

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW092121\
 Data File : VW020104.D
 Acq On : 21 Sep 2021 20:16
 Operator : SY/VA
 Sample : M3813-16
 Misc : 6.00g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 GB6W0

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: VW020104.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.154	35	41	68	rBV	90376	514007	35.52%	4.367%
2	2.361	70	75	86	rVB	118512	240591	16.62%	2.044%
3	2.898	157	163	176	rVB	86014	210352	14.53%	1.787%
4	3.312	229	231	233	rVB2	339	296	0.02%	0.003%
5	3.465	254	256	258	rBV2	270	295	0.02%	0.003%
6	3.599	275	278	281	rVB2	309	365	0.03%	0.003%
7	3.715	293	297	299	rBV3	761	1033	0.07%	0.009%
8	3.897	325	327	332	rBV3	287	474	0.03%	0.004%
9	4.025	335	348	373	rBV	162439	529439	36.58%	4.498%
10	4.306	390	394	395	rVB2	227	254	0.02%	0.002%
11	4.391	399	408	416	rBV	6269	17247	1.19%	0.147%
12	4.544	430	433	436	rVB2	146	198	0.01%	0.002%
13	4.611	441	444	445	rBV2	185	200	0.01%	0.002%
14	4.684	450	456	463	rVV4	759	1889	0.13%	0.016%
15	4.922	484	495	513	rVB3	19902	68994	4.77%	0.586%
16	5.092	519	523	524	rBV3	685	787	0.05%	0.007%
17	5.354	563	566	567	rBV2	359	337	0.02%	0.003%
18	5.434	577	579	581	rVB2	316	253	0.02%	0.002%
19	5.659	613	616	619	rVB	216	236	0.02%	0.002%
20	5.799	637	639	645	rVV3	407	667	0.05%	0.006%
21	5.946	654	663	675	rVB4	4653	14634	1.01%	0.124%
22	6.464	746	748	751	rVB	189	205	0.01%	0.002%
23	6.494	751	753	757	rBV2	203	300	0.02%	0.003%
24	6.610	769	772	773	rBV	313	334	0.02%	0.003%
25	6.909	813	821	831	rVB4	2084	6038	0.42%	0.051%
26	7.080	840	849	871	rBV	39032	117428	8.11%	0.998%
27	7.342	890	892	894	rBV2	262	238	0.02%	0.002%
28	7.537	921	924	929	rBV3	251	424	0.03%	0.004%
29	7.653	932	943	954	rBV	260034	624610	43.16%	5.306%
30	7.763	959	961	965	rBV3	281	282	0.02%	0.002%
31	7.891	979	982	986	rVB3	404	470	0.03%	0.004%
32	7.952	986	992	993	rBV2	581	809	0.06%	0.007%
33	8.281	1036	1046	1062	rBV2	499297	1447272	100.00%	12.295%
34	8.476	1074	1078	1080	rBV2	229	234	0.02%	0.002%
35	8.549	1085	1090	1092	rBV2	618	905	0.06%	0.008%
36	8.622	1099	1102	1107	rBV3	335	624	0.04%	0.005%

