

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW052424\
 Data File : VW028727.D
 Acq On : 24 May 2024 12:38
 Operator : SY/MD
 Sample : P2569-22
 Misc : 4.28g/10mL/MSVOA_W/SOIL/A
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 BH6A8

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\SFAMWLM050224SMA.M
 Title : SFAM01.0

Signal : TIC: VW028727.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.478	259	261	263	rBV3	926	992	0.54%	0.075%
2	3.533	264	270	281	rVB2	17601	43057	23.63%	3.273%
3	3.710	297	299	301	rBV3	651	504	0.28%	0.038%
4	3.905	330	331	336	rVB5	945	762	0.42%	0.058%
5	4.027	344	351	363	rVB2	13542	36561	20.06%	2.779%
6	4.216	376	382	394	rVB2	13135	37043	20.33%	2.816%
7	4.515	427	431	432	rBV3	805	1064	0.58%	0.081%
8	4.600	443	445	448	rBV4	537	643	0.35%	0.049%
9	5.070	520	522	525	rVB3	875	716	0.39%	0.054%
10	5.234	547	549	552	rBV4	671	608	0.33%	0.046%
11	5.313	560	562	564	rBV3	787	733	0.40%	0.056%
12	5.435	578	582	584	rBV3	593	538	0.30%	0.041%
13	5.515	591	595	598	rVB3	1002	1358	0.75%	0.103%
14	5.557	598	602	604	rBV5	682	957	0.53%	0.073%
15	5.582	604	606	607	rBV	614	412	0.23%	0.031%
16	5.691	623	624	628	rVB3	608	717	0.39%	0.054%
17	5.728	628	630	633	rBV3	702	810	0.44%	0.062%
18	5.783	637	639	641	rBV3	483	439	0.24%	0.033%
19	6.264	715	718	720	rBV3	757	632	0.35%	0.048%
20	6.338	728	730	735	rVB4	634	901	0.49%	0.068%
21	6.374	735	736	738	rBV	783	643	0.35%	0.049%
22	6.557	764	766	769	rVB3	775	714	0.39%	0.054%
23	6.588	769	771	773	rBV	525	502	0.28%	0.038%
24	6.679	784	786	788	rBV2	605	723	0.40%	0.055%
25	6.758	796	799	805	rBV3	625	1375	0.75%	0.105%
26	6.929	826	827	830	rBV	682	796	0.44%	0.061%
27	7.026	841	843	845	rBV3	621	469	0.26%	0.036%
28	7.136	848	861	870	rBV5	7363	31432	17.25%	2.389%
29	7.648	935	945	956	rBV	31702	80955	44.42%	6.153%
30	7.789	964	968	969	rBV3	811	870	0.48%	0.066%
31	7.837	974	976	980	rVB4	809	908	0.50%	0.069%
32	7.886	982	984	988	rVB4	540	560	0.31%	0.043%
33	8.014	1002	1005	1007	rBV3	836	1169	0.64%	0.089%
34	8.112	1020	1021	1024	rVB	610	490	0.27%	0.037%
35	8.148	1024	1027	1029	rBV2	638	814	0.45%	0.062%
36	8.209	1034	1037	1039	rBV3	752	897	0.49%	0.068%

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM050224SMA.M
 Title : SFAM01.0

