

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW051023\
 Data File : VW025920.D
 Acq On : 10 May 2023 11:03
 Operator : SY/MD
 Sample : 02612-38
 Misc : 3.72g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 JREJ2

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\SFAMWLM050123SMA.M
 Title : SFAM01.0

Signal : TIC: VW025920.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	92	rVB	139623	362616	11.47%	1.578%
2	2.668	121	128	141	rBV2	70663	201619	6.38%	0.877%
3	2.893	158	165	181	rVB	117686	317140	10.03%	1.380%
4	3.192	212	214	217	rBV4	2803	3406	0.11%	0.015%
5	3.387	242	246	249	rBV6	3713	5144	0.16%	0.022%
6	3.735	301	303	307	rVB4	2185	2528	0.08%	0.011%
7	4.021	337	350	362	rBV	310438	1031307	32.62%	4.487%
8	4.204	371	380	399	rVB	423019	1195415	37.81%	5.201%
9	4.832	480	483	486	rBV5	2184	2832	0.09%	0.012%
10	4.923	486	498	511	rVV2	29875	118786	3.76%	0.517%
11	5.125	527	531	534	rBV6	2206	3649	0.12%	0.016%
12	5.222	546	547	552	rVB5	1801	2160	0.07%	0.009%
13	5.393	572	575	578	rBV5	1961	2578	0.08%	0.011%
14	5.460	584	586	588	rVB3	1919	1799	0.06%	0.008%
15	5.527	593	597	599	rBV5	1501	1843	0.06%	0.008%
16	5.679	619	622	623	rBV3	2137	2675	0.08%	0.012%
17	5.698	623	625	628	rVB4	1740	1860	0.06%	0.008%
18	5.734	628	631	632	rBV3	2057	2262	0.07%	0.010%
19	5.880	650	655	656	rBV5	2380	3361	0.11%	0.015%
20	5.941	657	665	675	rVB2	23457	72319	2.29%	0.315%
21	6.021	675	678	679	rBV3	2143	1880	0.06%	0.008%
22	6.173	700	703	706	rVB5	1701	2324	0.07%	0.010%
23	6.228	708	712	713	rBV3	1284	1721	0.05%	0.007%
24	6.399	739	740	743	rVV3	1729	2016	0.06%	0.009%
25	6.478	748	753	756	rBV7	1677	3163	0.10%	0.014%
26	6.600	771	773	775	rVB3	2023	1932	0.06%	0.008%
27	7.075	843	851	865	rBV	89040	264632	8.37%	1.151%
28	7.295	884	887	890	rBV5	1452	1820	0.06%	0.008%
29	7.380	897	901	902	rVB3	1530	1648	0.05%	0.007%
30	7.411	904	906	910	rBV6	1836	2365	0.07%	0.010%
31	7.502	919	921	923	rVV3	1861	1901	0.06%	0.008%
32	7.527	923	925	928	rVV4	1824	2190	0.07%	0.010%
33	7.648	935	945	958	rVV	521189	1283675	40.61%	5.585%
34	7.758	961	963	965	rBV3	1629	1794	0.06%	0.008%
35	7.831	971	975	978	rVB6	1373	2305	0.07%	0.010%
36	7.898	984	986	989	rBV4	1353	2037	0.06%	0.009%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM050123SMA.M
 Title : SFAM01.0