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 Title : SFAM01.0

37	8.701	1107	1115	1119	rBV4	603	1239	0.09%	0.011%
38	8.848	1128	1139	1152	rBV	513121	984896	68.05%	8.367%
39	9.049	1167	1172	1183	rVB4	3576	7720	0.53%	0.066%
40	9.128	1183	1185	1188	rVB2	256	263	0.02%	0.002%
41	9.153	1188	1189	1192	rBV2	269	283	0.02%	0.002%
42	9.201	1195	1197	1200	rVB3	321	268	0.02%	0.002%
43	9.274	1200	1209	1226	rBV	330768	685532	47.37%	5.824%
44	9.409	1226	1231	1240	rVB2	9492	19882	1.37%	0.169%
45	9.524	1248	1250	1253	rVB2	551	544	0.04%	0.005%
46	9.659	1270	1272	1274	rBV3	413	434	0.03%	0.004%
47	9.854	1302	1304	1306	rBV	249	253	0.02%	0.002%
48	10.037	1327	1334	1345	rBV	176879	313886	21.69%	2.667%
49	10.323	1373	1381	1388	rBV	682687	1202870	83.11%	10.219%
50	10.390	1388	1392	1398	rVB2	18484	31955	2.21%	0.271%
51	10.494	1405	1409	1411	rBV3	545	893	0.06%	0.008%
52	10.579	1416	1423	1434	rBV	120221	207180	14.32%	1.760%
53	10.707	1438	1444	1452	rVV	27973	49726	3.44%	0.422%
54	10.829	1461	1464	1467	rBV3	218	335	0.02%	0.003%
55	10.927	1472	1480	1497	rBV	167638	286596	19.80%	2.435%
56	11.073	1498	1504	1515	rVB	87155	142504	9.85%	1.211%
57	11.256	1533	1534	1537	rBV2	417	350	0.02%	0.003%
58	11.286	1537	1539	1540	rVV2	389	220	0.02%	0.002%
59	11.299	1540	1541	1545	rVV2	282	287	0.02%	0.002%
60	11.353	1548	1550	1554	rVV2	329	357	0.02%	0.003%
61	11.481	1566	1571	1572	rBV	225	369	0.03%	0.003%
62	11.530	1577	1579	1583	rVB	241	215	0.01%	0.002%
63	11.573	1584	1586	1588	rBV	387	323	0.02%	0.003%
64	11.634	1588	1596	1606	rBV	725990	1231065	85.06%	10.458%
65	11.805	1619	1624	1627	rBV	4698	7250	0.50%	0.062%
66	11.957	1643	1649	1651	rBV4	829	1378	0.10%	0.012%
67	12.048	1659	1664	1667	rBV2	320	402	0.03%	0.003%
68	12.097	1667	1672	1674	rBV3	607	1043	0.07%	0.009%
69	12.243	1693	1696	1698	rBV2	374	535	0.04%	0.005%
70	12.341	1706	1712	1719	rBV2	10386	15918	1.10%	0.135%
71	12.432	1722	1727	1729	rBV3	416	464	0.03%	0.004%
72	12.463	1729	1732	1734	rBV	280	284	0.02%	0.002%
73	12.603	1747	1755	1763	rBV2	54779	95250	6.58%	0.809%
74	12.695	1763	1770	1777	rBV	268523	440466	30.43%	3.742%
75	12.859	1793	1797	1799	rBV3	421	725	0.05%	0.006%
76	12.890	1799	1802	1805	rBV4	751	1088	0.08%	0.009%

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 Title : SFAM01.0

77	13.012	1820	1822	1823	rBV2	554	465	0.03%	0.004%
78	13.103	1833	1837	1842	rVB4	1544	2258	0.16%	0.019%
79	13.237	1857	1859	1860	rBV2	511	260	0.02%	0.002%
80	13.402	1879	1886	1892	rBV3	5566	10303	0.71%	0.088%
81	13.469	1896	1897	1899	rBV	386	326	0.02%	0.003%
82	13.560	1904	1912	1919	rVV	715831	1125397	77.76%	9.561%
83	13.646	1922	1926	1933	rVB	24560	40241	2.78%	0.342%
84	13.853	1953	1960	1969	rBV	625442	988308	68.29%	8.396%
85	14.066	1990	1995	2004	rVB	22512	37163	2.57%	0.316%
86	14.322	2033	2037	2042	rVB4	7175	10577	0.73%	0.090%
87	14.475	2060	2062	2063	rBV2	314	264	0.02%	0.002%
88	14.627	2084	2087	2090	rBV4	358	633	0.04%	0.005%
89	14.725	2099	2103	2106	rVB3	741	1027	0.07%	0.009%
90	14.950	2136	2140	2144	rVB4	1806	3007	0.21%	0.026%
91	15.036	2152	2154	2157	rBV3	280	253	0.02%	0.002%
92	15.133	2168	2170	2173	rBV3	343	286	0.02%	0.002%
93	15.176	2173	2177	2183	rVV6	1287	2010	0.14%	0.017%
94	15.340	2202	2204	2206	rBV3	324	394	0.03%	0.003%
95	15.487	2223	2228	2238	rVB	3771	7208	0.50%	0.061%
96	15.767	2270	2274	2276	rBV3	415	612	0.04%	0.005%
97	15.798	2276	2279	2281	rVB3	751	932	0.06%	0.008%
98	16.096	2324	2328	2333	rVB3	476	834	0.06%	0.007%
99	16.462	2386	2388	2389	rBV	312	206	0.01%	0.002%
100	16.737	2432	2433	2435	rBV	360	348	0.02%	0.003%