37	8.276	1039	1048	1067	rVB3	52066	182247	100.00%	13.852%
38	8.410	1067	1070	1073	rBV5	990	1485	0.81%	0.113%
39	8.526	1087	1089	1093	rBV5	607	913	0.50%	0.069%
40	8.563	1093	1095	1097	rBV3	692	696	0.38%	0.053%
41	8.758	1126	1127	1132	rVB5	841	646	0.35%	0.049%
42	8.843	1132	1141	1152	rBV	45465	96372	52.88%	7.325%
43	9.185	1195	1197	1199	rBV3	585	657	0.36%	0.050%
44	9.276	1203	1212	1221	rBV	46870	101858	55.89%	7.742%
45	9.343	1221	1223	1226	rVB4	784	611	0.34%	0.046%
46	9.502	1245	1249	1252	rBV5	786	1330	0.73%	0.101%
47	9.550	1255	1257	1260	rVV4	683	937	0.51%	0.071%
48	9.642	1271	1272	1276	rBV4	645	722	0.40%	0.055%
49	9.745	1287	1289	1292	rBV3	807	765	0.42%	0.058%
50	9.922	1316	1318	1320	rBV2	597	563	0.31%	0.043%
51	9.983	1326	1328	1330	rBV2	826	883	0.48%	0.067%
52	10.032	1330	1336	1345	rVB2	12485	24404	13.39%	1.855%
53	10.130	1345	1352	1362	rBV	63628	131575	72.20%	10.001%
54	10.325	1377	1384	1391	rVB	61643	113423	62.24%	8.621%
55	10.380	1391	1393	1395	rBV3	1214	1147	0.63%	0.087%
56	10.489	1409	1411	1412	rBV	739	634	0.35%	0.048%
57	10.581	1421	1426	1432	rVB	8480	14969	8.21%	1.138%
58	10.697	1442	1445	1450	rBV3	1771	3002	1.65%	0.228%
59	10.794	1457	1461	1463	rBV3	731	1170	0.64%	0.089%
60	10.837	1466	1468	1470	rBV3	675	591	0.32%	0.045%
61	10.928	1481	1483	1486	rBV4	2194	2981	1.64%	0.227%
62	11.190	1524	1526	1530	rVB4	1160	1107	0.61%	0.084%
63	11.227	1530	1532	1533	rBV	627	470	0.26%	0.036%
64	11.264	1536	1538	1544	rVB7	726	1239	0.68%	0.094%
65	11.434	1564	1566	1568	rVB3	683	523	0.29%	0.040%
66	11.629	1591	1598	1607	rBV	65463	115623	63.44%	8.788%
67	11.776	1620	1622	1626	rVB3	577	560	0.31%	0.043%
68	11.885	1638	1640	1641	rBV2	534	433	0.24%	0.033%
69	11.934	1645	1648	1651	rBV3	856	908	0.50%	0.069%
70	11.965	1651	1653	1655	rBV3	988	684	0.38%	0.052%
71	11.989	1655	1657	1658	rBV2	674	412	0.23%	0.031%
72	12.044	1664	1666	1669	rBV2	547	570	0.31%	0.043%
73	12.074	1669	1671	1673	rBV2	664	670	0.37%	0.051%
74	12.208	1691	1693	1694	rBV	573	529	0.29%	0.040%
75	12.294	1704	1707	1708	rBV2	869	944	0.52%	0.072%
76	12.416	1723	1727	1730	rBV3	490	783	0.43%	0.060%

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77	12.458	1732	1734	1738	rVB5	715	731	0.40%	0.056%
78	12.538	1746	1747	1750	rVB3	613	523	0.29%	0.040%
79	12.605	1750	1758	1763	rBV3	2550	6010	3.30%	0.457%
80	12.647	1763	1765	1766	rBV2	520	468	0.26%	0.036%
81	12.690	1766	1772	1780	rVB	39891	68293	37.47%	5.191%
82	12.794	1787	1789	1790	rBV2	577	442	0.24%	0.034%
83	12.928	1807	1811	1813	rBV4	1031	1313	0.72%	0.100%
84	12.983	1818	1820	1823	rVB3	563	500	0.27%	0.038%
85	13.208	1852	1857	1866	rVB3	2296	4833	2.65%	0.367%
86	13.403	1887	1889	1892	rVB	951	696	0.38%	0.053%
87	13.507	1902	1906	1907	rBV4	673	721	0.40%	0.055%
88	13.556	1907	1914	1921	rBV	45677	79366	43.55%	6.032%
89	13.653	1928	1930	1932	rBV2	512	479	0.26%	0.036%
90	13.848	1955	1962	1969	rBV	46950	78161	42.89%	5.941%
91	13.964	1979	1981	1983	rBV2	552	518	0.28%	0.039%
92	14.050	1994	1995	1996	rBV	1009	659	0.36%	0.050%
93	14.141	2005	2010	2017	rBV6	2222	3770	2.07%	0.287%
94	14.306	2034	2037	2039	rBV2	690	703	0.39%	0.053%
95	14.708	2100	2103	2107	rBV4	681	833	0.46%	0.063%
96	15.135	2170	2173	2174	rBV2	1024	873	0.48%	0.066%
97	15.214	2184	2186	2189	rVB3	719	462	0.25%	0.035%
98	15.763	2274	2276	2279	rBV4	825	901	0.49%	0.068%
99	15.964	2307	2309	2310	rBV2	561	441	0.24%	0.034%
100	16.421	2382	2384	2388	rBV5	745	1162	0.64%	0.088%

