

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW083121\
 Data File : VW019959.D
 Acq On : 31 Aug 2021 15:35
 Operator : SY/VA
 Sample : M3579-16RE
 Misc : 4.68g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 GB6B8RE

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\SFAMWLM081821SMA.M
 Title : SFAM01.0

Signal : TIC: VW019959.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.361	70	75	86	rVB	102917	205113	17.02%	2.581%
2	2.507	95	99	109	rBV	25167	55613	4.61%	0.700%
3	2.898	156	163	180	rVB	89753	223082	18.51%	2.808%
4	3.288	226	227	230	rBV2	303	226	0.02%	0.003%
5	3.355	236	238	239	rBV2	312	213	0.02%	0.003%
6	3.398	239	245	250	rVV4	1439	3273	0.27%	0.041%
7	3.715	293	297	298	rBV2	559	759	0.06%	0.010%
8	4.025	336	348	361	rBV	120265	381631	31.66%	4.803%
9	4.397	401	409	415	rBV4	862	2438	0.20%	0.031%
10	4.617	444	445	447	rVB2	301	199	0.02%	0.003%
11	4.641	447	449	450	rBV	276	192	0.02%	0.002%
12	4.684	453	456	457	rBV3	333	277	0.02%	0.003%
13	4.806	473	476	478	rBV	218	214	0.02%	0.003%
14	4.922	484	495	514	rBV4	9678	34144	2.83%	0.430%
15	5.129	526	529	531	rBV2	167	226	0.02%	0.003%
16	5.196	538	540	542	rBV3	244	225	0.02%	0.003%
17	5.952	656	664	671	rVB6	1897	5535	0.46%	0.070%
18	6.092	685	687	689	rBV2	308	339	0.03%	0.004%
19	6.226	707	709	712	rBV2	258	225	0.02%	0.003%
20	6.336	726	727	731	rVB2	195	205	0.02%	0.003%
21	6.909	813	821	829	rVV5	2212	6518	0.54%	0.082%
22	7.086	842	850	874	rBV	31584	107701	8.93%	1.355%
23	7.269	878	880	882	rBV2	294	265	0.02%	0.003%
24	7.415	901	904	907	rVB3	180	262	0.02%	0.003%
25	7.549	921	926	932	rBV4	636	1544	0.13%	0.019%
26	7.653	932	943	959	rVB	215532	520740	43.20%	6.554%
27	8.037	1002	1006	1007	rBV	278	343	0.03%	0.004%
28	8.073	1010	1012	1015	rBV2	387	397	0.03%	0.005%
29	8.159	1024	1026	1031	rVB2	450	511	0.04%	0.006%
30	8.281	1036	1046	1064	rBV2	392604	1205440	100.00%	15.171%
31	8.439	1071	1072	1075	rVB	504	374	0.03%	0.005%
32	8.476	1075	1078	1079	rBV2	423	481	0.04%	0.006%
33	8.555	1086	1091	1100	rVB5	3522	8359	0.69%	0.105%
34	8.622	1100	1102	1107	rBV3	317	494	0.04%	0.006%
35	8.708	1110	1116	1123	rBV5	2190	5294	0.44%	0.067%
36	8.848	1130	1139	1154	rBV	397474	771465	64.00%	9.709%