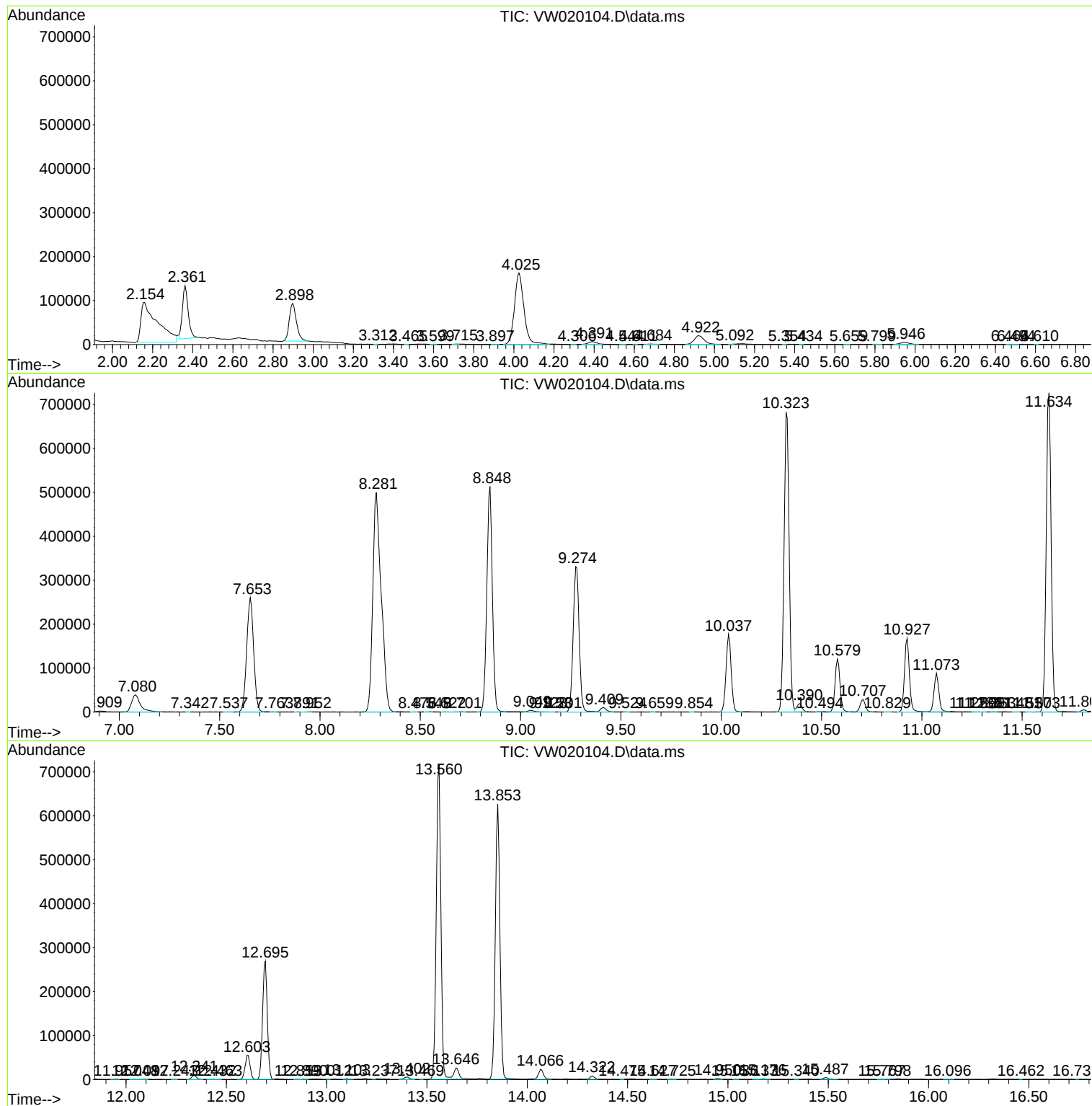
Sum of corrected areas: 11771281

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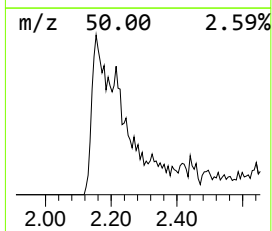
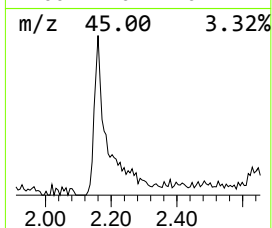
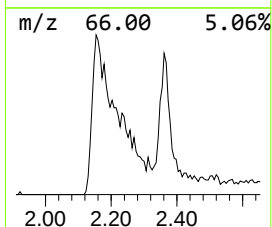
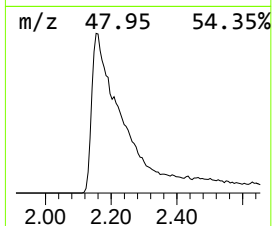
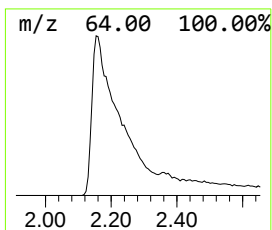
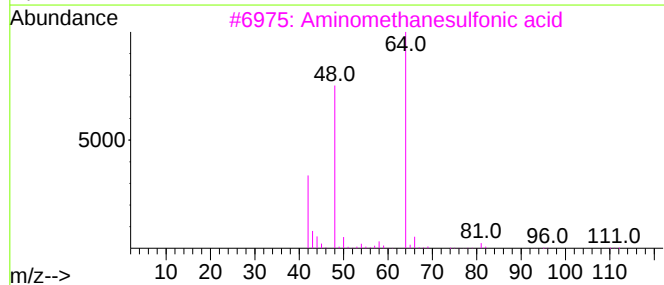
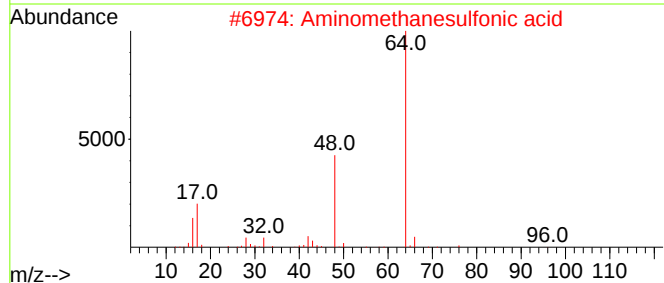