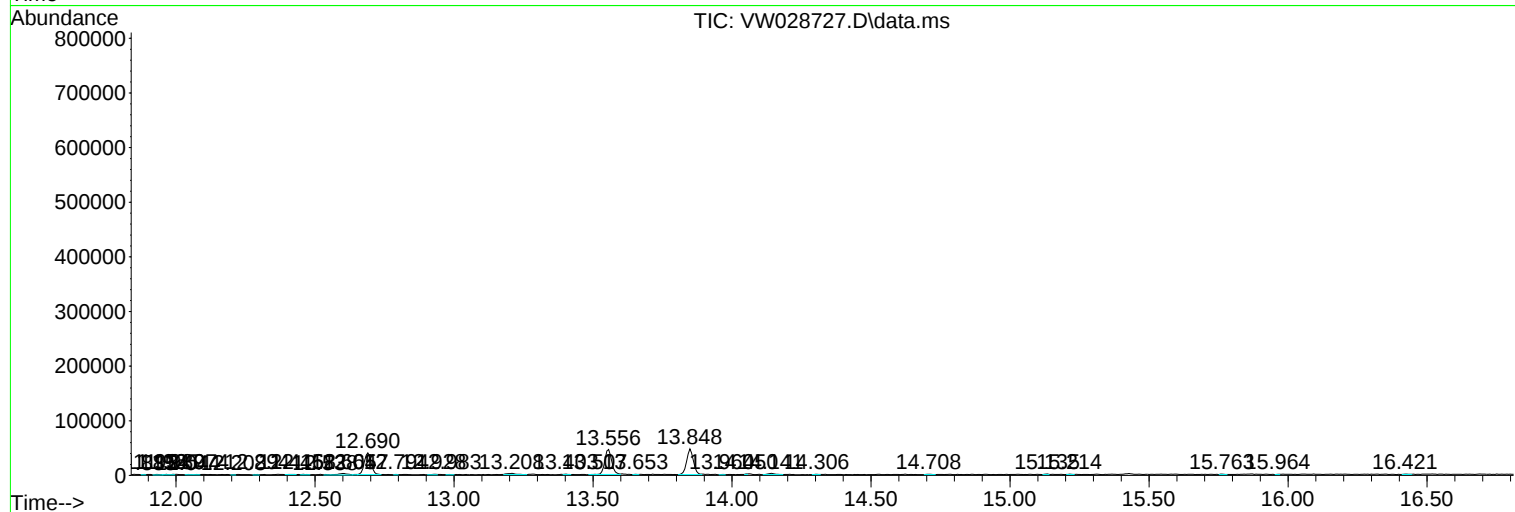
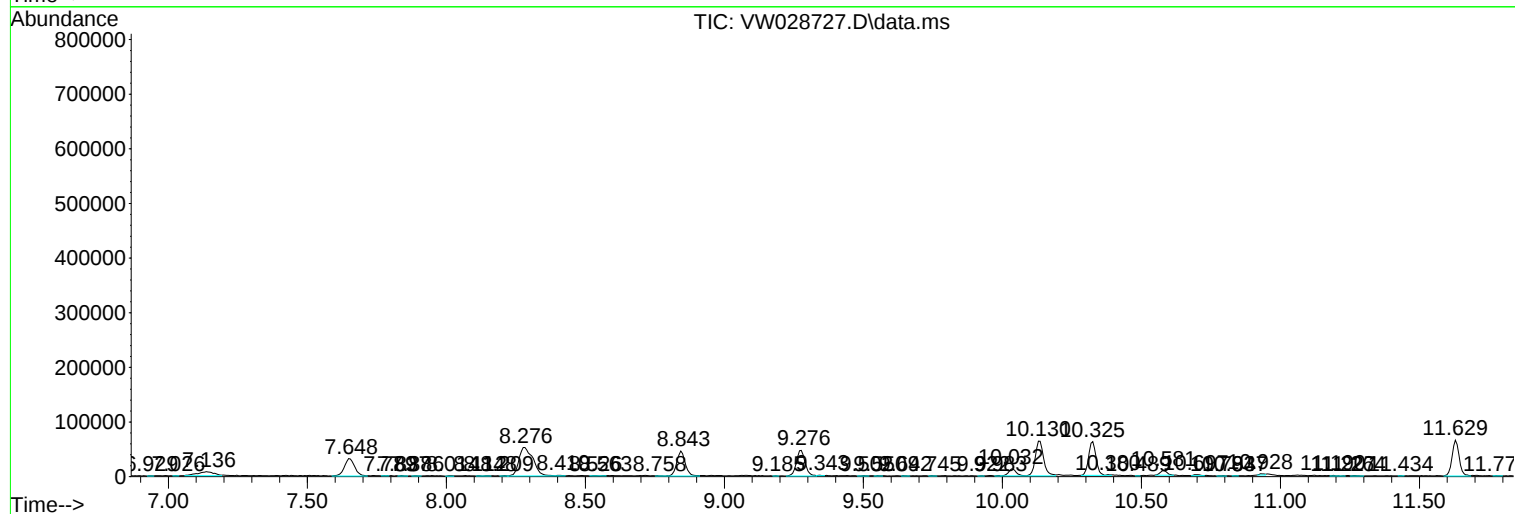
