

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW092121\
 Data File : VW020105.D
 Acq On : 21 Sep 2021 20:40
 Operator : SY/VA
 Sample : M3813-17
 Misc : 5.51g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 GB6W1

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\SFAMWLM092121SMA.M
 Title : SFAM01.0

Signal : TIC: VW020105.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.203	36	49	69	rBV	91833	603613	41.30%	5.002%
2	2.361	71	75	90	rVB	122658	267062	18.27%	2.213%
3	2.898	157	163	180	rVB	88835	224048	15.33%	1.857%
4	3.666	287	289	293	rVB2	242	215	0.01%	0.002%
5	3.903	325	328	335	rVB3	339	518	0.04%	0.004%
6	4.025	335	348	385	rBV2	165375	560338	38.34%	4.643%
7	4.269	385	388	389	rBV4	339	407	0.03%	0.003%
8	4.318	394	396	397	rVB	379	171	0.01%	0.001%
9	4.336	397	399	401	rBV	221	189	0.01%	0.002%
10	4.391	401	408	419	rVB4	1464	4487	0.31%	0.037%
11	4.525	427	430	431	rVB2	297	225	0.02%	0.002%
12	4.568	434	437	438	rBV2	149	172	0.01%	0.001%
13	4.672	452	454	458	rVB2	268	333	0.02%	0.003%
14	4.720	458	462	465	rBV3	131	239	0.02%	0.002%
15	4.745	465	466	469	rVV2	251	195	0.01%	0.002%
16	4.922	484	495	517	rVB2	18438	65195	4.46%	0.540%
17	5.129	520	529	544	rVB4	1593	5519	0.38%	0.046%
18	5.318	558	560	563	rBV2	132	181	0.01%	0.001%
19	5.946	655	663	675	rVB4	5175	15420	1.06%	0.128%
20	6.110	687	690	691	rBV	322	359	0.02%	0.003%
21	6.220	706	708	710	rBV	254	243	0.02%	0.002%
22	6.263	713	715	717	rVV2	187	177	0.01%	0.001%
23	6.714	785	789	791	rBV2	200	304	0.02%	0.003%
24	6.903	812	820	831	rBV3	5584	16293	1.11%	0.135%
25	7.080	839	849	866	rBV2	41375	130193	8.91%	1.079%
26	7.220	870	872	874	rVB2	338	222	0.02%	0.002%
27	7.470	909	913	915	rBV	190	175	0.01%	0.001%
28	7.549	924	926	928	rVV2	354	385	0.03%	0.003%
29	7.653	932	943	955	rBV	255649	623720	42.68%	5.169%
30	7.891	979	982	985	rVB2	405	394	0.03%	0.003%
31	7.964	989	994	996	rBV3	537	1020	0.07%	0.008%
32	8.073	1010	1012	1014	rBV	201	200	0.01%	0.002%
33	8.281	1035	1046	1063	rBV2	493960	1461459	100.00%	12.111%
34	8.512	1080	1084	1087	rBV2	441	578	0.04%	0.005%
35	8.543	1087	1089	1090	rBV	359	322	0.02%	0.003%
36	8.628	1100	1103	1107	rVB2	429	607	0.04%	0.005%

