

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW050923\
 Data File : VW025905.D
 Acq On : 09 May 2023 14:04
 Operator : SY/MD
 Sample : 02612-28
 Misc : 3.56g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 JREG9

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: VW025905.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.143	37	42	46	rBV	42530	81140	2.53%	0.342%
2	2.363	72	78	94	rVB	146780	376169	11.74%	1.586%
3	2.667	122	128	142	rBV	130264	338467	10.56%	1.427%
4	2.899	158	166	185	rVB	147396	410002	12.79%	1.729%
5	3.381	243	245	247	rBV3	1616	1781	0.06%	0.008%
6	3.527	265	269	276	rVB9	2937	6647	0.21%	0.028%
7	3.686	290	295	296	rBV5	1992	2265	0.07%	0.010%
8	3.765	306	308	311	rVB4	1670	1847	0.06%	0.008%
9	3.795	311	313	316	rBV4	2142	2431	0.08%	0.010%
10	3.881	320	327	332	rBV4	3682	10151	0.32%	0.043%
11	3.948	336	338	340	rBV3	1434	1749	0.05%	0.007%
12	4.021	340	350	361	rBV	340309	1050428	32.78%	4.429%
13	4.204	371	380	395	rBV	590726	1616960	50.46%	6.818%
14	4.911	486	496	508	rBV2	38308	138685	4.33%	0.585%
15	5.063	518	521	522	rBV3	1829	1728	0.05%	0.007%
16	5.112	525	529	530	rBV4	2755	3952	0.12%	0.017%
17	5.307	557	561	563	rBV5	1492	1736	0.05%	0.007%
18	5.429	579	581	583	rVV3	1547	1931	0.06%	0.008%
19	5.545	596	600	603	rBV5	1766	2718	0.08%	0.011%
20	5.655	615	618	621	rVB5	1356	1779	0.06%	0.008%
21	5.691	621	624	627	rBV5	1464	1988	0.06%	0.008%
22	5.758	633	635	641	rVV7	1741	3290	0.10%	0.014%
23	5.807	641	643	648	rVB6	2005	2388	0.07%	0.010%
24	5.941	656	665	673	rBV4	13630	42537	1.33%	0.179%
25	6.167	698	702	703	rBV3	1640	1738	0.05%	0.007%
26	6.252	713	716	717	rBV3	1831	2106	0.07%	0.009%
27	6.423	738	744	747	rBV7	1146	2493	0.08%	0.011%
28	6.490	752	755	757	rVB4	1674	2048	0.06%	0.009%
29	6.667	782	784	787	rVB4	2009	1788	0.06%	0.008%
30	6.776	800	802	807	rBV6	1614	1988	0.06%	0.008%
31	6.929	823	827	828	rVV4	2185	2597	0.08%	0.011%
32	7.075	843	851	857	rBV	85292	239503	7.47%	1.010%
33	7.648	934	945	957	rVB	525824	1292935	40.35%	5.452%
34	7.782	962	967	969	rBV5	2104	2819	0.09%	0.012%
35	7.898	982	986	988	rBV5	1130	1670	0.05%	0.007%
36	7.977	997	999	1005	rVB7	1801	2855	0.09%	0.012%