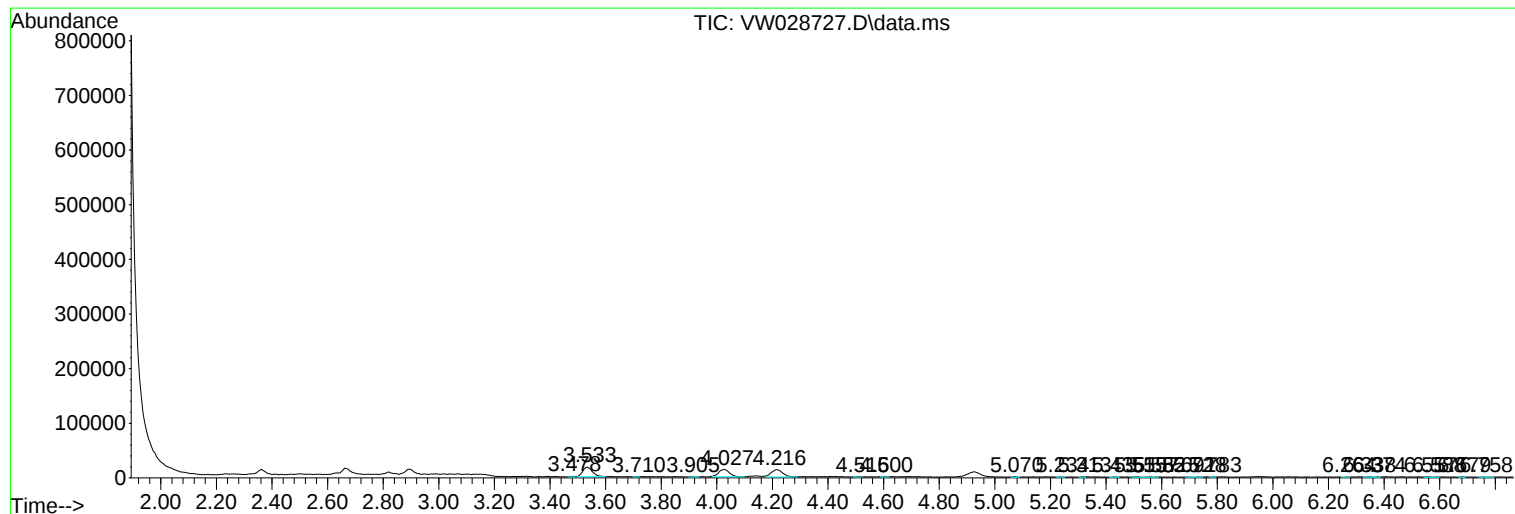
Sum of corrected areas: 1315658