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 Title : SFAM01.0

37	8.695	1110	1114	1116	rBV3	904	1290	0.09%	0.011%
38	8.848	1130	1139	1153	rBV	481824	940370	64.34%	7.793%
39	9.049	1166	1172	1182	rBV3	7373	15344	1.05%	0.127%
40	9.134	1185	1186	1190	rVB2	235	170	0.01%	0.001%
41	9.274	1199	1209	1220	rBV	338221	689262	47.16%	5.712%
42	9.409	1226	1231	1243	rVB2	13657	26058	1.78%	0.216%
43	9.494	1243	1245	1247	rVV3	177	193	0.01%	0.002%
44	9.518	1247	1249	1253	rVB2	341	377	0.03%	0.003%
45	9.591	1259	1261	1265	rVB2	291	252	0.02%	0.002%
46	9.665	1270	1273	1278	rBV4	330	439	0.03%	0.004%
47	9.701	1278	1279	1284	rVB3	208	213	0.01%	0.002%
48	9.817	1292	1298	1300	rBV2	269	303	0.02%	0.003%
49	9.890	1309	1310	1314	rBV3	223	281	0.02%	0.002%
50	10.037	1327	1334	1346	rBV	179135	321169	21.98%	2.661%
51	10.226	1362	1365	1369	rVB2	236	318	0.02%	0.003%
52	10.262	1369	1371	1372	rBV2	244	177	0.01%	0.001%
53	10.323	1373	1381	1388	rVV	674109	1201995	82.25%	9.961%
54	10.390	1388	1392	1400	rVB	25892	46019	3.15%	0.381%
55	10.500	1406	1410	1412	rBV2	514	799	0.05%	0.007%
56	10.518	1412	1413	1415	rVV	696	449	0.03%	0.004%
57	10.579	1416	1423	1435	rVV	124595	217089	14.85%	1.799%
58	10.707	1438	1444	1456	rVV	29589	54105	3.70%	0.448%
59	10.817	1459	1462	1466	rVB3	217	321	0.02%	0.003%
60	10.927	1473	1480	1494	rBV	184175	312518	21.38%	2.590%
61	11.073	1497	1504	1513	rBV	134684	217735	14.90%	1.804%
62	11.384	1553	1555	1556	rBV	356	243	0.02%	0.002%
63	11.439	1562	1564	1569	rVB3	320	451	0.03%	0.004%
64	11.536	1578	1580	1583	rBV	222	298	0.02%	0.002%
65	11.567	1583	1585	1588	rBV3	252	243	0.02%	0.002%
66	11.634	1588	1596	1605	rBV	705896	1180714	80.79%	9.784%
67	11.811	1619	1625	1628	rBV3	2175	4027	0.28%	0.033%
68	12.061	1664	1666	1667	rBV	202	187	0.01%	0.002%
69	12.091	1668	1671	1679	rVV5	1107	2216	0.15%	0.018%
70	12.176	1681	1685	1691	rVB3	569	754	0.05%	0.006%
71	12.237	1692	1695	1698	rVB2	634	899	0.06%	0.007%
72	12.262	1698	1699	1701	rBV2	305	298	0.02%	0.002%
73	12.341	1706	1712	1721	rVV2	18235	29539	2.02%	0.245%
74	12.445	1728	1729	1732	rBV	200	169	0.01%	0.001%
75	12.554	1743	1747	1748	rBV2	207	211	0.01%	0.002%
76	12.609	1748	1756	1763	rBV	66413	113296	7.75%	0.939%

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 Title : SFAM01.0

77	12.695	1763	1770	1777	rBV	282123	470474	32.19%	3.899%
78	12.835	1791	1793	1795	rBV2	247	270	0.02%	0.002%
79	12.859	1795	1797	1800	rVB	315	304	0.02%	0.003%
80	12.932	1807	1809	1810	rBV2	869	542	0.04%	0.004%
81	13.005	1819	1821	1822	rBV2	479	479	0.03%	0.004%
82	13.097	1832	1836	1841	rBV5	1063	2061	0.14%	0.017%
83	13.396	1879	1885	1895	rVV3	8192	15561	1.06%	0.129%
84	13.475	1895	1898	1900	rBV3	599	708	0.05%	0.006%
85	13.560	1904	1912	1919	rBV	693042	1084658	74.22%	8.988%
86	13.646	1923	1926	1933	rVB2	16168	25350	1.73%	0.210%
87	13.853	1952	1960	1973	rBV	626893	1006014	68.84%	8.337%
88	14.066	1990	1995	2004	rVB2	26803	46047	3.15%	0.382%
89	14.322	2032	2037	2043	rBV3	10731	16857	1.15%	0.140%
90	14.426	2052	2054	2058	rVB2	807	638	0.04%	0.005%
91	14.499	2063	2066	2067	rBV3	717	719	0.05%	0.006%
92	14.786	2111	2113	2116	rBV2	401	371	0.03%	0.003%
93	14.871	2125	2127	2128	rBV	411	243	0.02%	0.002%
94	14.950	2136	2140	2146	rVB5	3946	6341	0.43%	0.053%
95	15.182	2174	2178	2181	rBV3	2381	3451	0.24%	0.029%
96	15.401	2211	2214	2219	rVB7	1193	1495	0.10%	0.012%
97	15.487	2223	2228	2235	rVB	7075	12503	0.86%	0.104%
98	15.962	2300	2306	2312	rVB4	892	1857	0.13%	0.015%
99	16.328	2359	2366	2370	rBV6	1974	4359	0.30%	0.036%
100	16.450	2385	2386	2387	rBV	477	251	0.02%	0.002%

