

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW082724\
 Data File : VW030042.D
 Acq On : 27 Aug 2024 14:21
 Operator : SY/MD
 Sample : P3675-19
 Misc : 5.63g/10mL/MSVOA_W/SOIL/A
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 DCYA1

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\SFAMWLM082624SMA.M

Title : SFAM01.0

Signal : TIC: VW030042.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	71	78	96	rBV	51830	146117	14.95%	1.931%
2	2.899	159	166	184	rVB	38108	112961	11.56%	1.493%
3	3.387	242	246	253	rVB5	1928	4734	0.48%	0.063%
4	3.576	273	277	278	rBV	258	366	0.04%	0.005%
5	3.594	278	280	283	rVV2	338	355	0.04%	0.005%
6	3.625	283	285	287	rVV	256	209	0.02%	0.003%
7	3.734	297	303	313	rVB6	2128	6509	0.67%	0.086%
8	3.844	320	321	323	rBV	199	187	0.02%	0.002%
9	4.021	339	350	364	rBV	98847	345387	35.33%	4.565%
10	4.832	481	483	485	rVB2	181	171	0.02%	0.002%
11	4.923	485	498	526	rBV3	31480	131813	13.48%	1.742%
12	5.179	538	540	542	rBV2	325	204	0.02%	0.003%
13	5.216	545	546	555	rBV2	233	562	0.06%	0.007%
14	5.325	562	564	568	rVB	183	179	0.02%	0.002%
15	5.405	575	577	578	rVB	309	194	0.02%	0.003%
16	5.490	590	591	594	rBV2	187	172	0.02%	0.002%
17	5.649	615	617	622	rBV2	182	278	0.03%	0.004%
18	5.703	625	626	628	rBV	148	130	0.01%	0.002%
19	5.740	628	632	633	rVV2	179	185	0.02%	0.002%
20	5.789	633	640	649	rVV5	1512	4797	0.49%	0.063%
21	5.941	656	665	675	rVB5	2837	8397	0.86%	0.111%
22	6.112	685	693	694	rBV3	855	1295	0.13%	0.017%
23	6.283	719	721	722	rBV2	192	150	0.02%	0.002%
24	6.411	741	742	746	rBV	161	175	0.02%	0.002%
25	6.606	772	774	784	rVB3	651	1201	0.12%	0.016%
26	6.697	784	789	791	rBV2	250	390	0.04%	0.005%
27	6.904	816	823	834	rBV3	2154	6610	0.68%	0.087%
28	7.087	845	853	866	rBV2	26257	84468	8.64%	1.116%
29	7.551	924	929	931	rBV2	264	421	0.04%	0.006%
30	7.648	934	945	959	rBV	167252	399432	40.86%	5.279%
31	7.910	986	988	990	rBV	155	162	0.02%	0.002%
32	8.081	1013	1016	1019	rBV2	113	190	0.02%	0.003%
33	8.105	1019	1020	1025	rVB2	185	159	0.02%	0.002%
34	8.154	1025	1028	1029	rBV	212	166	0.02%	0.002%
35	8.276	1038	1048	1065	rBV2	339100	977514	100.00%	12.920%
36	8.477	1079	1081	1085	rBV2	103	130	0.01%	0.002%