37	8.276	1037	1048	1065	rBV2	1101686	3161255	100.00%	13.753%
38	8.453	1074	1077	1082	rVB7	1639	1698	0.05%	0.007%
39	8.618	1102	1104	1105	rBV2	2075	2030	0.06%	0.009%
40	8.843	1130	1141	1154	rBV	1127134	2225320	70.39%	9.681%
41	9.075	1176	1179	1181	rVV4	2475	2692	0.09%	0.012%
42	9.148	1189	1191	1195	rVB4	1826	2114	0.07%	0.009%
43	9.197	1197	1199	1202	rBV4	1825	1992	0.06%	0.009%
44	9.270	1204	1211	1220	rBV	743394	1505860	47.63%	6.551%
45	9.490	1245	1247	1251	rVB5	1973	2480	0.08%	0.011%
46	9.575	1258	1261	1262	rBV3	1969	2053	0.06%	0.009%
47	9.666	1274	1276	1279	rBV4	2771	2575	0.08%	0.011%
48	9.965	1321	1325	1326	rBV4	1526	1788	0.06%	0.008%
49	10.032	1329	1336	1346	rVV	345269	630090	19.93%	2.741%
50	10.136	1347	1353	1355	rVV2	27839	51639	1.63%	0.225%
51	10.185	1356	1361	1374	rVV	56327	167891	5.31%	0.730%
52	10.325	1376	1384	1391	rVV	1461535	2589668	81.92%	11.266%
53	10.386	1391	1394	1401	rVV2	22839	42739	1.35%	0.186%
54	10.441	1401	1403	1406	rVB4	2284	1957	0.06%	0.009%
55	10.575	1417	1425	1437	rVB	227447	392337	12.41%	1.707%
56	10.703	1440	1446	1451	rBV2	20893	40095	1.27%	0.174%
57	10.849	1466	1470	1475	rVB8	2592	5305	0.17%	0.023%
58	10.922	1475	1482	1500	rBV	317019	576322	18.23%	2.507%
59	11.215	1528	1530	1533	rBV4	1655	1915	0.06%	0.008%
60	11.245	1533	1535	1539	rVB5	2556	2565	0.08%	0.011%
61	11.331	1546	1549	1552	rVB5	1963	2320	0.07%	0.010%
62	11.361	1552	1554	1557	rVB4	2323	1905	0.06%	0.008%
63	11.398	1557	1560	1566	rBV7	2970	5581	0.18%	0.024%
64	11.629	1590	1598	1607	rBV	1418846	2379124	75.26%	10.350%
65	11.727	1612	1614	1619	rVB6	5652	6985	0.22%	0.030%
66	11.837	1626	1632	1638	rBV9	6001	12452	0.39%	0.054%
67	11.965	1650	1653	1657	rBV6	1510	2477	0.08%	0.011%
68	12.032	1663	1664	1668	rVB4	1665	1730	0.05%	0.008%
69	12.166	1682	1686	1689	rVV6	2164	3753	0.12%	0.016%
70	12.452	1731	1733	1735	rBV3	1692	1932	0.06%	0.008%
71	12.526	1741	1745	1748	rVB6	2319	3105	0.10%	0.014%
72	12.605	1752	1758	1763	rVV	24084	39889	1.26%	0.174%
73	12.690	1765	1772	1779	rVV	452287	741794	23.47%	3.227%
74	12.751	1780	1782	1787	rVB3	6832	9129	0.29%	0.040%
75	12.940	1811	1813	1815	rVB3	2821	1925	0.06%	0.008%
76	13.044	1826	1830	1834	rVB7	2300	3032	0.10%	0.013%

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 Title : SFAM01.0

77	13.123	1841	1843	1845	rVB3	2383	2370	0.07%	0.010%
78	13.208	1850	1857	1861	rBV	17375	37963	1.20%	0.165%
79	13.410	1885	1890	1893	rVB7	3617	5622	0.18%	0.024%
80	13.452	1893	1897	1898	rBV4	2768	3411	0.11%	0.015%
81	13.556	1907	1914	1923	rVV	1092125	1740174	55.05%	7.571%
82	13.647	1924	1929	1938	rVB	37226	62883	1.99%	0.274%
83	13.849	1955	1962	1979	rVB2	856026	1428377	45.18%	6.214%
84	14.025	1988	1991	1992	rBV3	2139	2822	0.09%	0.012%
85	14.062	1992	1997	2004	rVB	31983	55568	1.76%	0.242%
86	14.184	2015	2017	2018	rBV2	1922	1673	0.05%	0.007%
87	14.220	2020	2023	2028	rVV6	5321	10500	0.33%	0.046%
88	14.318	2036	2039	2047	rVV10	7106	13819	0.44%	0.060%
89	14.379	2047	2049	2051	rVV3	1869	1804	0.06%	0.008%
90	14.422	2052	2056	2059	rVV6	4725	6562	0.21%	0.029%
91	14.617	2086	2088	2092	rVB5	3922	4179	0.13%	0.018%
92	15.043	2154	2158	2161	rVB6	1903	2786	0.09%	0.012%
93	15.123	2165	2171	2175	rBV9	3578	7617	0.24%	0.033%
94	15.428	2216	2221	2226	rVV	18775	30292	0.96%	0.132%
95	15.476	2227	2229	2235	rVB3	7125	11688	0.37%	0.051%
96	15.879	2293	2295	2301	rVB7	2278	2486	0.08%	0.011%
97	15.958	2306	2308	2309	rBV2	2817	2152	0.07%	0.009%
98	16.159	2339	2341	2347	rVB7	1653	2199	0.07%	0.010%
99	16.220	2347	2351	2352	rBV4	1785	2259	0.07%	0.010%
100	16.726	2431	2434	2435	rBV2	1936	2238	0.07%	0.010%