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 Title : SFAM01.0

37	9.079	1171	1177	1181	rBV2	1317	2580	0.21%	0.032%
38	9.134	1184	1186	1190	rVB2	280	303	0.03%	0.004%
39	9.274	1198	1209	1222	rBV	277483	572448	47.49%	7.204%
40	9.415	1226	1232	1238	rVB3	6711	12315	1.02%	0.155%
41	9.500	1244	1246	1248	rBV2	333	286	0.02%	0.004%
42	9.524	1248	1250	1252	rBV2	471	301	0.02%	0.004%
43	9.634	1267	1268	1269	rBV	283	199	0.02%	0.003%
44	9.665	1269	1273	1280	rVB3	1117	2231	0.19%	0.028%
45	9.726	1280	1283	1284	rBV2	201	219	0.02%	0.003%
46	9.744	1284	1286	1287	rBV	293	214	0.02%	0.003%
47	9.902	1307	1312	1317	rVB5	529	871	0.07%	0.011%
48	9.969	1321	1323	1326	rVB2	195	230	0.02%	0.003%
49	10.037	1326	1334	1343	rBV	139895	246056	20.41%	3.097%
50	10.213	1361	1363	1366	rVB3	301	229	0.02%	0.003%
51	10.329	1373	1382	1388	rBV	480850	840924	69.76%	10.583%
52	10.390	1388	1392	1399	rVB	22453	41078	3.41%	0.517%
53	10.445	1399	1401	1402	rVB2	403	252	0.02%	0.003%
54	10.457	1402	1403	1408	rBV2	285	248	0.02%	0.003%
55	10.506	1408	1411	1413	rBV3	440	637	0.05%	0.008%
56	10.579	1416	1423	1432	rBV	89803	156012	12.94%	1.963%
57	10.707	1437	1444	1451	rVB2	5215	9442	0.78%	0.119%
58	10.866	1462	1470	1475	rBV	155781	275103	22.82%	3.462%
59	10.927	1475	1480	1496	rVV	117773	200689	16.65%	2.526%
60	11.073	1498	1504	1511	rVV2	24096	41472	3.44%	0.522%
61	11.146	1514	1516	1519	rVB2	633	461	0.04%	0.006%
62	11.177	1519	1521	1523	rBV3	351	275	0.02%	0.003%
63	11.201	1523	1525	1528	rBV2	420	377	0.03%	0.005%
64	11.286	1537	1539	1544	rVB2	236	237	0.02%	0.003%
65	11.335	1545	1547	1550	rBV2	243	197	0.02%	0.002%
66	11.634	1588	1596	1605	rVV	473242	777534	64.50%	9.786%
67	11.731	1610	1612	1618	rVB3	1978	2297	0.19%	0.029%
68	11.780	1618	1620	1622	rVB	346	246	0.02%	0.003%
69	11.841	1622	1630	1640	rBV2	22010	43665	3.62%	0.550%
70	12.054	1663	1665	1666	rBV	434	320	0.03%	0.004%
71	12.115	1673	1675	1678	rVB2	342	283	0.02%	0.004%
72	12.164	1678	1683	1690	rVB3	6224	10421	0.86%	0.131%
73	12.237	1690	1695	1699	rVB3	411	655	0.05%	0.008%
74	12.341	1707	1712	1718	rVB2	2758	4302	0.36%	0.054%
75	12.493	1733	1737	1738	rBV	165	219	0.02%	0.003%
76	12.603	1750	1755	1762	rVB3	5380	9058	0.75%	0.114%

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 Title : SFAM01.0

77	12.695	1762	1770	1777	rBV	218347	356844	29.60%	4.491%
78	12.756	1777	1780	1785	rVB2	736	914	0.08%	0.012%
79	12.804	1785	1788	1792	rBV2	255	263	0.02%	0.003%
80	12.871	1796	1799	1802	rVV2	548	537	0.04%	0.007%
81	12.938	1807	1810	1814	rVB3	1086	1444	0.12%	0.018%
82	13.103	1834	1837	1841	rVB2	918	1059	0.09%	0.013%
83	13.274	1858	1865	1874	rVB5	2811	6732	0.56%	0.085%
84	13.402	1880	1886	1890	rBV4	2141	3315	0.28%	0.042%
85	13.512	1900	1904	1905	rBV2	790	872	0.07%	0.011%
86	13.560	1905	1912	1923	rVV	247670	406880	33.75%	5.121%
87	13.853	1953	1960	1967	rBV	222186	354960	29.45%	4.467%
88	14.018	1984	1987	1989	rBV3	678	887	0.07%	0.011%
89	14.066	1992	1995	2001	rVB3	1870	3285	0.27%	0.041%
90	14.298	2030	2033	2034	rBV3	379	445	0.04%	0.006%
91	14.322	2034	2037	2043	rVB4	2571	3749	0.31%	0.047%
92	14.456	2057	2059	2061	rBV2	226	252	0.02%	0.003%
93	14.517	2067	2069	2072	rBV2	567	602	0.05%	0.008%
94	14.841	2118	2122	2125	rBV3	340	453	0.04%	0.006%
95	15.170	2174	2176	2180	rVB3	793	1028	0.09%	0.013%
96	16.084	2324	2326	2331	rVB2	462	450	0.04%	0.006%
97	16.127	2331	2333	2338	rBV3	550	640	0.05%	0.008%
98	16.218	2346	2348	2349	rBV	369	208	0.02%	0.003%
99	16.261	2353	2355	2357	rBV	381	288	0.02%	0.004%
100	16.346	2368	2369	2372	rBV3	373	465	0.04%	0.006%

