

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW053124\
 Data File : VW028942.D
 Acq On : 31 May 2024 14:49
 Operator : SY/MD
 Sample : P2647-12
 Misc : 4.97g/10mL/MSVOA_W/SOIL/B
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 BHBS6

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: VW028942.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.363	72	78	93	rVB	81695	171094	11.69%	1.801%
2	2.899	158	166	181	rBV	65512	180313	12.32%	1.898%
3	3.308	227	233	238	rVB7	2240	4754	0.32%	0.050%
4	3.387	244	246	256	rVB7	1768	3439	0.24%	0.036%
5	3.527	258	269	283	rBV	56564	166379	11.37%	1.751%
6	3.862	322	324	326	rVB2	879	744	0.05%	0.008%
7	3.887	326	328	330	rBV3	580	633	0.04%	0.007%
8	4.021	339	350	360	rBV	149377	430970	29.46%	4.537%
9	4.118	360	366	375	rVV	55980	156115	10.67%	1.643%
10	4.210	376	381	392	rVB	17813	46453	3.18%	0.489%
11	4.387	402	410	423	rVB3	7189	23391	1.60%	0.246%
12	4.649	451	453	454	rBV	969	740	0.05%	0.008%
13	4.923	487	498	511	rVV2	21485	75709	5.17%	0.797%
14	5.716	623	628	630	rBV5	558	953	0.07%	0.010%
15	5.819	642	645	650	rVB4	1198	1279	0.09%	0.013%
16	5.856	650	651	654	rBV3	515	609	0.04%	0.006%
17	5.941	656	665	679	rVB3	7669	25665	1.75%	0.270%
18	6.222	707	711	713	rBV5	621	1010	0.07%	0.011%
19	6.270	715	719	723	rVB6	623	895	0.06%	0.009%
20	6.423	741	744	746	rBV3	676	901	0.06%	0.009%
21	6.569	766	768	773	rBV5	665	664	0.05%	0.007%
22	6.673	782	785	787	rVB4	717	672	0.05%	0.007%
23	6.691	787	788	791	rVB3	680	614	0.04%	0.006%
24	6.728	791	794	798	rVB4	807	1011	0.07%	0.011%
25	6.783	800	803	807	rBV5	656	989	0.07%	0.010%
26	6.880	817	819	823	rBV4	667	1061	0.07%	0.011%
27	6.929	823	827	828	rBV2	595	577	0.04%	0.006%
28	7.075	843	851	857	rBV	40218	118962	8.13%	1.252%
29	7.362	894	898	899	rBV3	693	669	0.05%	0.007%
30	7.392	899	903	904	rBV3	529	572	0.04%	0.006%
31	7.648	934	945	958	rBV	255671	634826	43.39%	6.682%
32	8.276	1038	1048	1065	rBV2	490512	1463009	100.00%	15.400%
33	8.532	1086	1090	1091	rVV3	716	710	0.05%	0.007%
34	8.557	1091	1094	1100	rVB8	1329	2617	0.18%	0.028%
35	8.691	1114	1116	1118	rBV3	1279	1325	0.09%	0.014%
36	8.843	1132	1141	1158	rVV	411225	821452	56.15%	8.647%