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Integrator: RTE

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

37	8.160	1028	1029	1033	rVB4	1802	1789	0.06%	0.008%
38	8.203	1033	1036	1037	rBV3	1727	2028	0.06%	0.009%
39	8.276	1037	1048	1063	rBV2	1100934	3204468	100.00%	13.512%
40	8.514	1084	1087	1089	rBV3	1656	2166	0.07%	0.009%
41	8.557	1091	1094	1097	rVV4	2780	3743	0.12%	0.016%
42	8.624	1101	1105	1108	rVB6	1693	2559	0.08%	0.011%
43	8.843	1131	1141	1153	rBV	1094014	2163906	67.53%	9.124%
44	9.056	1172	1176	1177	rBV4	4261	5290	0.17%	0.022%
45	9.276	1203	1212	1221	rBV	747988	1528177	47.69%	6.444%
46	9.563	1256	1259	1262	rBV4	2062	3210	0.10%	0.014%
47	9.764	1290	1292	1295	rVB4	1646	1695	0.05%	0.007%
48	9.953	1320	1323	1326	rBV5	1776	2627	0.08%	0.011%
49	10.032	1329	1336	1347	rVV	320446	593802	18.53%	2.504%
50	10.136	1347	1353	1355	rVV2	31143	58970	1.84%	0.249%
51	10.184	1356	1361	1373	rVV2	59114	172656	5.39%	0.728%
52	10.318	1376	1383	1392	rVV	1419828	2581314	80.55%	10.884%
53	10.386	1392	1394	1403	rVB2	13614	20001	0.62%	0.084%
54	10.483	1407	1410	1411	rBV3	2128	2467	0.08%	0.010%
55	10.575	1418	1425	1435	rBV	203595	358494	11.19%	1.512%
56	10.703	1439	1446	1453	rBV2	56704	110099	3.44%	0.464%
57	10.757	1453	1455	1457	rVV3	3920	4078	0.13%	0.017%
58	10.855	1470	1471	1476	rVB5	1854	2126	0.07%	0.009%
59	10.922	1476	1482	1495	rBV	310340	554517	17.30%	2.338%
60	11.062	1500	1505	1510	rVV2	26611	47572	1.48%	0.201%
61	11.434	1561	1566	1575	rVB2	14132	27481	0.86%	0.116%
62	11.629	1591	1598	1607	rBV	1401003	2303741	71.89%	9.714%
63	11.788	1620	1624	1626	rBV5	1392	1907	0.06%	0.008%
64	11.843	1628	1633	1639	rVB8	5064	10262	0.32%	0.043%
65	11.934	1645	1648	1649	rBV3	2652	3093	0.10%	0.013%
66	11.965	1652	1653	1656	rVV3	2774	2456	0.08%	0.010%
67	12.093	1671	1674	1676	rBV4	1634	2002	0.06%	0.008%
68	12.330	1711	1713	1715	rBV3	1683	1795	0.06%	0.008%
69	12.428	1727	1729	1732	rVB4	1626	1919	0.06%	0.008%
70	12.464	1732	1735	1736	rBV3	2906	2766	0.09%	0.012%
71	12.519	1741	1744	1748	rBV6	2014	3359	0.10%	0.014%
72	12.605	1751	1758	1764	rVB	39491	70469	2.20%	0.297%
73	12.690	1764	1772	1779	rBV	460855	743913	23.21%	3.137%
74	12.751	1779	1782	1788	rVB3	7637	12586	0.39%	0.053%
75	12.891	1803	1805	1806	rBV2	1884	1829	0.06%	0.008%
76	12.928	1806	1811	1818	rVB7	8898	17503	0.55%	0.074%

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 Title : SFAM01.0

77	12.983	1818	1820	1822	rVB3	2482	2054	0.06%	0.009%
78	13.037	1822	1829	1832	rBV8	2650	5053	0.16%	0.021%
79	13.111	1837	1841	1849	rVB10	5766	12643	0.39%	0.053%
80	13.202	1849	1856	1864	rBV5	13819	32927	1.03%	0.139%
81	13.294	1867	1871	1876	rVB6	5801	9133	0.29%	0.039%
82	13.391	1882	1887	1889	rBV5	1967	3693	0.12%	0.016%
83	13.446	1894	1896	1897	rBV2	3037	2786	0.09%	0.012%
84	13.556	1907	1914	1924	rBV	1079278	1653223	51.59%	6.971%
85	13.641	1924	1928	1934	rVB	23514	39197	1.22%	0.165%
86	13.848	1955	1962	1971	rBV	867335	1410525	44.02%	5.948%
87	14.062	1992	1997	2004	rVB	21332	35852	1.12%	0.151%
88	14.318	2031	2039	2049	rBV	7183	21823	0.68%	0.092%
89	14.415	2049	2055	2061	rBV4	12825	24173	0.75%	0.102%
90	14.690	2097	2100	2102	rBV4	1977	2501	0.08%	0.011%
91	14.714	2102	2104	2108	rVB5	3589	5354	0.17%	0.023%
92	14.818	2119	2121	2124	rVV3	2044	1720	0.05%	0.007%
93	14.988	2147	2149	2153	rBV4	4453	5742	0.18%	0.024%
94	15.129	2169	2172	2174	rBV4	1903	2001	0.06%	0.008%
95	15.433	2214	2222	2227	rBV3	19249	41035	1.28%	0.173%
96	15.677	2260	2262	2266	rBV5	2063	2502	0.08%	0.011%
97	15.763	2272	2276	2278	rBV5	2662	4198	0.13%	0.018%
98	15.921	2297	2302	2305	rBV7	3558	7080	0.22%	0.030%
99	15.952	2305	2307	2312	rVV6	3198	4821	0.15%	0.020%
100	16.025	2314	2319	2335	rVB3	47627	94045	2.93%	0.397%