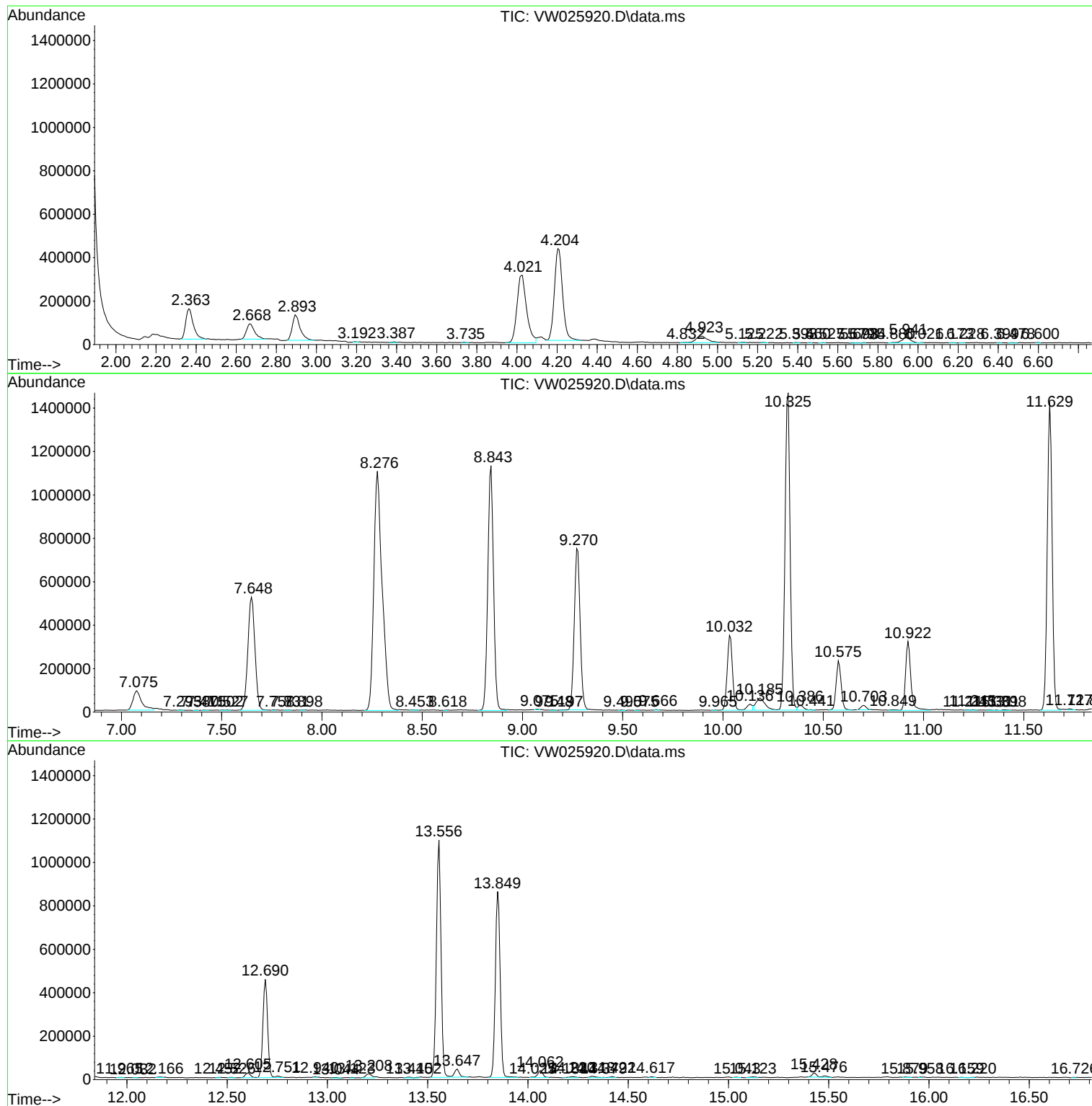
Sum of corrected areas: 22985659

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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM050123SMA.M
Quant Title : SFAM01.0