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM050224SMA.M
Quant Title : SFAM01.0

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



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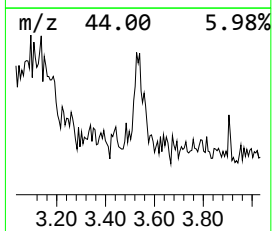
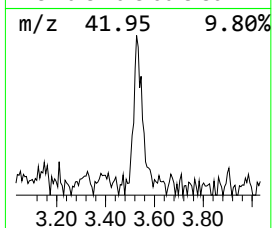
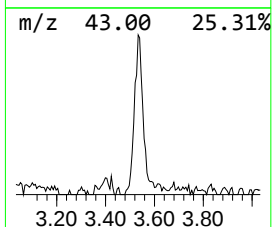
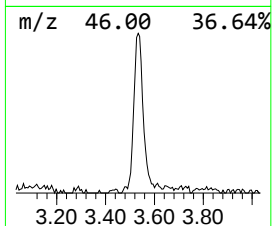
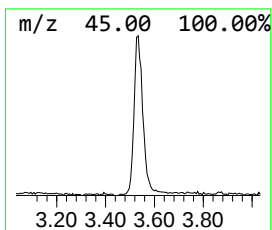
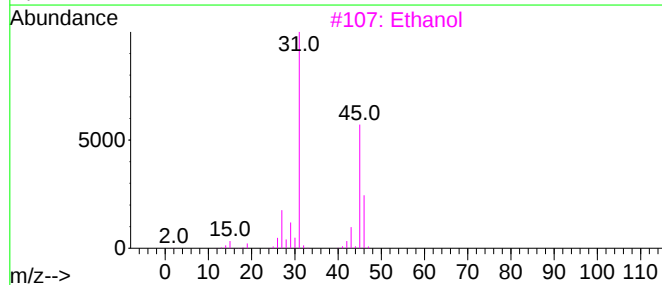
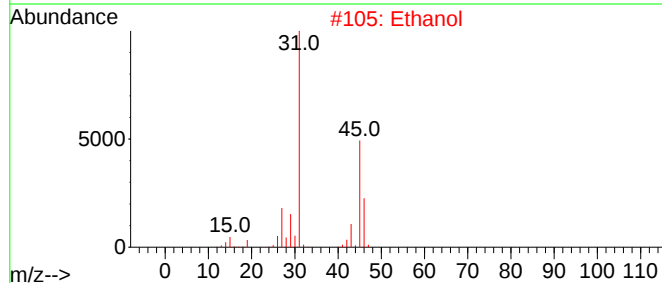
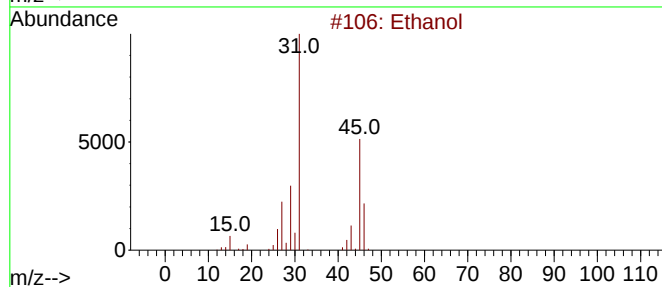
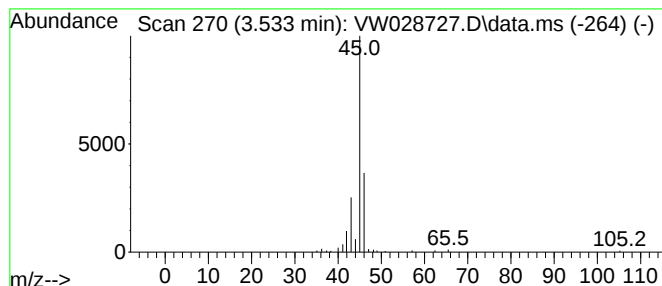
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM050224SMA.M
Quant Title : SFAM01.0

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

Peak Number 1 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.533	11.17 ug/L	43057	1,4-Difluorobenzene	8.843

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol			46	C2H6O	000064-17-5	56
2	Ethanol			46	C2H6O	000064-17-5	40
3	Ethanol			46	C2H6O	000064-17-5	9
4	Ethanol			46	C2H6O	000064-17-5	9
5	Dimethyl ether			46	C2H6O	000115-10-6	9