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

37	9.020	1168	1170	1172	rBV3	1085	800	0.05%	0.008%
38	9.081	1173	1180	1184	rBV8	1366	3306	0.23%	0.035%
39	9.270	1200	1211	1220	rBV	354169	734624	50.21%	7.733%
40	9.569	1256	1260	1263	rVB4	558	616	0.04%	0.006%
41	9.666	1272	1276	1281	rVB8	1474	2753	0.19%	0.029%
42	9.959	1320	1324	1325	rVB4	711	712	0.05%	0.007%
43	10.032	1325	1336	1344	rBV	140110	257827	17.62%	2.714%
44	10.130	1345	1352	1360	rVB	89580	169508	11.59%	1.784%
45	10.325	1375	1384	1399	rBV	613435	1091203	74.59%	11.486%
46	10.514	1409	1415	1416	rBV7	1301	2502	0.17%	0.026%
47	10.575	1419	1425	1436	rVV	84974	151935	10.39%	1.599%
48	10.697	1440	1445	1451	rVV	10834	19049	1.30%	0.201%
49	10.770	1454	1457	1462	rVB6	787	926	0.06%	0.010%
50	10.861	1467	1472	1474	rBV3	1412	1921	0.13%	0.020%
51	10.922	1476	1482	1496	rVV	139322	273996	18.73%	2.884%
52	11.068	1500	1506	1516	rVV4	11907	33979	2.32%	0.358%
53	11.166	1520	1522	1527	rVB6	1254	1962	0.13%	0.021%
54	11.294	1540	1543	1548	rVV6	808	924	0.06%	0.010%
55	11.428	1562	1565	1573	rVB7	1176	2415	0.17%	0.025%
56	11.526	1579	1581	1583	rVB3	920	798	0.05%	0.008%
57	11.556	1583	1586	1589	rBV4	707	906	0.06%	0.010%
58	11.629	1589	1598	1607	rBV	508788	851981	58.23%	8.968%
59	11.830	1627	1631	1638	rVB9	2089	4647	0.32%	0.049%
60	11.946	1643	1650	1660	rBV3	13644	29326	2.00%	0.309%
61	12.032	1662	1664	1666	rVB3	891	749	0.05%	0.008%
62	12.160	1682	1685	1693	rBV7	1549	3453	0.24%	0.036%
63	12.404	1723	1725	1728	rVB2	605	657	0.04%	0.007%
64	12.458	1731	1734	1735	rBV3	1153	1143	0.08%	0.012%
65	12.605	1750	1758	1764	rVV3	10110	18942	1.29%	0.199%
66	12.690	1764	1772	1779	rVV	223816	376186	25.71%	3.960%
67	12.788	1786	1788	1792	rVB4	561	675	0.05%	0.007%
68	12.830	1792	1795	1797	rVB4	746	743	0.05%	0.008%
69	12.849	1797	1798	1802	rBV4	498	704	0.05%	0.007%
70	12.928	1807	1811	1816	rBV6	2411	4200	0.29%	0.044%
71	13.019	1824	1826	1828	rBV3	692	741	0.05%	0.008%
72	13.129	1840	1844	1847	rBV5	626	1024	0.07%	0.011%
73	13.208	1850	1857	1863	rBV3	15374	29139	1.99%	0.307%
74	13.281	1867	1869	1879	rVB8	3130	6384	0.44%	0.067%
75	13.367	1879	1883	1888	rBV2	4047	8173	0.56%	0.086%
76	13.556	1901	1914	1927	rBV	313733	522467	35.71%	5.500%

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 Title : SFAM01.0

77	13.739	1942	1944	1945	rBV	893	689	0.05%	0.007%
78	13.757	1945	1947	1954	rVB6	1390	2382	0.16%	0.025%
79	13.848	1954	1962	1970	rBV	309139	501198	34.26%	5.276%
80	13.940	1975	1977	1981	rVV5	1537	1989	0.14%	0.021%
81	14.062	1991	1997	2006	rBV	6612	10699	0.73%	0.113%
82	14.184	2016	2017	2022	rVB5	707	771	0.05%	0.008%
83	14.226	2022	2024	2026	rBV3	643	766	0.05%	0.008%
84	14.306	2033	2037	2039	rBV4	586	712	0.05%	0.007%
85	14.714	2101	2104	2111	rVB7	1073	2004	0.14%	0.021%
86	14.793	2114	2117	2120	rBV3	573	664	0.05%	0.007%
87	15.129	2169	2172	2174	rVB3	593	746	0.05%	0.008%
88	15.269	2193	2195	2198	rVV4	608	595	0.04%	0.006%
89	15.318	2201	2203	2207	rVB5	592	617	0.04%	0.006%
90	15.427	2215	2221	2226	rBV2	6668	11661	0.80%	0.123%
91	15.476	2227	2229	2233	rVB4	1017	1332	0.09%	0.014%
92	15.622	2250	2253	2256	rBV5	580	672	0.05%	0.007%
93	15.708	2265	2267	2270	rBV3	593	578	0.04%	0.006%
94	15.854	2289	2291	2293	rVV3	646	631	0.04%	0.007%
95	15.885	2295	2296	2299	rVB3	808	633	0.04%	0.007%
96	16.317	2366	2367	2370	rVB3	703	582	0.04%	0.006%
97	16.354	2370	2373	2378	rBV6	620	926	0.06%	0.010%
98	16.470	2389	2392	2393	rBV3	622	620	0.04%	0.007%
99	16.659	2418	2423	2425	rBV3	955	1526	0.10%	0.016%
100	16.714	2429	2432	2433	rBV3	1078	1134	0.08%	0.012%