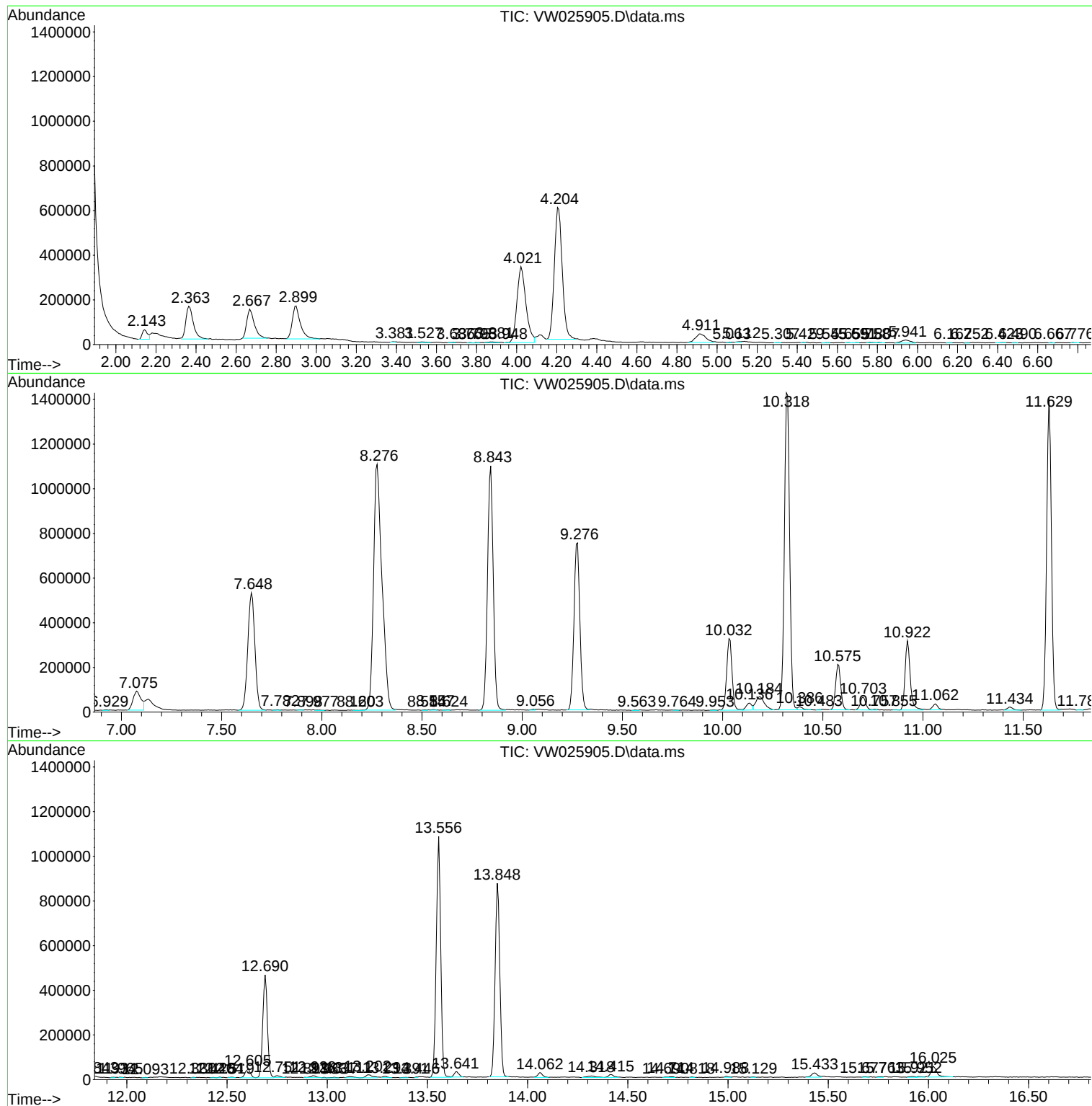
Sum of corrected areas: 23716225

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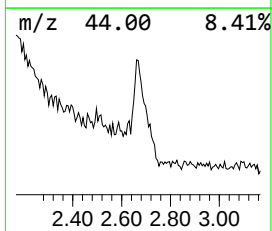
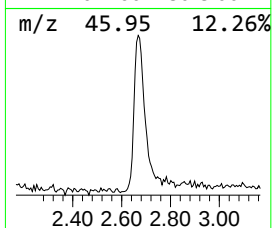
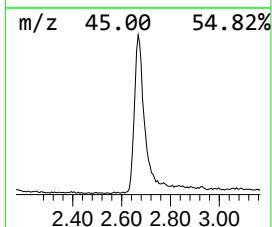
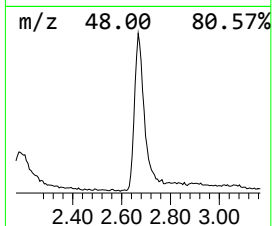
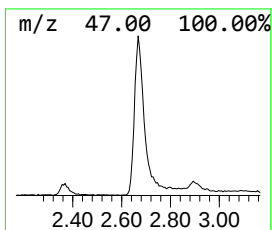
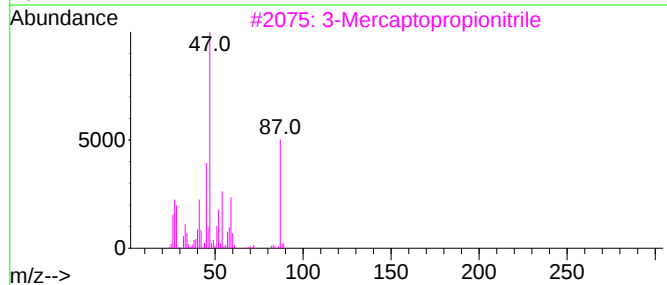
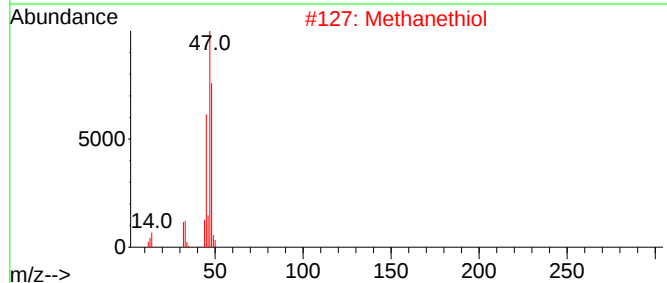
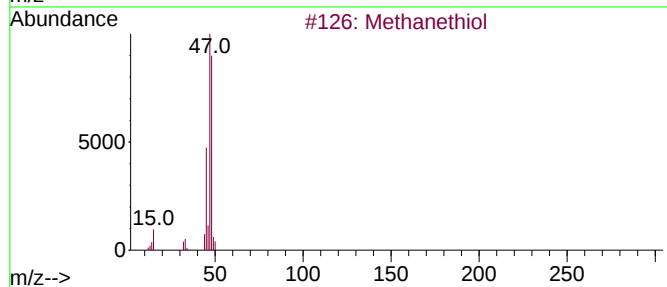
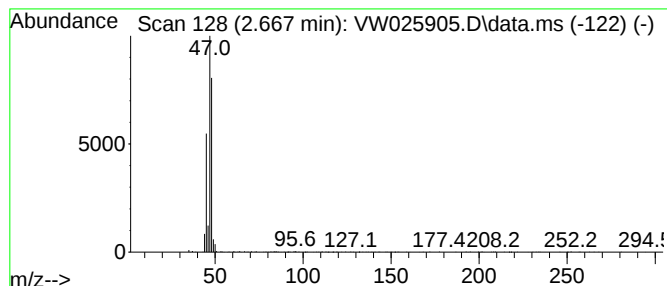
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM050123SMA.M
Quant Title : SFAM01.0

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.
2.667	3.91 ug/L	338467	1,4-Difluorobenzene	8.843

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanethiol	48	CH4S	000074-93-1	90
2			Methanethiol	48	CH4S	000074-93-1	90
3			3-Mercaptopropionitrile	87	C3H5NS	001001-58-7	28
4			Acetic acid, mercapto-	92	C2H4O2S	000068-11-1	28
5			Acetic acid, mercapto-	92	C2H4O2S	000068-11-1	9