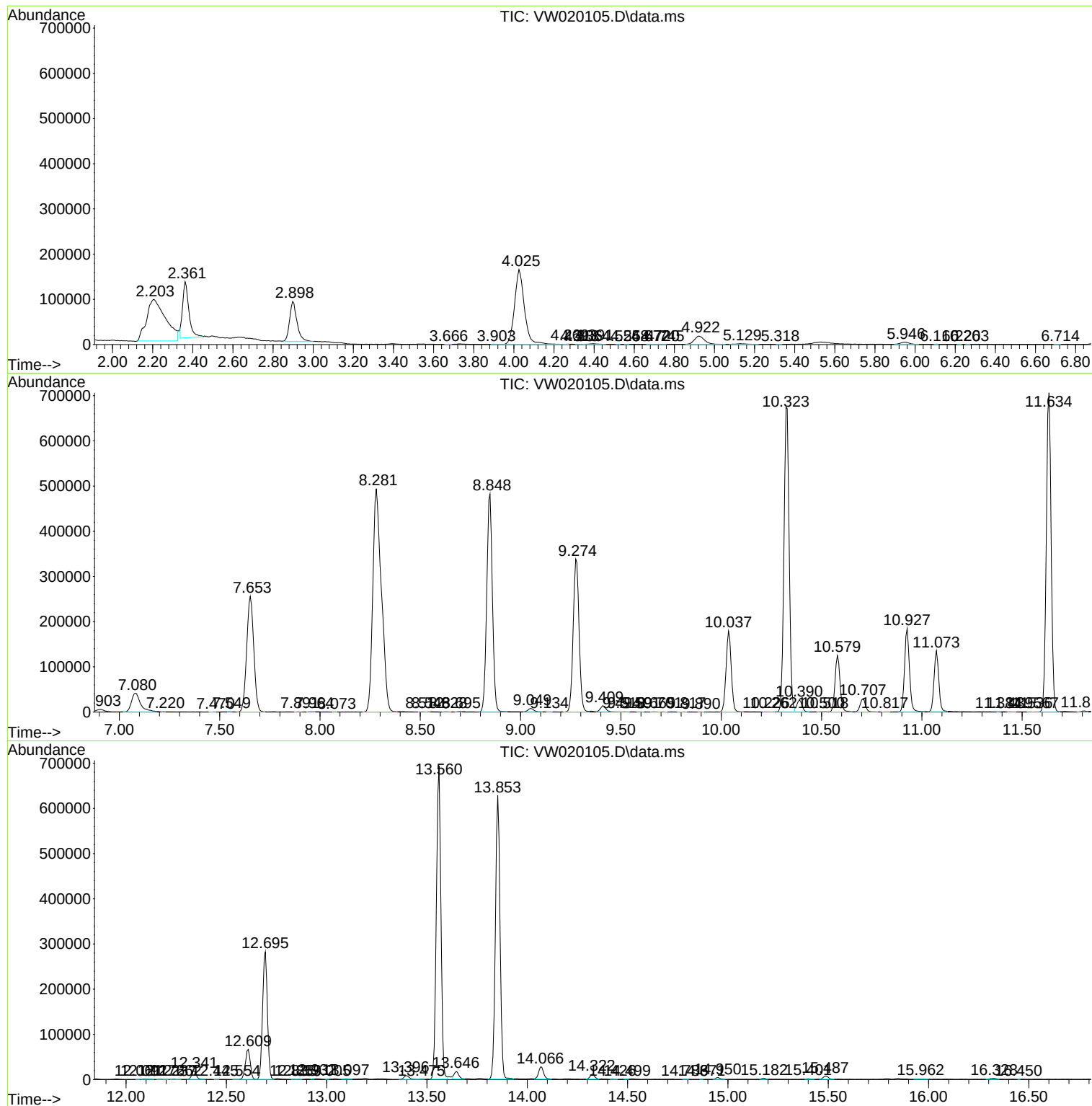
Sum of corrected areas: 12067522

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM092121SMA.M
Quant Title : SFAM01.0