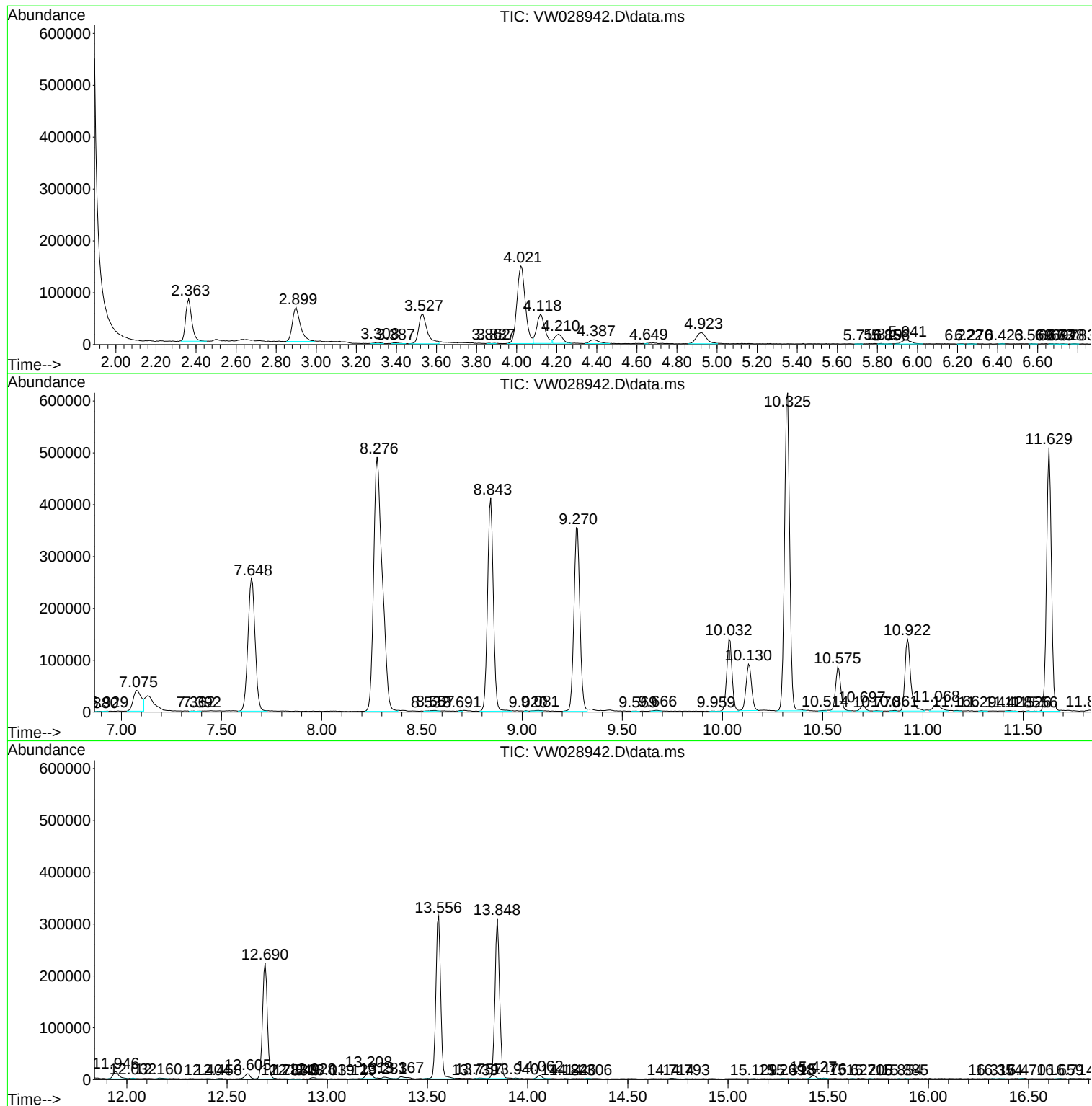
Sum of corrected areas: 9499899

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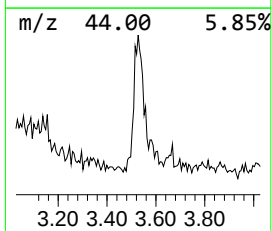
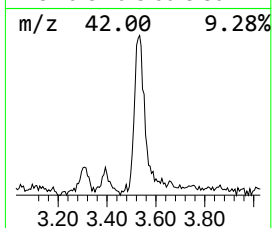
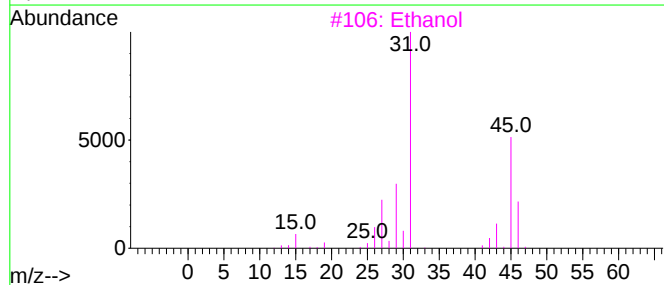
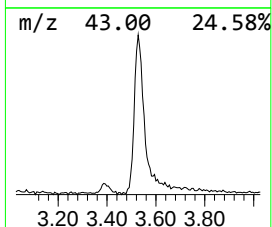
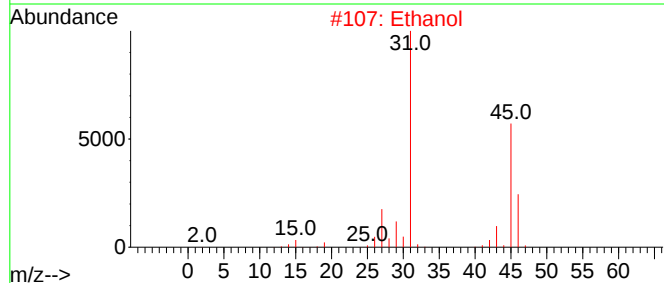
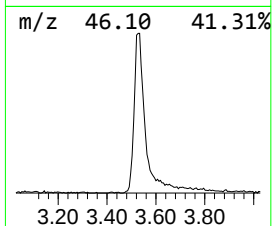
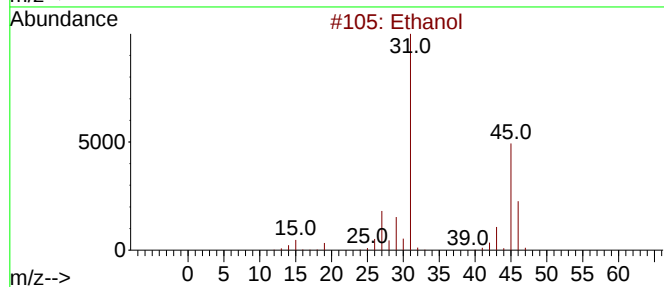
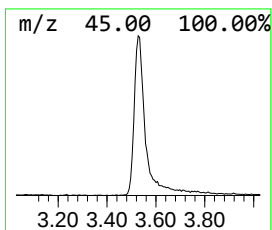
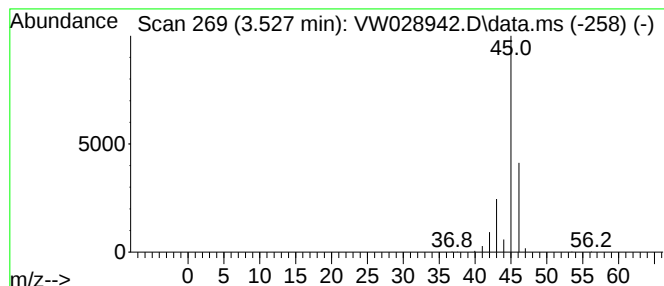
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM050224SMA.M
Quant Title : SFAM01.0

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

Peak Number 1 Ethanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.527	5.06 ug/L	166379	1,4-Difluorobenzene	8.843

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol			46	C2H6O	000064-17-5	83
2	Ethanol			46	C2H6O	000064-17-5	74
3	Ethanol			46	C2H6O	000064-17-5	64
4	Dimethyl ether			46	C2H6O	000115-10-6	9
5	Dimethyl ether			46	C2H6O	000115-10-6	9