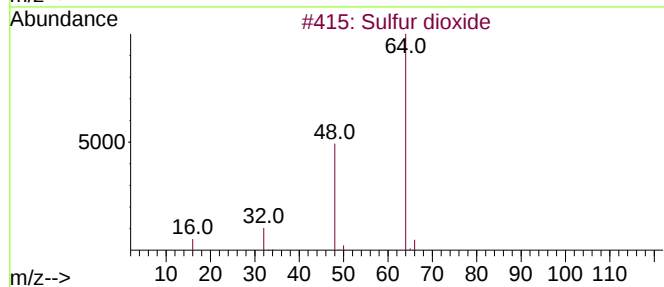
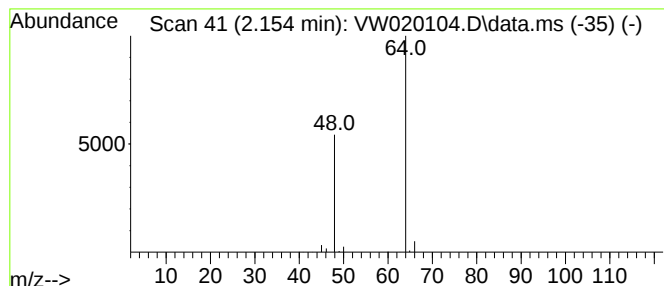
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM092121SMA.M
Quant Title : SFAM01.0

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.
2.154	13.05 ug/L	514007	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	64
4			Sulfur dioxide	64	O2S	007446-09-5	9
5			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9