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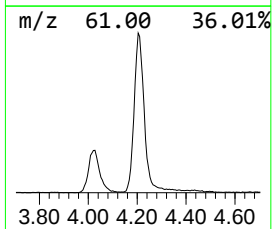
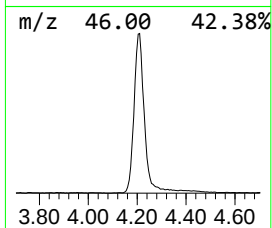
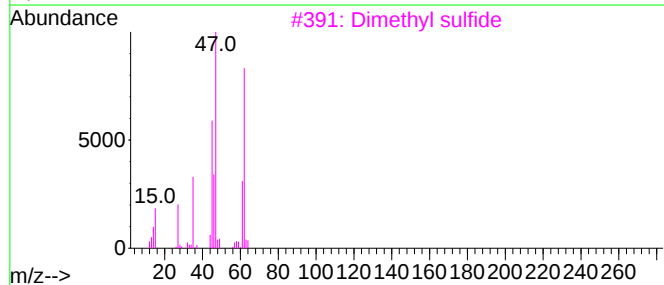
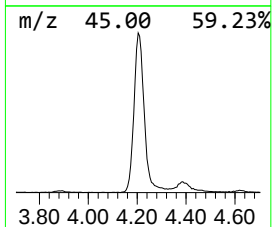
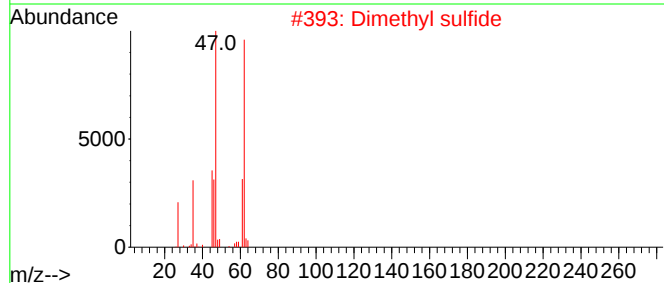
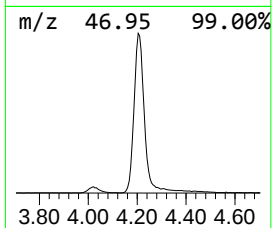
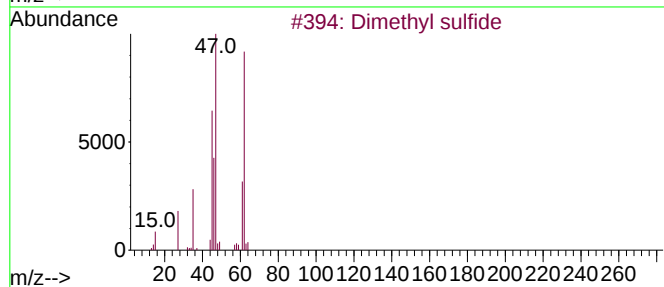
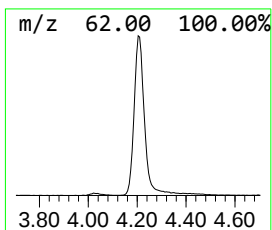
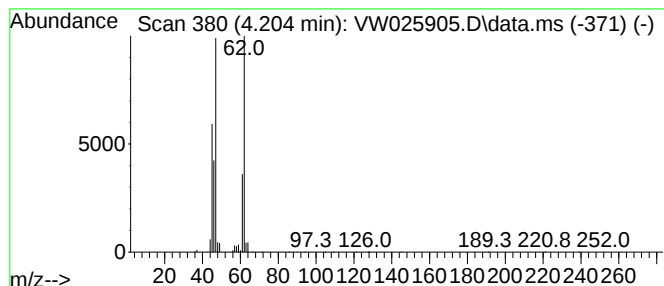
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM050123SMA.M
Quant Title : SFAM01.0

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	18.68 ug/L	1616960	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	91
5			Dimethyl sulfide	62	C2H6S	000075-18-3	91