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



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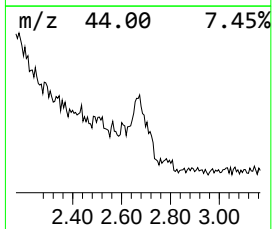
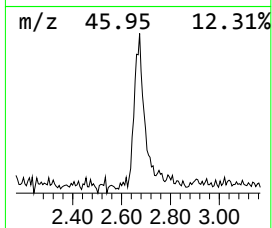
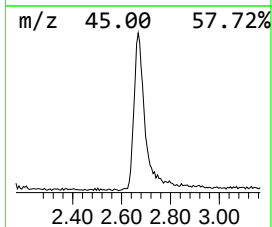
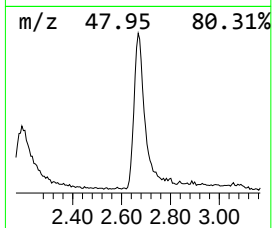
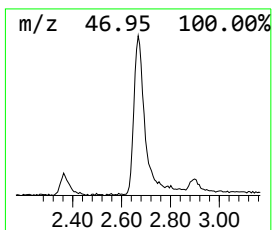
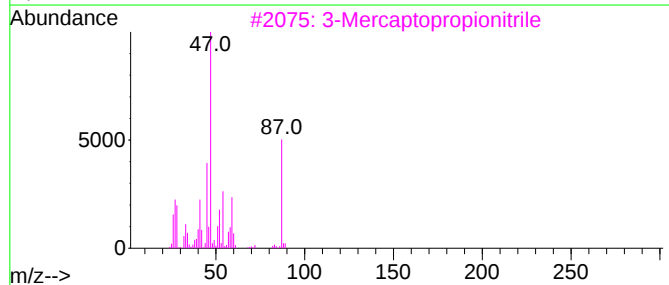
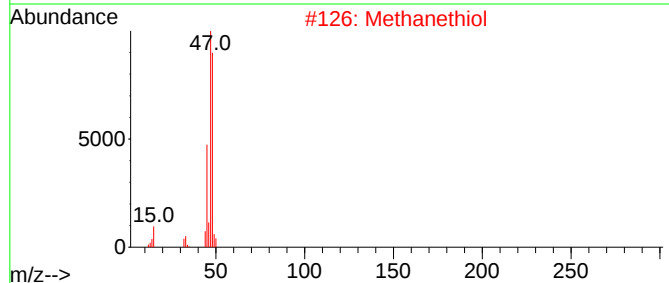
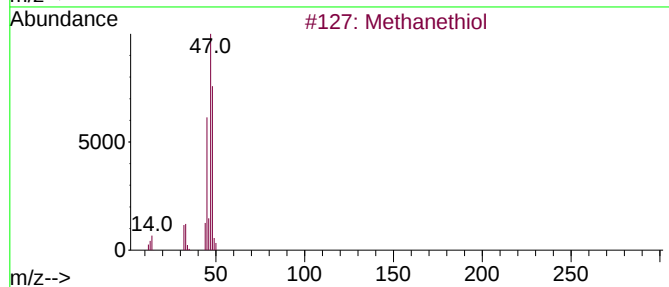
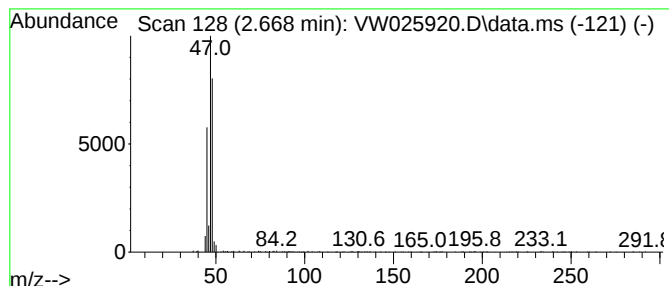
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM050123SMA.M
Quant Title : SFAM01.0

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

Peak Number 1 Methanethiol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.668	2.27 ug/L	201619	1,4-Difluorobenzene	8.843

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanethiol	48	CH4S	000074-93-1	83
2			Methanethiol	48	CH4S	000074-93-1	80
3			3-Mercaptopropionitrile	87	C3H5NS	001001-58-7	28
4			Methional	104	C4H8OS	003268-49-3	9
5			Acetic acid, mercapto-	92	C2H4O2S	000068-11-1	9