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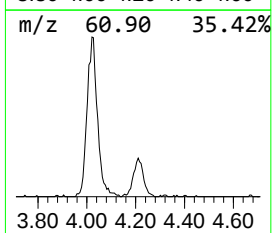
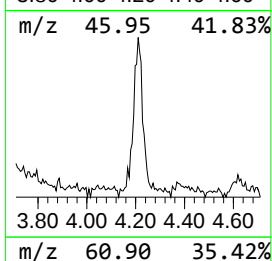
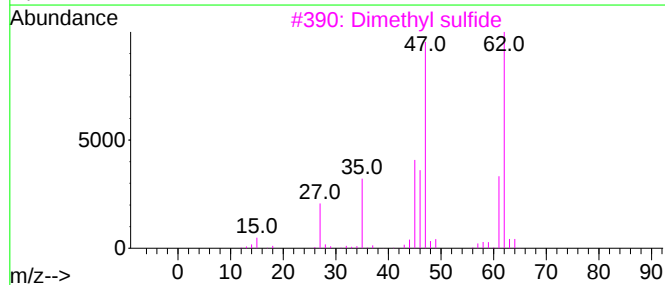
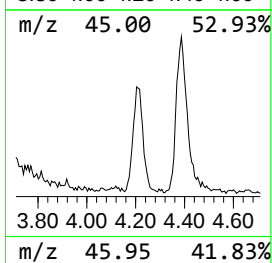
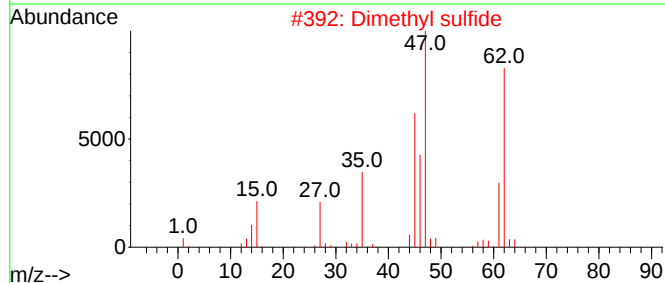
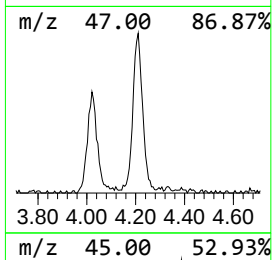
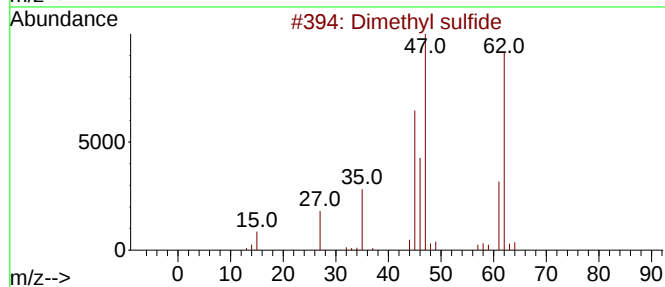
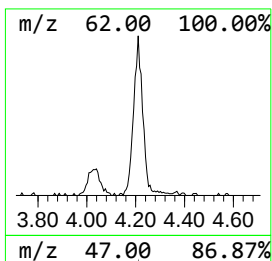
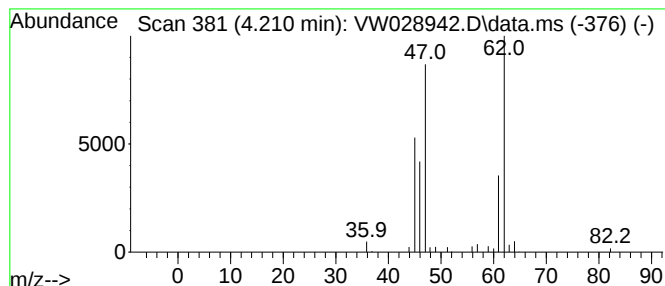
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM050224SMA.M
Quant Title : SFAM01.0

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

Peak Number 2 Dimethyl sulfide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.210	1.41 ug/L	46453	1,4-Difluorobenzene	8.843

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl sulfide	62	C2H6S	000075-18-3	91
2			Dimethyl sulfide	62	C2H6S	000075-18-3	91
3			Dimethyl sulfide	62	C2H6S	000075-18-3	91
4			Dimethyl sulfide	62	C2H6S	000075-18-3	91
5			Borane-methyl sulfide complex	76	C2H9BS	013292-87-0	74