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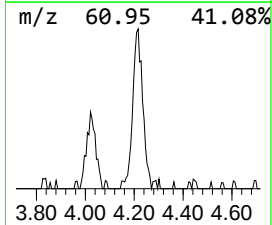
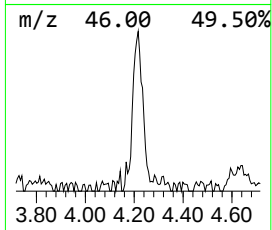
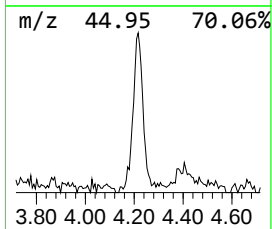
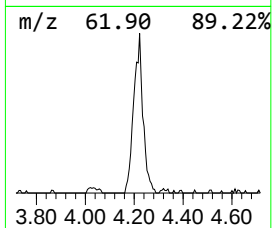
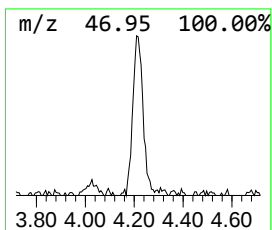
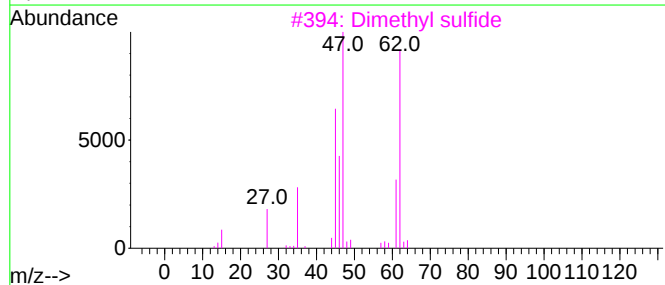
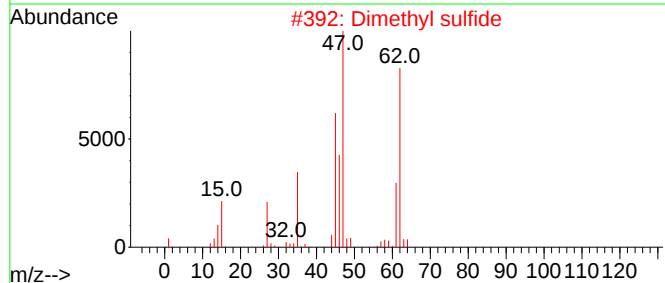
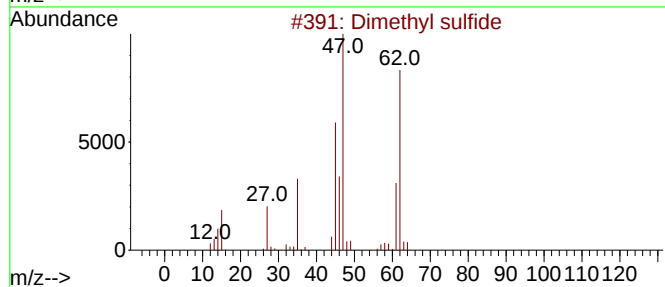
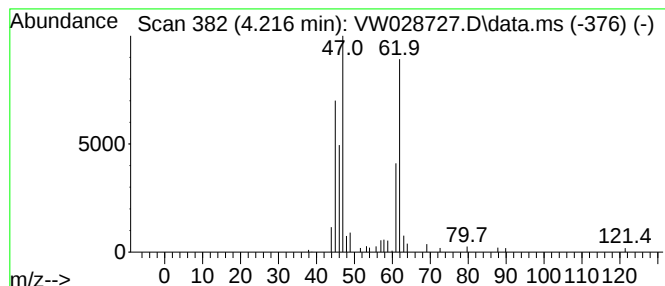
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM050224SMA.M
Quant Title : SFAM01.0

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

Peak Number 2 Dimethyl sulfide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.216	9.61 ug/L	37043	1,4-Difluorobenzene	8.843

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl sulfide	62	C2H6S	000075-18-3	94
2			Dimethyl sulfide	62	C2H6S	000075-18-3	94
3			Dimethyl sulfide	62	C2H6S	000075-18-3	91
4			Dimethyl sulfide	62	C2H6S	000075-18-3	90
5			Borane-methyl sulfide complex	76	C2H9BS	013292-87-0	83