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Instrument :
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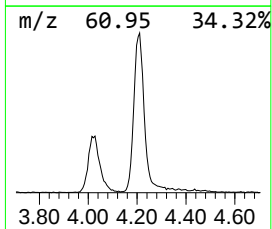
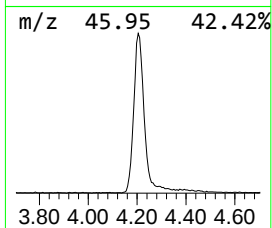
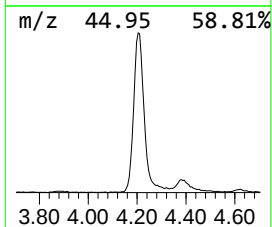
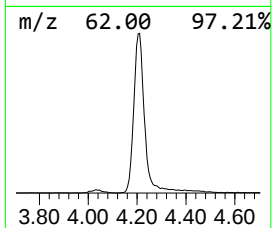
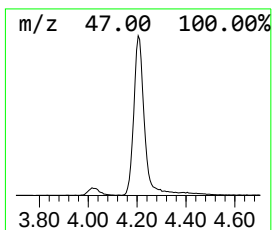
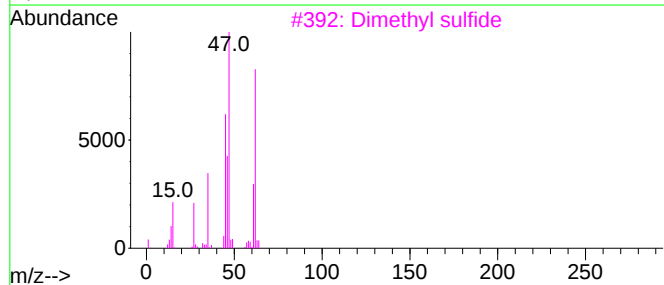
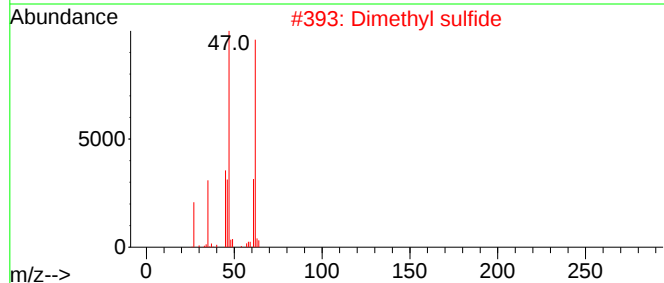
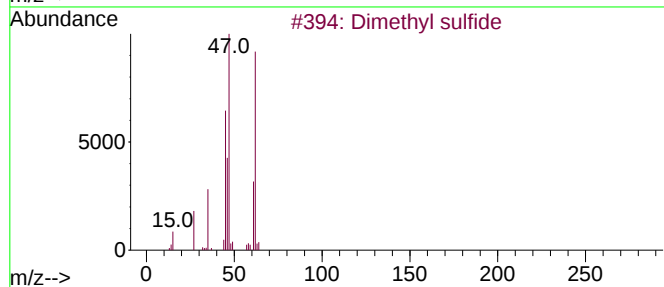
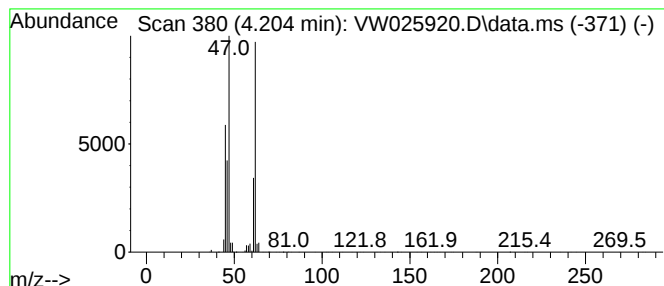
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM050123SMA.M
Quant Title : SFAM01.0

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

Peak Number 2 Dimethyl sulfide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.204	13.43 ug/L	1195420	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	94
4			Dimethyl sulfide	62	C2H6S	000075-18-3	94
5			Dimethyl sulfide	62	C2H6S	000075-18-3	94