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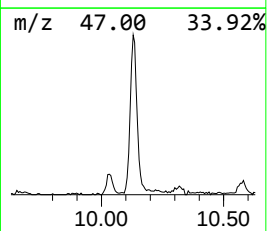
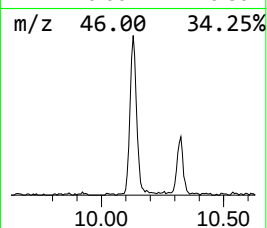
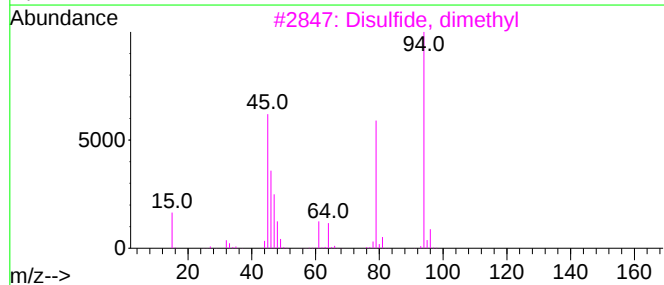
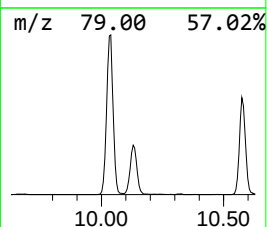
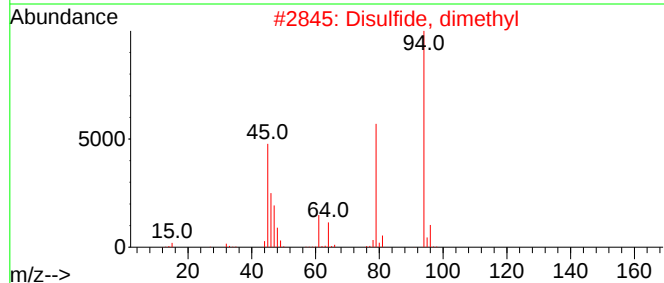
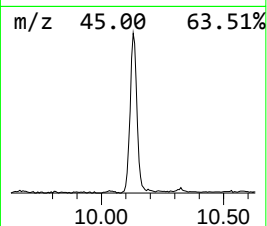
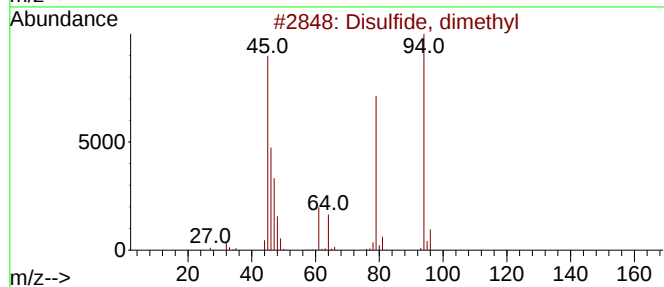
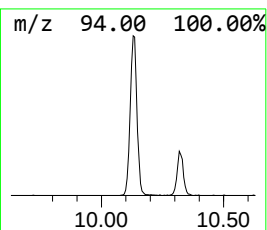
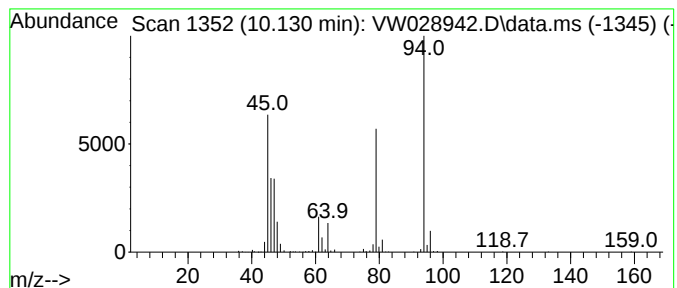
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM050224SMA.M
Quant Title : SFAM01.0

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

Peak Number 4 Disulfide, dimethyl Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.130	5.16 ug/L	169508	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	95
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\VW053124\
Data File : VW028942.D
Acq On : 31 May 2024 14:49
Operator : SY/MD
Sample : P2647-12
Misc : 4.97g/10mL/MSVOA_W/SOIL/B
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
BHBS6