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



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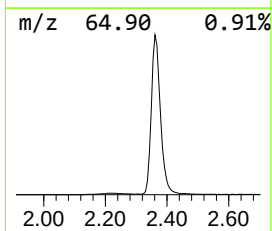
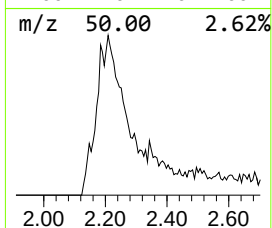
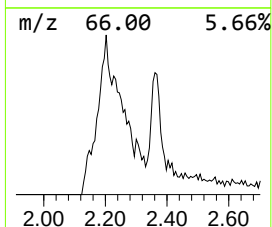
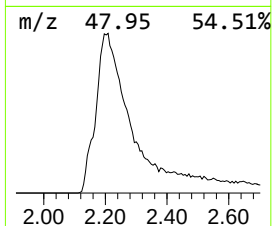
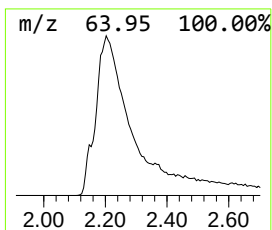
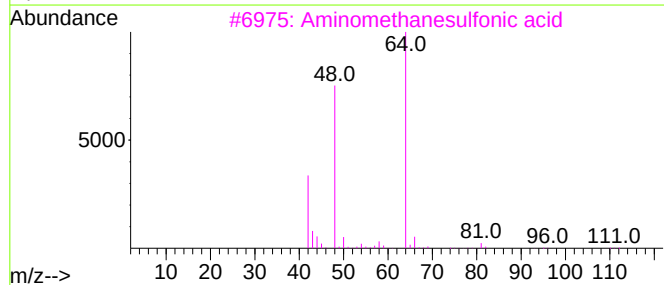
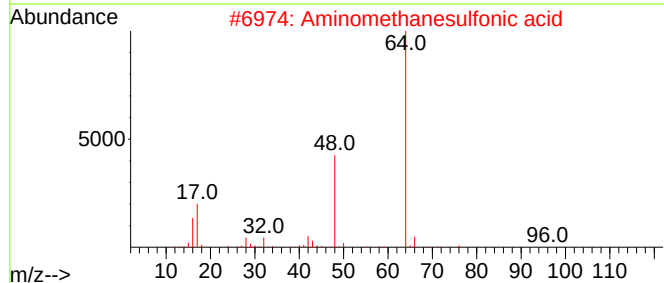
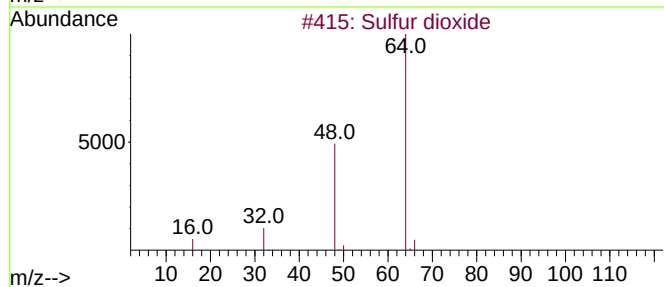
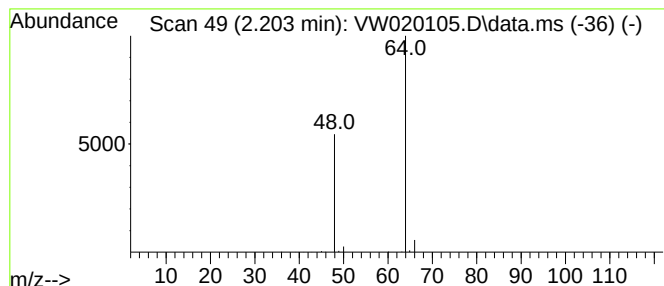
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM092121SMA.M
Quant Title : SFAM01.0

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.203	16.05 ug/L	603613	1,4-Difluorobenzene	8.848

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	25
4			Sulfur dioxide	64	O2S	007446-09-5	9
5			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9