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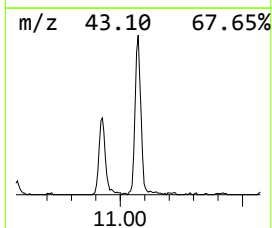
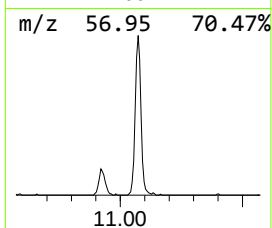
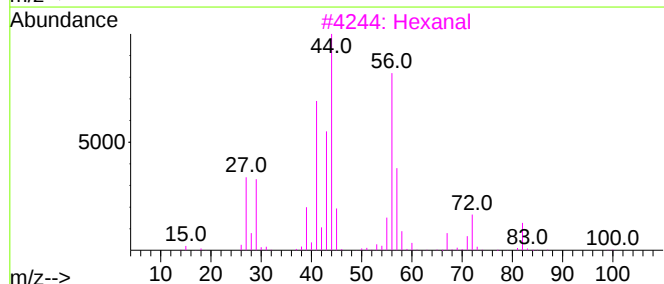
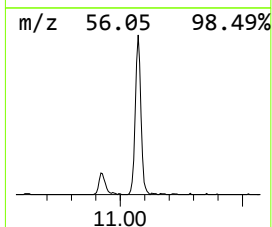
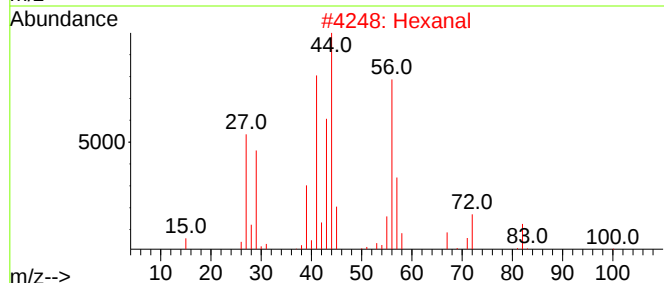
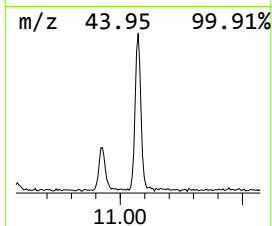
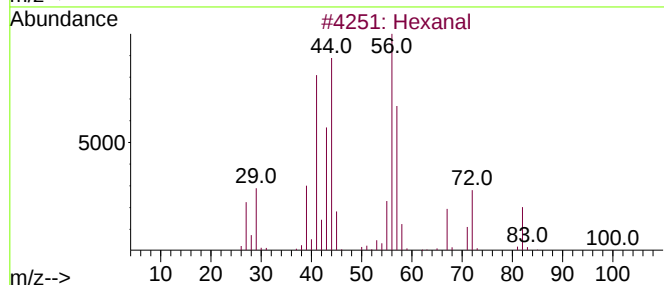
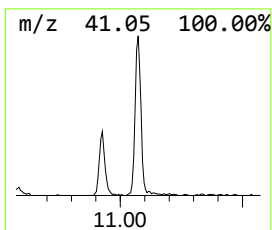
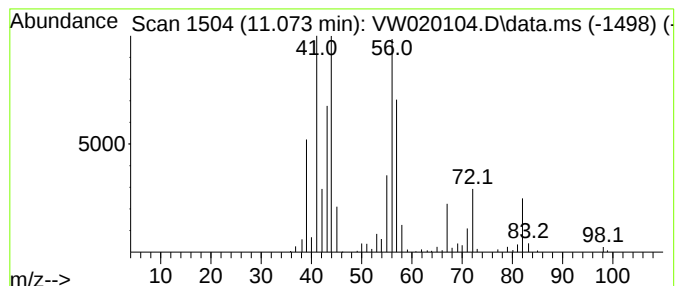
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Quant Title : SFAM01.0

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	2.89 ug/L	142504	Chlorobenzene-d5	11.634

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	80
2	Hexanal			100	C6H12O	000066-25-1	59
3	Hexanal			100	C6H12O	000066-25-1	53
4	Hexanal			100	C6H12O	000066-25-1	53
5	Hexanal			100	C6H12O	000066-25-1	45



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.154	13.1	ug/L	514007	1	8.848	984896	25.0
Hexanal	11.073	2.9	ug/L	142504	2	11.634	1231070	25.0