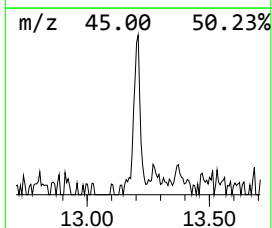
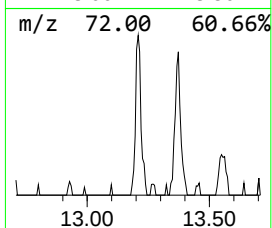
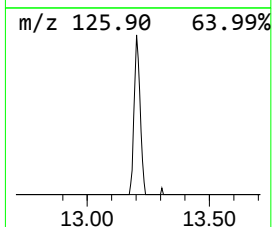
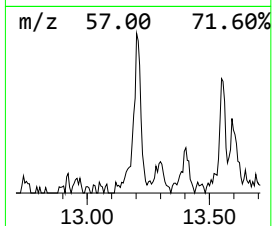
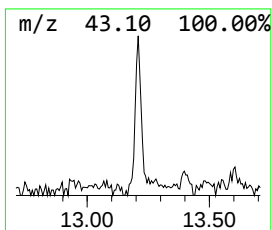
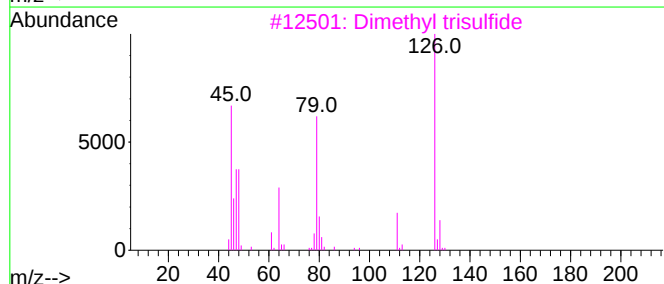
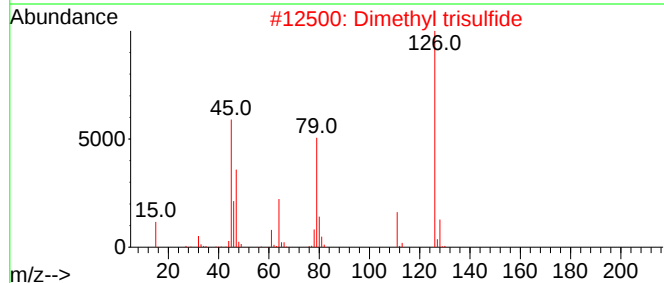
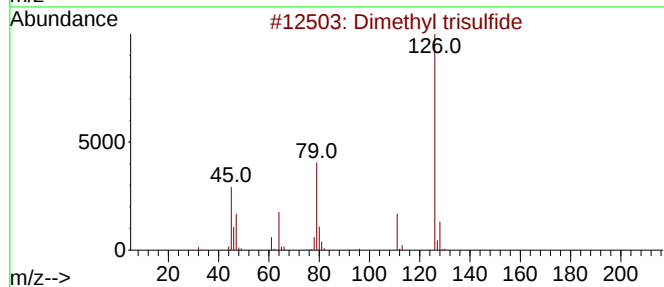
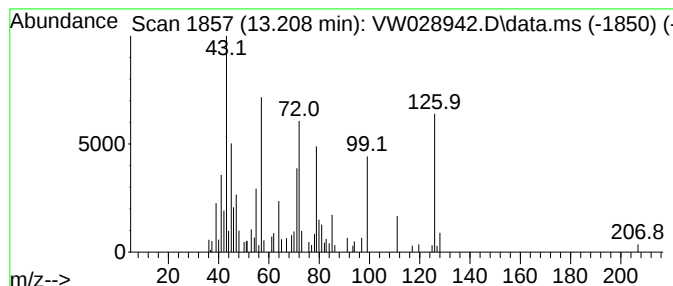
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Quant Title : SFAM01.0

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

Peak Number 5 Dimethyl trisulfide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.208	1.39 ug/L	29139	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl trisulfide	126	C2H6S3	003658-80-8	90
2			Dimethyl trisulfide	126	C2H6S3	003658-80-8	89
3			Dimethyl trisulfide	126	C2H6S3	003658-80-8	70
4			Dimethyl trisulfide	126	C2H6S3	003658-80-8	55
5			3-Octanone	128	C8H16O	000106-68-3	30



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Instrument :
MSVOA_W
ClientSampleId :
BHBS6

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	3.527	5.1	ug/L	166379	1	8.843	821452	25.0
Dimethyl sulfide	4.210	1.4	ug/L	46453	1	8.843	821452	25.0
Disulfide, dime...	10.130	5.2	ug/L	169508	1	8.843	821452	25.0
Dimethyl trisul...	13.208	1.4	ug/L	29139	3	13.556	522467	25.0