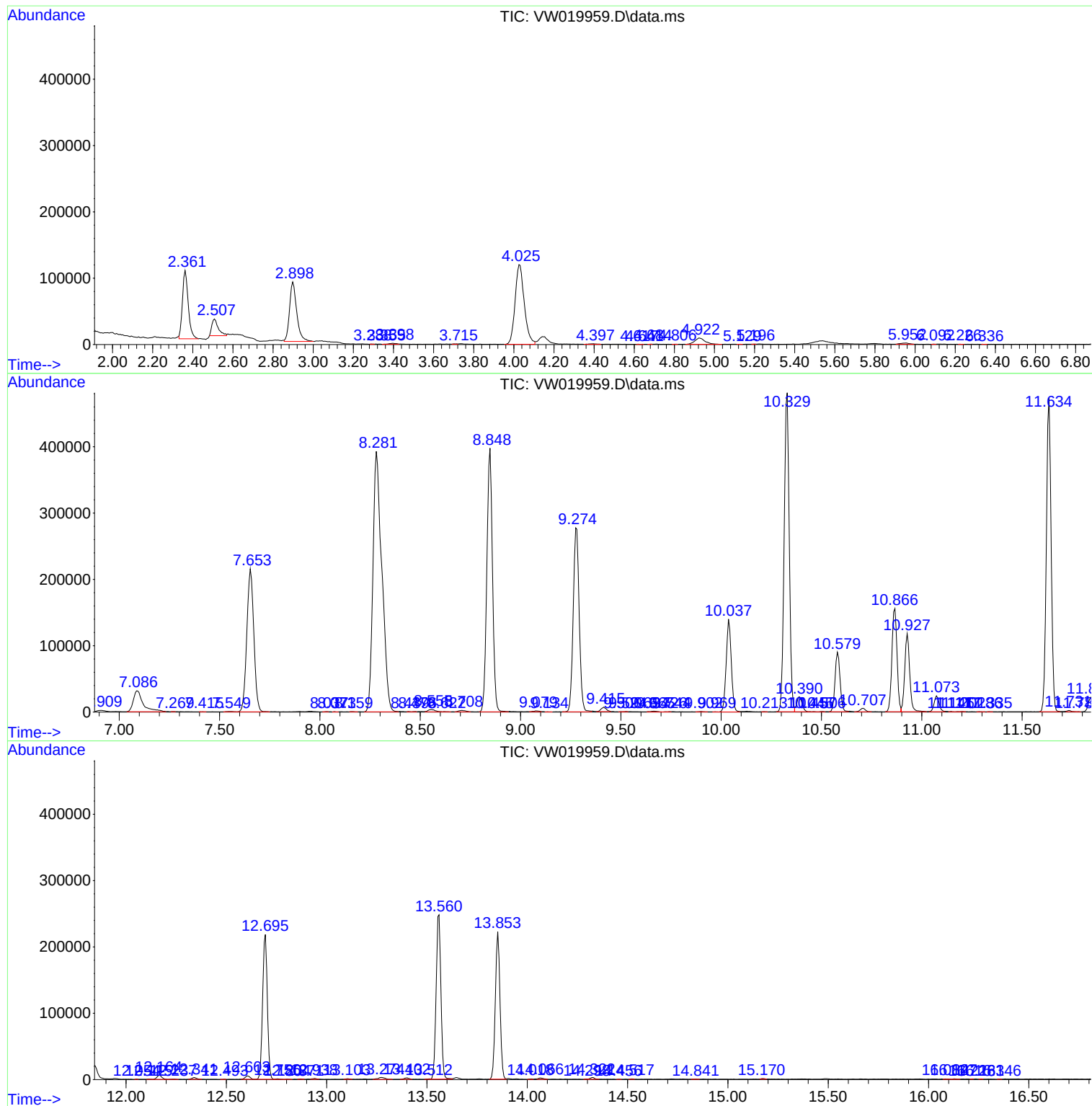
Sum of corrected areas: 7945775

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM081821SMA.M
Quant Title : SFAM01.0