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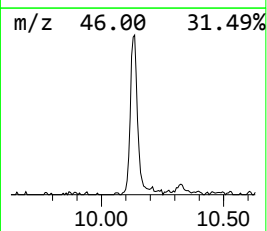
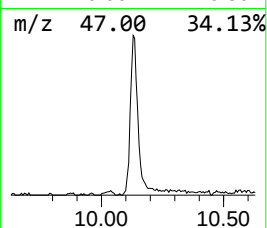
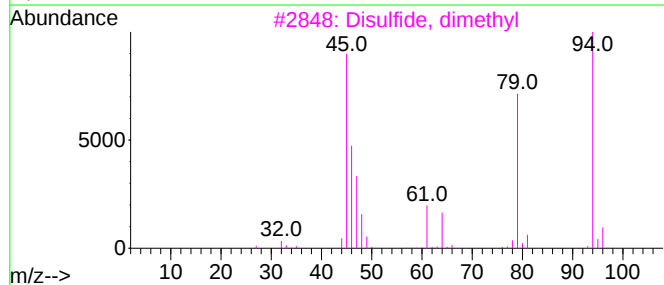
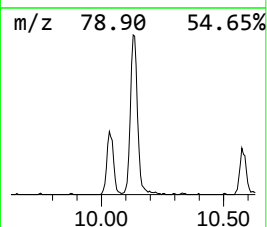
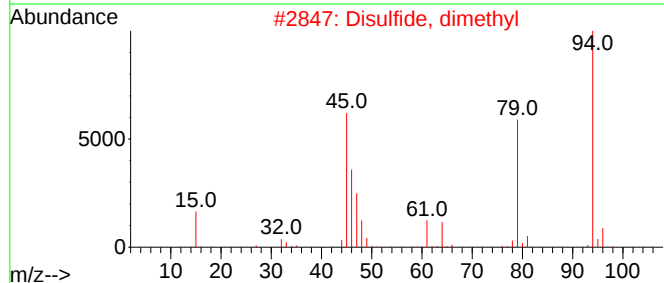
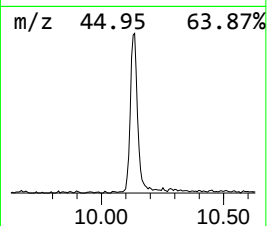
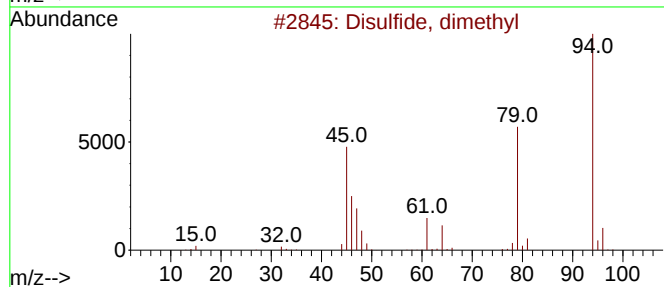
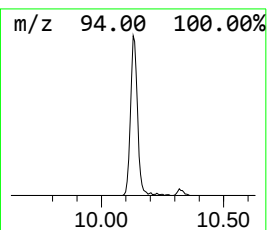
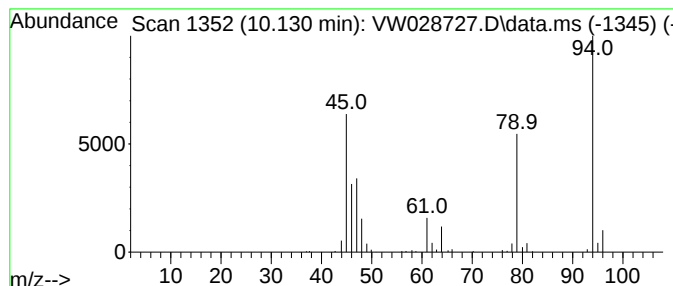
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Quant Title : SFAM01.0

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

Peak Number 4 Disulfide, dimethyl Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.130	34.13 ug/L	131575	1,4-Difluorobenzene	8.843

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Disulfide, dimethyl	94	C2H6S2	000624-92-0	96
2			Disulfide, dimethyl	94	C2H6S2	000624-92-0	94
3			Disulfide, dimethyl	94	C2H6S2	000624-92-0	94
4			Disulfide, dimethyl	94	C2H6S2	000624-92-0	91
5			Disulfide, dimethyl	94	C2H6S2	000624-92-0	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW052424\
Data File : VW028727.D
Acq On : 24 May 2024 12:38
Operator : SY/MD
Sample : P2569-22
Misc : 4.28g/10mL/MSVOA_W/SOIL/A
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
BH6A8