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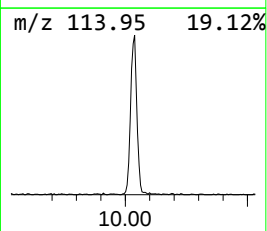
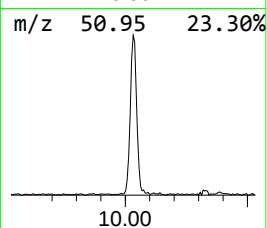
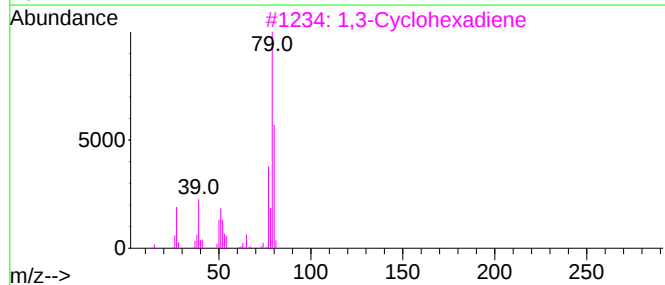
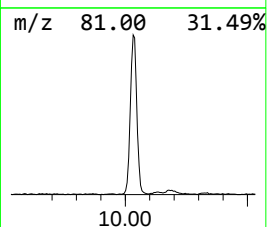
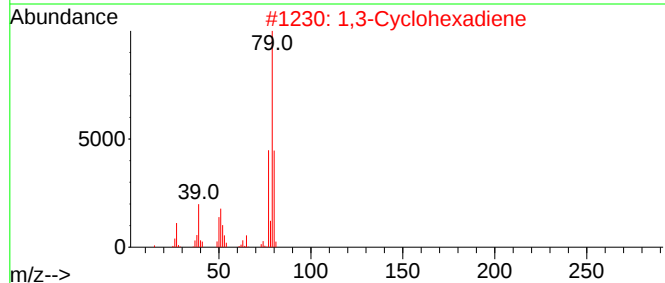
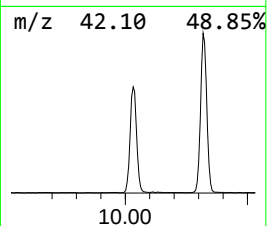
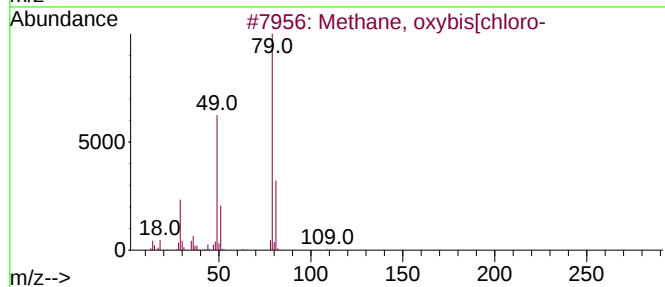
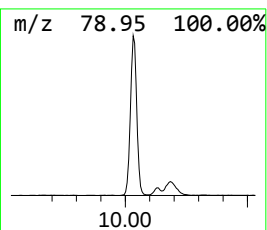
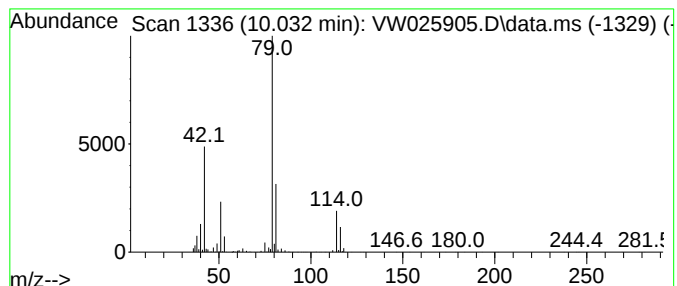
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Quant Title : SFAM01.0

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

Peak Number 3 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.032	6.86 ug/L	593802	1,4-Difluorobenzene	8.843

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methane, oxybis[chloro-	114	C2H4Cl2O	000542-88-1	37
2			1,3-Cyclohexadiene	80	C6H8	000592-57-4	25
3			1,3-Cyclohexadiene	80	C6H8	000592-57-4	25
4			Thiophosgene	114	CCl2S	000463-71-8	16
5			3-Thiatricyclo[3.1.1.0(2,4)]heptane	112	C6H8S	1000221-37-0	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW050923\
Data File : VW025905.D
Acq On : 09 May 2023 14:04
Operator : SY/MD
Sample : 02612-28
Misc : 3.56g/10mL/MSVOA_W/SOIL
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
JREG9