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



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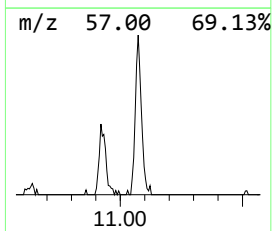
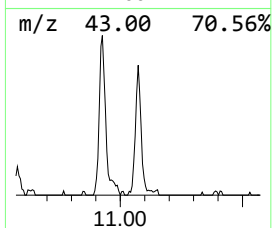
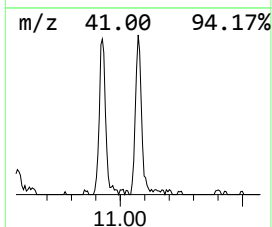
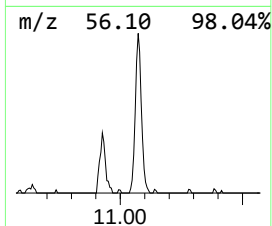
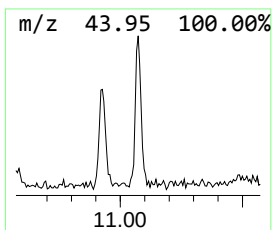
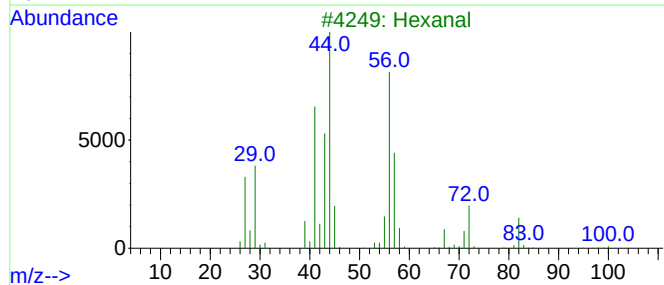
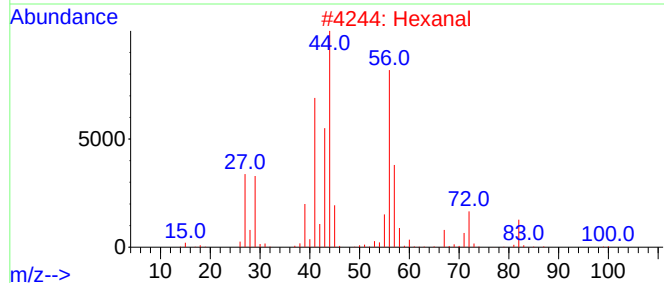
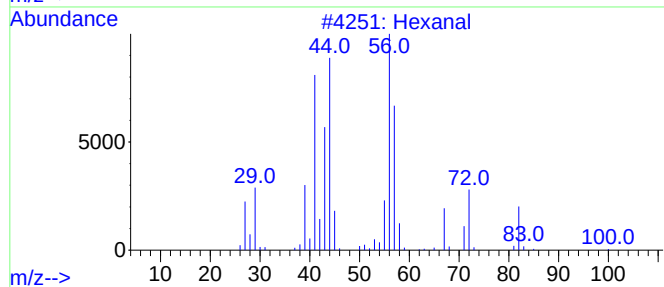
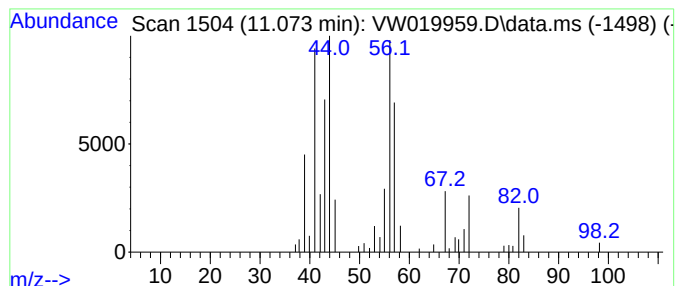
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM081821SMA.M
Quant Title : SFAM01.0

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

Peak Number 3 Hexanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.073	1.33 ug/L	41472	Chlorobenzene-d5	11.634

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	64
2	Hexanal			100	C6H12O	000066-25-1	59
3	Hexanal			100	C6H12O	000066-25-1	59
4	Hexanal			100	C6H12O	000066-25-1	53
5	Hexanal			100	C6H12O	000066-25-1	45



