	019975-56-5	53
2			1,2,4-Triazole, 3,5-dithioxo-	133	C2H3N3S2	005650-03-3	53
3			4-Oxo-5-methoxycarbonylthio-3-th...	238	C7H10O5S2	1000454-99-9	53
4			Rhodanine	133	C3H3NOS2	000141-84-4	42
5			3-Methylthiazolidine-2-thione	133	C4H7NS2	001908-87-8	40



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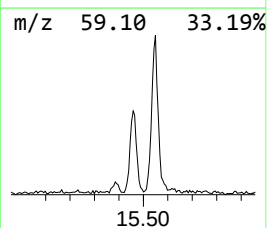
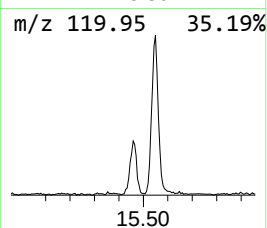
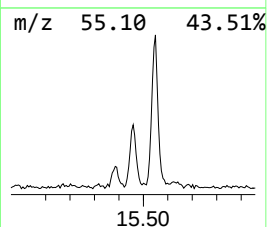
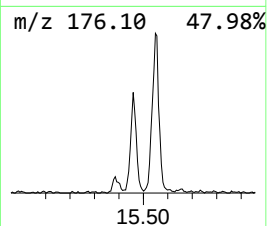
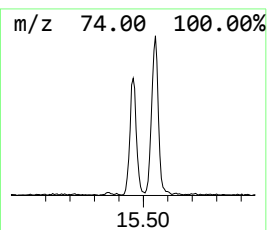
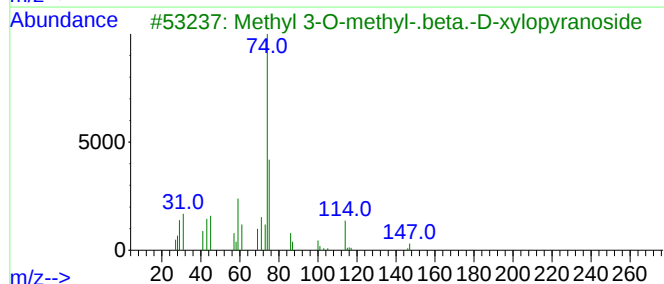
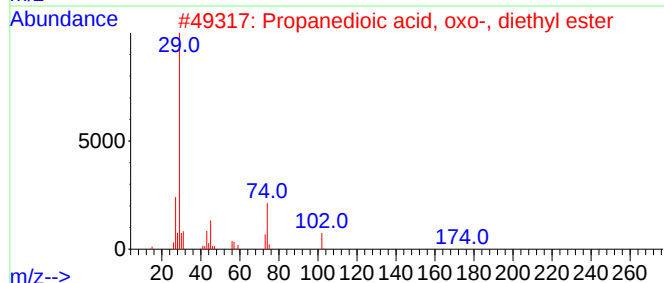
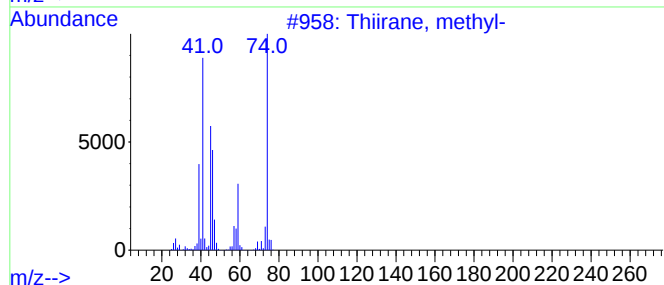
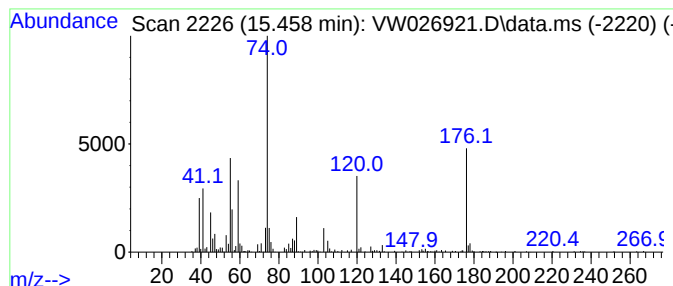
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Quant Title : SFAM01.0

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.
15.458	3.48 ug/L	159325	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiirane, methyl-	74	C3H6S	001072-43-1	38
2			Propanedioic acid, oxo-, diethyl...	174	C7H10O5	000609-09-6	23
3			Methyl 3-O-methyl-.beta.-D-xylop...	178	C7H14O5	007381-10-4	23
4			D-Phenylalanine	165	C9H11NO2	000673-06-3	23
5			Thiirane, methyl-	74	C3H6S	001072-43-1	17



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW082523\
Data File : VW026921.D
Acq On : 26 Aug 2023 02:40
Operator : SY/MD
Sample : 04175-09
Misc : 5.76g/10mL/MSVOA_W/SOIL
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
EZYK3