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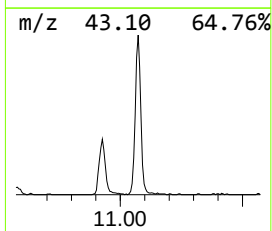
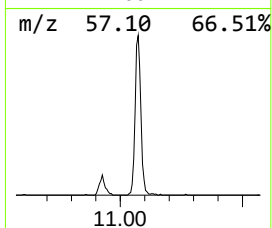
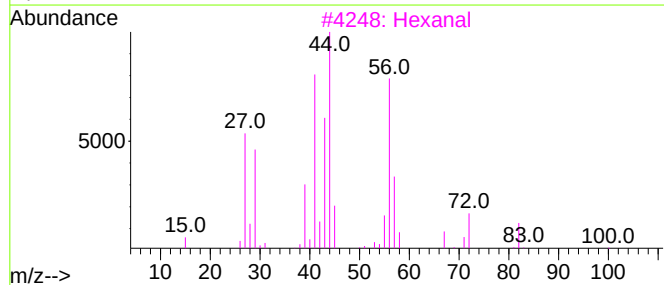
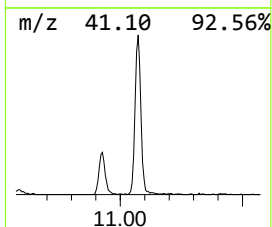
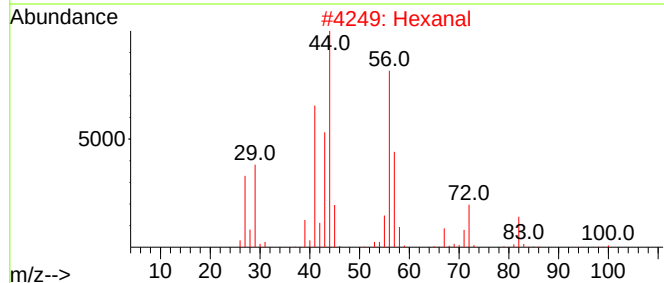
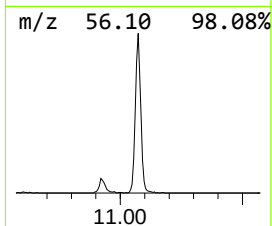
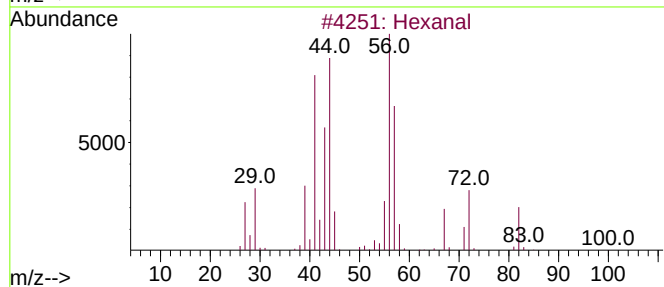
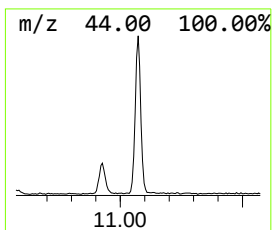
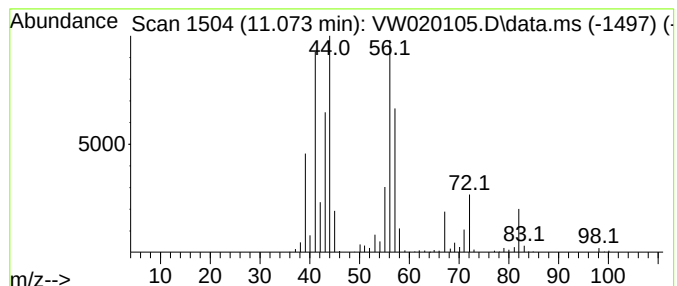
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Quant Title : SFAM01.0

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

Peak Number 3 Hexanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.073	4.61 ug/L	217735	Chlorobenzene-d5	11.634

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	95
2	Hexanal			100	C6H12O	000066-25-1	81
3	Hexanal			100	C6H12O	000066-25-1	64
4	Hexanal			100	C6H12O	000066-25-1	64
5	Hexanal			100	C6H12O	000066-25-1	59



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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
Sulfur dioxide	2.203	16.1	ug/L	603613	1	8.848	940370	25.0
Hexanal	11.073	4.6	ug/L	217735	2	11.634	1180710	25.0