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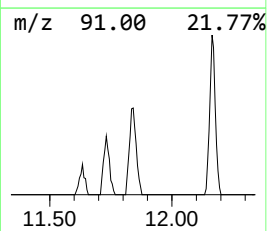
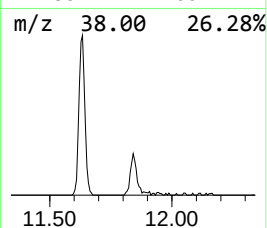
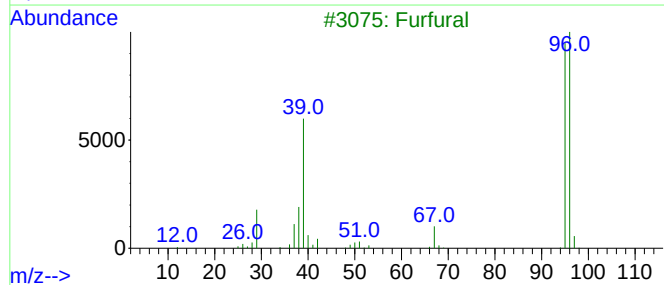
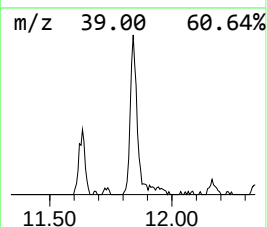
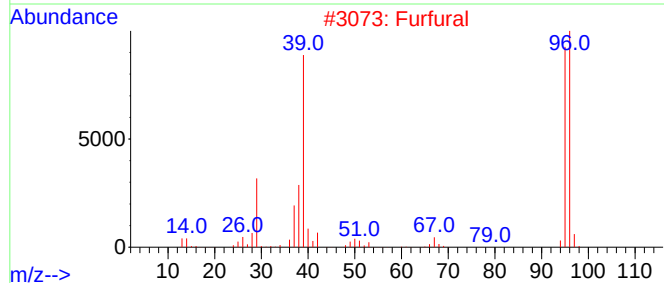
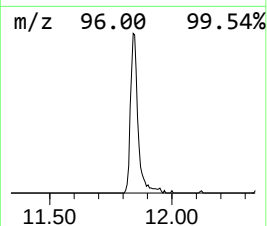
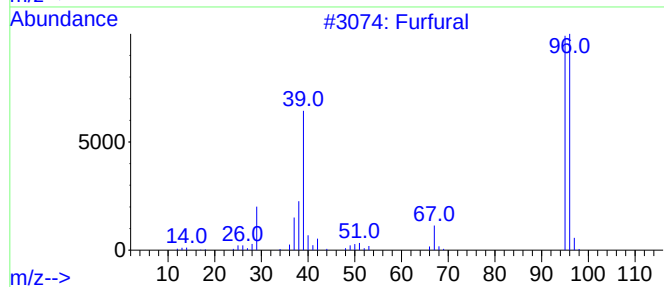
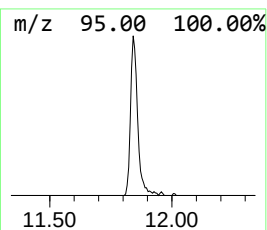
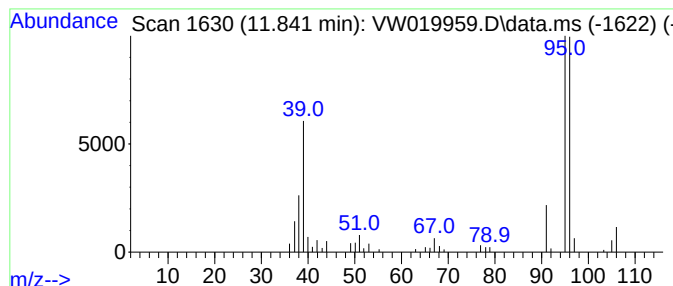
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM081821SMA.M
Quant Title : SFAM01.0

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

Peak Number 4 Furfural Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.841	1.40 ug/L	43665	Chlorobenzene-d5	11.634

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furfural	96	C5H4O2	000098-01-1	91
2			Furfural	96	C5H4O2	000098-01-1	91
3			Furfural	96	C5H4O2	000098-01-1	91
4			3-Furaldehyde	96	C5H4O2	000498-60-2	64
5			Furfural	96	C5H4O2	000098-01-1	64



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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
Hexanal	11.073	1.3	ug/L	41472	2	11.634	777534	25.0
Furfural	11.841	1.4	ug/L	43665	2	11.634	777534	25.0