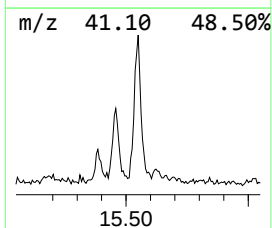
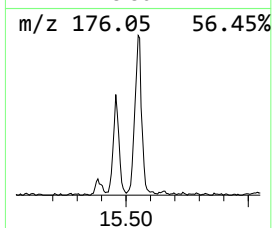
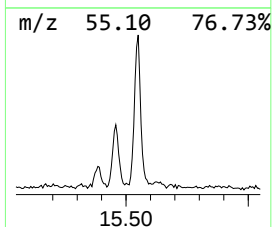
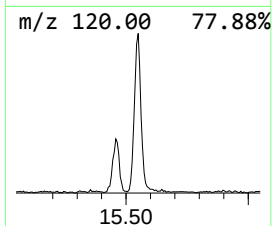
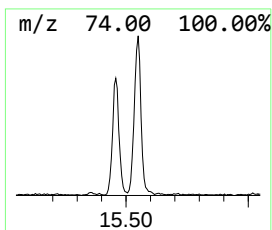
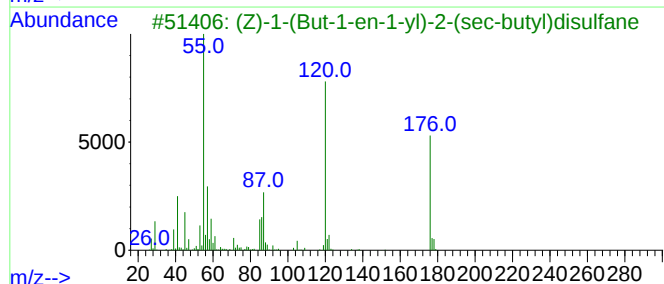
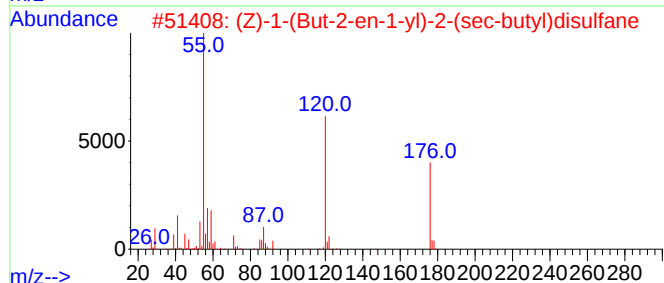
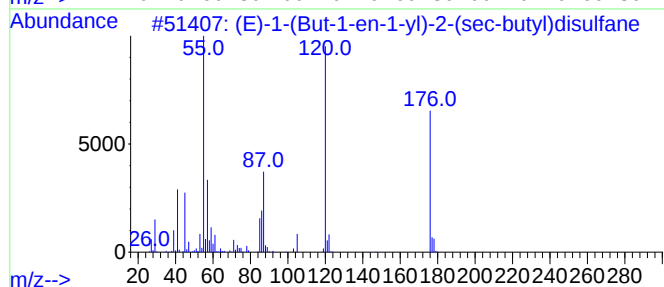
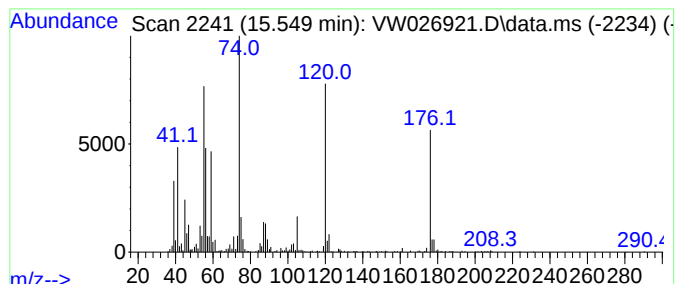
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Quant Title : SFAM01.0

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.
15.549	6.76 ug/L	309479	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-1-(But-1-en-1-yl)-2-(sec-but...	176	C8H16S2	110690-22-7	41		
2	(Z)-1-(But-2-en-1-yl)-2-(sec-but...	176	C8H16S2	110690-23-8	41		
3	(Z)-1-(But-1-en-1-yl)-2-(sec-but...	176	C8H16S2	110690-21-6	38		
4	(E)-1-(But-2-en-1-yl)-2-(sec-but...	176	C8H16S2	110690-24-9	38		
5	1,3-Dithiane	120	C4H8S2	000505-23-7	35		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW082523\
Data File : VW026921.D
Acq On : 26 Aug 2023 02:40
Operator : SY/MD
Sample : 04175-09
Misc : 5.76g/10mL/MSVOA_W/SOIL
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
EZYK3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM081023SMA.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
2,2-Dimethylthi...	8.746	1.4	ug/L	56508	1	8.843	1030200	25.0
Thiazole, 4,5-d...	15.385	1.4	ug/L	62703	3	13.556	1144640	25.0
unknown-01	15.458	3.5	ug/L	159325	3	13.556	1144640	25.0
unknown-02	15.549	6.8	ug/L	309479	3	13.556	1144640	25.0