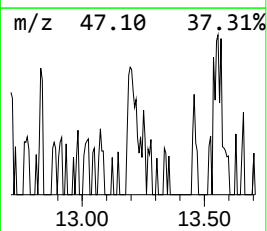
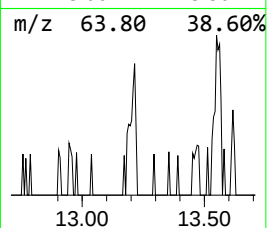
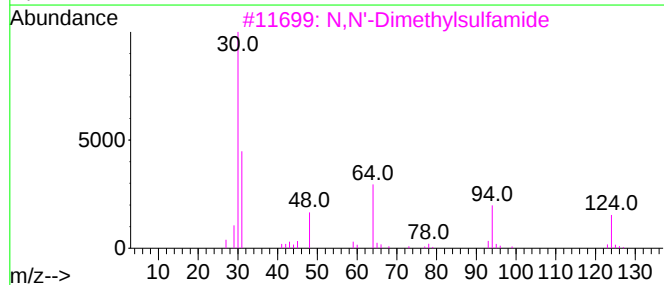
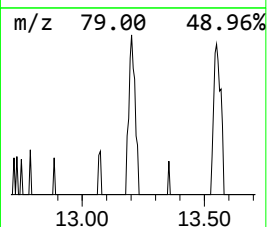
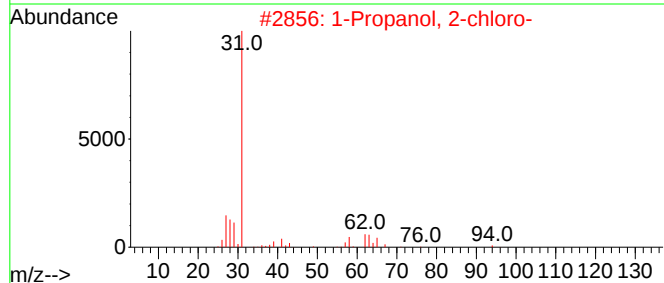
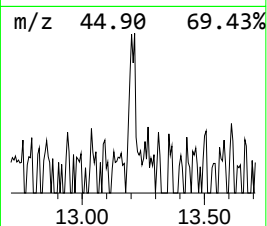
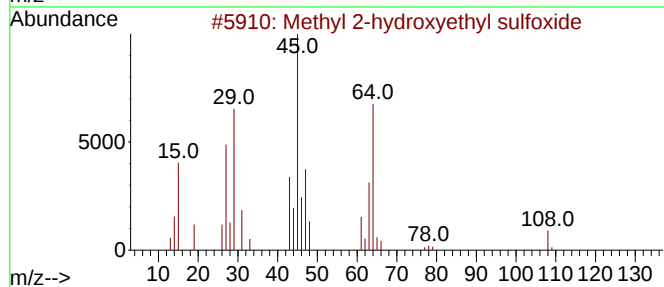
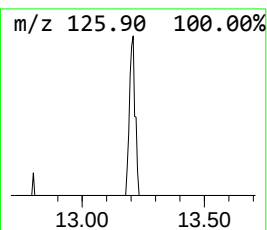
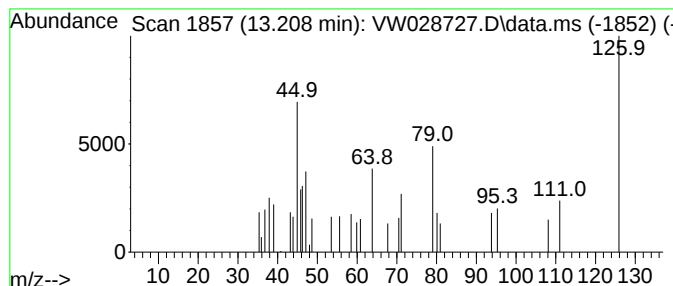
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Quant Title : SFAM01.0

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

Peak Number 6 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.208	1.52 ug/L	4833	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl 2-hydroxyethyl sulfoxide	108	C3H8O2S	021281-74-3	10
2			1-Propanol, 2-chloro-	94	C3H7ClO	000078-89-7	4
3			N,N'-Dimethylsulfamide	124	C2H8N2O2S	022504-72-9	4
4			Isopropyl Alcohol	60	C3H8O	000067-63-0	4
5			Ethanamine, N,N-difluoro-	81	C2H5F2N	000758-18-9	4



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW052424\
Data File : VW028727.D
Acq On : 24 May 2024 12:38
Operator : SY/MD
Sample : P2569-22
Misc : 4.28g/10mL/MSVOA_W/SOIL/A
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
BH6A8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM050224SMA.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
Ethanol	3.533	11.2	ug/L	43057	1	8.843	96372	25.0
Dimethyl sulfide	4.216	9.6	ug/L	37043	1	8.843	96372	25.0
Disulfide, dime...	10.130	34.1	ug/L	131575	1	8.843	96372	25.0
unknown-01	13.208	1.5	ug/L	4833	3	13.556	79366	25.0