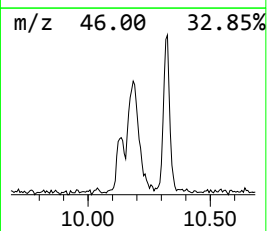
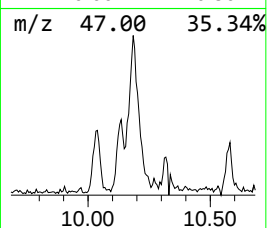
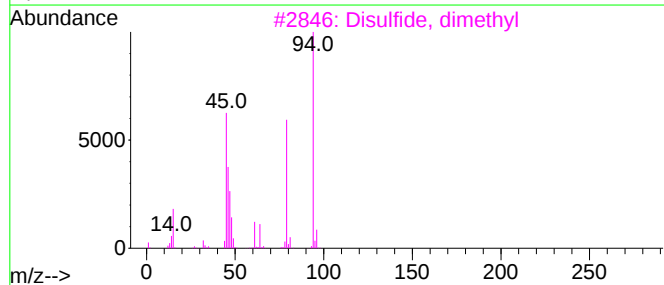
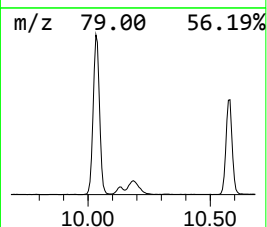
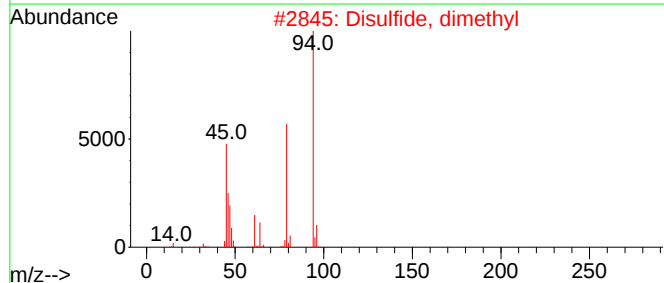
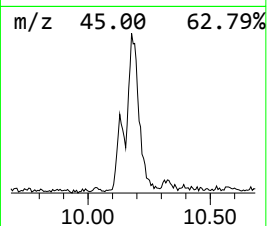
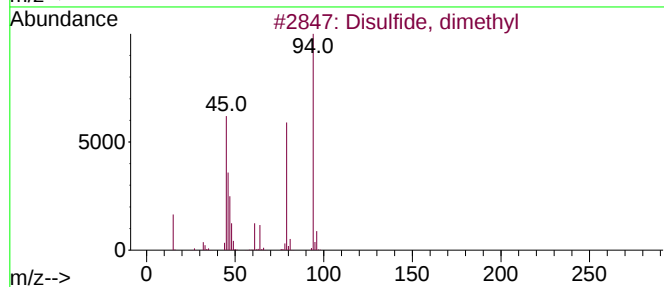
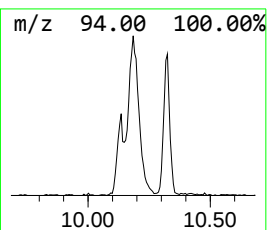
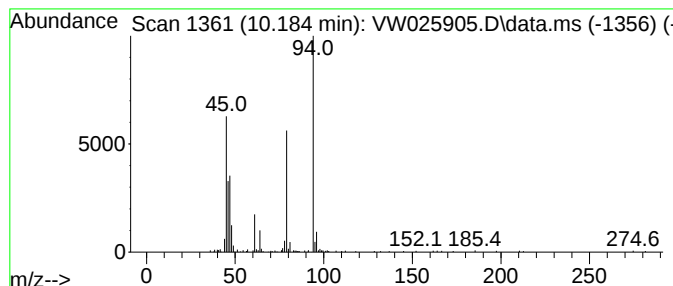
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Quant Title : SFAM01.0

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

Peak Number 4 Disulfide, dimethyl Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.184	1.99 ug/L	172656	1,4-Difluorobenzene	8.843

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Disulfide, dimethyl	94	C2H6S2	000624-92-0	94
2			Disulfide, dimethyl	94	C2H6S2	000624-92-0	94
3			Disulfide, dimethyl	94	C2H6S2	000624-92-0	91
4			Disulfide, dimethyl	94	C2H6S2	000624-92-0	91
5			Disulfide, dimethyl	94	C2H6S2	000624-92-0	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW050923\
Data File : VW025905.D
Acq On : 09 May 2023 14:04
Operator : SY/MD
Sample : 02612-28
Misc : 3.56g/10mL/MSVOA_W/SOIL
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
JREG9