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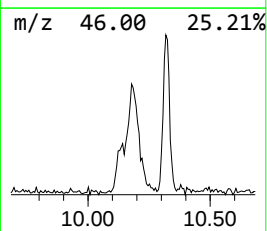
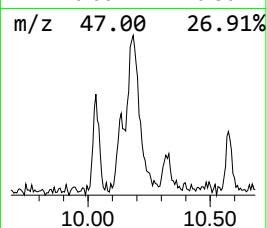
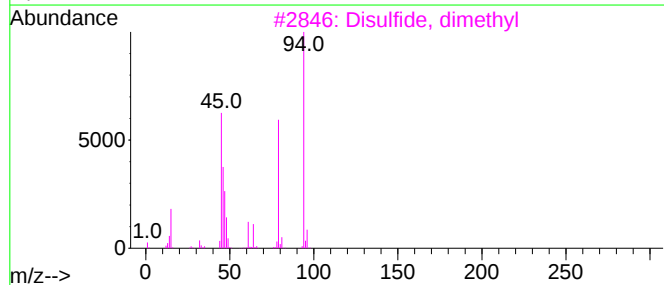
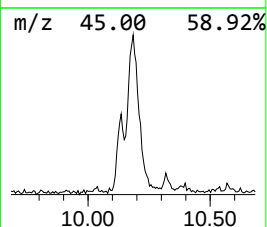
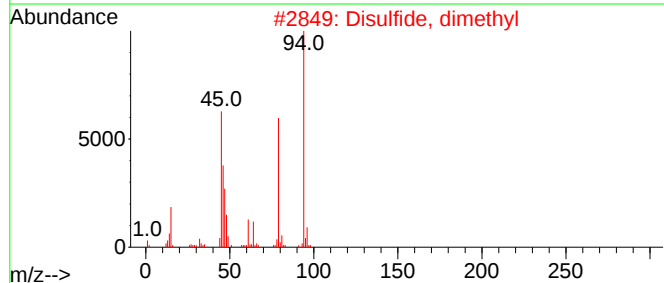
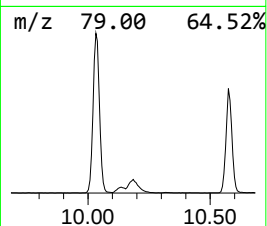
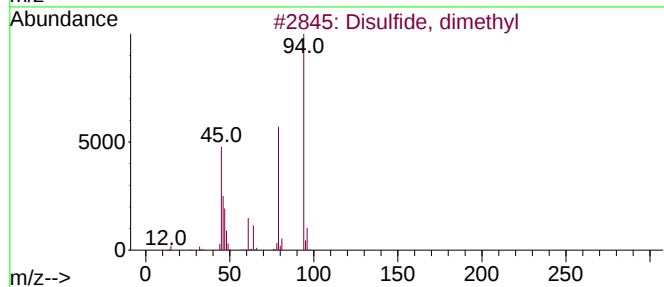
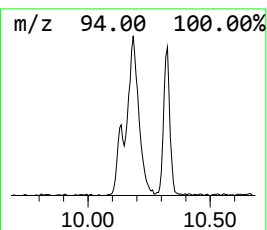
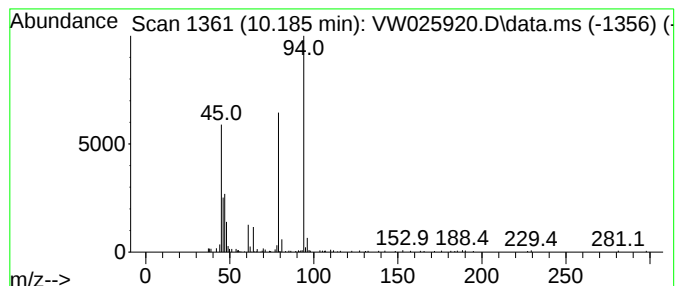
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Disulfide, dimethyl Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.185	1.89 ug/L	167891	1,4-Difluorobenzene	8.843

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Disulfide, dimethyl	94	C2H6S2	000624-92-0	90
2			Disulfide, dimethyl	94	C2H6S2	000624-92-0	72
3			Disulfide, dimethyl	94	C2H6S2	000624-92-0	72
4			Disulfide, dimethyl	94	C2H6S2	000624-92-0	72
5			Dimethyl sulfone	94	C2H6O2S	000067-71-0	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW051023\
Data File : VW025920.D
Acq On : 10 May 2023 11:03
Operator : SY/MD
Sample : 02612-38
Misc : 3.72g/10mL/MSVOA_W/SOIL
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
JREJ2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM050123SMA.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
Methanethiol	2.668	2.3	ug/L	201619	1	8.843	2225320	25.0
Dimethyl sulfide	4.204	13.4	ug/L	1195420	1	8.843	2225320	25.0
Disulfide, dime...	10.185	1.9	ug/L	167891	1	8.843	2225320	25.0