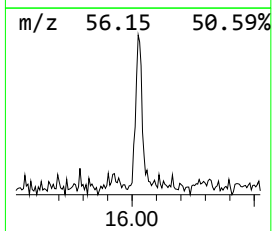
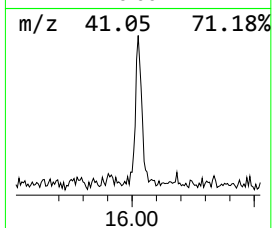
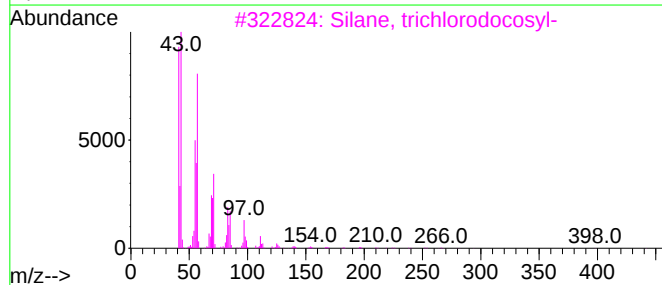
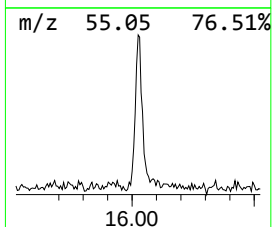
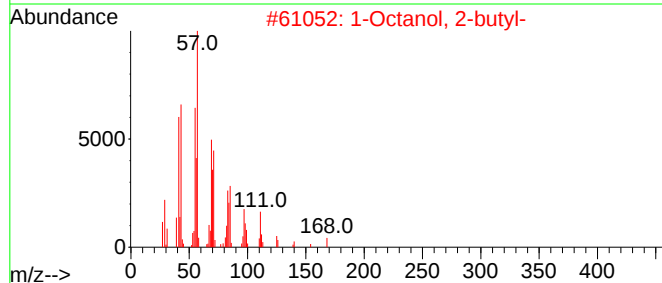
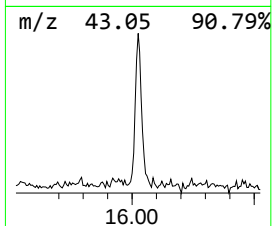
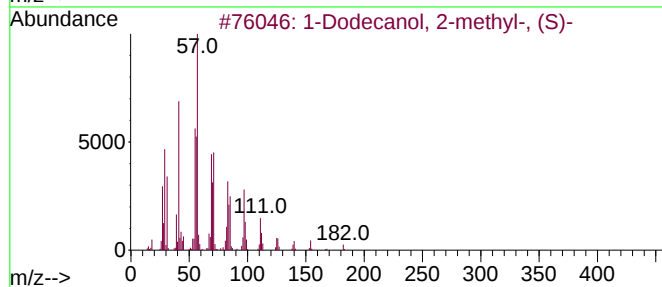
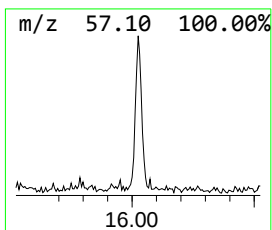
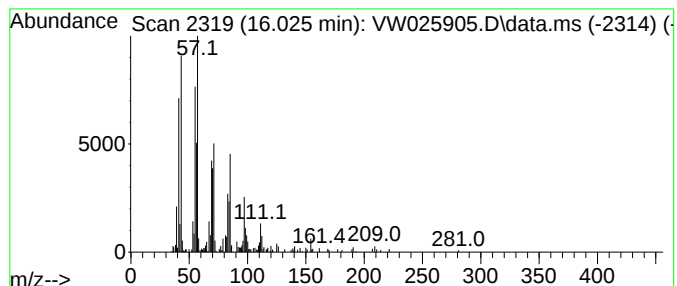
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Quant Title : SFAM01.0

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

Peak Number 5 1-Dodecanol, 2-methyl-, (S)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.025	1.42 ug/L	94045	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Dodecanol, 2-methyl-, (S)-	200	C13H28O	057289-26-6	86
2			1-Octanol, 2-butyl-	186	C12H26O	003913-02-8	80
3			Silane, trichlorodocosyl-	442	C22H45Cl3Si	007325-84-0	80
4			Cyclooctane, 1,2-dimethyl-	140	C10H20	013151-94-5	70
5			Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW050923\
Data File : VW025905.D
Acq On : 09 May 2023 14:04
Operator : SY/MD
Sample : 02612-28
Misc : 3.56g/10mL/MSVOA_W/SOIL
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
JREG9

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	2.667	3.9	ug/L	338467	1	8.843	2163910	25.0
Dimethyl sulfide	4.204	18.7	ug/L	1616960	1	8.843	2163910	25.0
unknown-01	10.032	6.9	ug/L	593802	1	8.843	2163910	25.0
Disulfide, dime...	10.184	2.0	ug/L	172656	1	8.843	2163910	25.0
1-Dodecanol, 2-...	16.025	1.4	ug/L	94045	3	13.556	1653220	25.0