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 Title : SFAM01.0

37	8.550	1085	1093	1100	rBV3	6890	16022	1.64%	0.212%
38	8.703	1111	1118	1126	rBV5	2886	7771	0.79%	0.103%
39	8.843	1131	1141	1152	rBV	403125	804650	82.32%	10.635%
40	9.050	1170	1175	1177	rBV4	853	1355	0.14%	0.018%
41	9.124	1186	1187	1191	rBV	301	223	0.02%	0.003%
42	9.276	1201	1212	1223	rBV	218003	451060	46.14%	5.962%
43	9.410	1228	1234	1242	rVB2	10007	20180	2.06%	0.267%
44	9.550	1252	1257	1262	rVB3	1206	2213	0.23%	0.029%
45	9.666	1274	1276	1279	rVB3	260	245	0.03%	0.003%
46	10.032	1329	1336	1346	rBV	117205	211795	21.67%	2.799%
47	10.129	1346	1352	1365	rVB3	7693	17551	1.80%	0.232%
48	10.245	1369	1371	1373	rBV	236	185	0.02%	0.002%
49	10.318	1375	1383	1391	rBV	444016	792286	81.05%	10.472%
50	10.501	1410	1413	1416	rBV4	383	531	0.05%	0.007%
51	10.575	1418	1425	1440	rBV	73100	130109	13.31%	1.720%
52	10.696	1440	1445	1451	rVV	8225	14283	1.46%	0.189%
53	10.806	1462	1463	1466	rBV	245	140	0.01%	0.002%
54	10.837	1466	1468	1469	rBV	232	185	0.02%	0.002%
55	10.922	1475	1482	1496	rBV	116982	207817	21.26%	2.747%
56	11.068	1500	1506	1520	rVB	94843	158641	16.23%	2.097%
57	11.282	1540	1541	1544	rVB2	427	347	0.04%	0.005%
58	11.312	1544	1546	1548	rBV2	183	151	0.02%	0.002%
59	11.391	1556	1559	1560	rBV2	198	177	0.02%	0.002%
60	11.465	1569	1571	1576	rVB3	424	624	0.06%	0.008%
61	11.568	1579	1588	1591	rBV3	2031	3928	0.40%	0.052%
62	11.629	1591	1598	1609	rVV	528997	878938	89.92%	11.617%
63	11.733	1613	1615	1618	rVB4	475	589	0.06%	0.008%
64	11.800	1624	1626	1627	rBV	321	318	0.03%	0.004%
65	11.843	1627	1633	1647	rVV	30865	64353	6.58%	0.851%
66	12.019	1658	1662	1668	rVB3	1954	3469	0.35%	0.046%
67	12.233	1691	1697	1703	rBV2	1668	3112	0.32%	0.041%
68	12.336	1708	1714	1720	rVV4	4191	7838	0.80%	0.104%
69	12.507	1737	1742	1751	rVB	6541	10453	1.07%	0.138%
70	12.605	1751	1758	1764	rVV	9836	15742	1.61%	0.208%
71	12.690	1765	1772	1780	rVV	156306	255649	26.15%	3.379%
72	12.751	1780	1782	1787	rVB4	672	856	0.09%	0.011%
73	12.891	1801	1805	1807	rVV4	478	875	0.09%	0.012%
74	12.934	1807	1812	1818	rVB3	4935	8541	0.87%	0.113%
75	13.038	1825	1829	1833	rVB	2326	2836	0.29%	0.037%
76	13.092	1833	1838	1843	rBV6	1989	4037	0.41%	0.053%

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 Title : SFAM01.0

77	13.153	1844	1848	1852	rVV4	2626	4325	0.44%	0.057%
78	13.208	1852	1857	1862	rVV4	4279	8055	0.82%	0.106%
79	13.269	1862	1867	1877	rVB3	7756	16954	1.73%	0.224%
80	13.397	1880	1888	1893	rBV4	3352	6033	0.62%	0.080%
81	13.452	1895	1897	1899	rBV2	239	245	0.03%	0.003%
82	13.495	1900	1904	1907	rBV4	1177	1645	0.17%	0.022%
83	13.556	1907	1914	1925	rVV	424606	685550	70.13%	9.061%
84	13.647	1926	1929	1934	rVB2	3188	4875	0.50%	0.064%
85	13.848	1955	1962	1969	rBV2	268332	450287	46.06%	5.952%
86	14.019	1984	1990	1992	rBV3	1962	3560	0.36%	0.047%
87	14.068	1993	1998	2007	rVB4	11077	21321	2.18%	0.282%
88	14.220	2019	2023	2027	rBV5	1250	2207	0.23%	0.029%
89	14.318	2034	2039	2046	rBV4	3757	6802	0.70%	0.090%
90	14.610	2085	2087	2092	rVB5	1050	1353	0.14%	0.018%
91	14.793	2115	2117	2123	rVB3	975	1134	0.12%	0.015%
92	14.860	2123	2128	2133	rBV5	1332	2329	0.24%	0.031%
93	14.946	2139	2142	2148	rVB4	2337	4030	0.41%	0.053%
94	15.019	2151	2154	2158	rBV3	431	626	0.06%	0.008%
95	15.165	2176	2178	2181	rBV3	662	672	0.07%	0.009%
96	15.348	2206	2208	2209	rBV	331	201	0.02%	0.003%
97	15.385	2212	2214	2215	rBV2	574	403	0.04%	0.005%
98	15.482	2226	2230	2232	rBV2	1517	2097	0.21%	0.028%
99	15.848	2285	2290	2295	rBV5	2344	4469	0.46%	0.059%
100	16.695	2427	2429	2431	rVB2	291	140	0.01%	0.002%

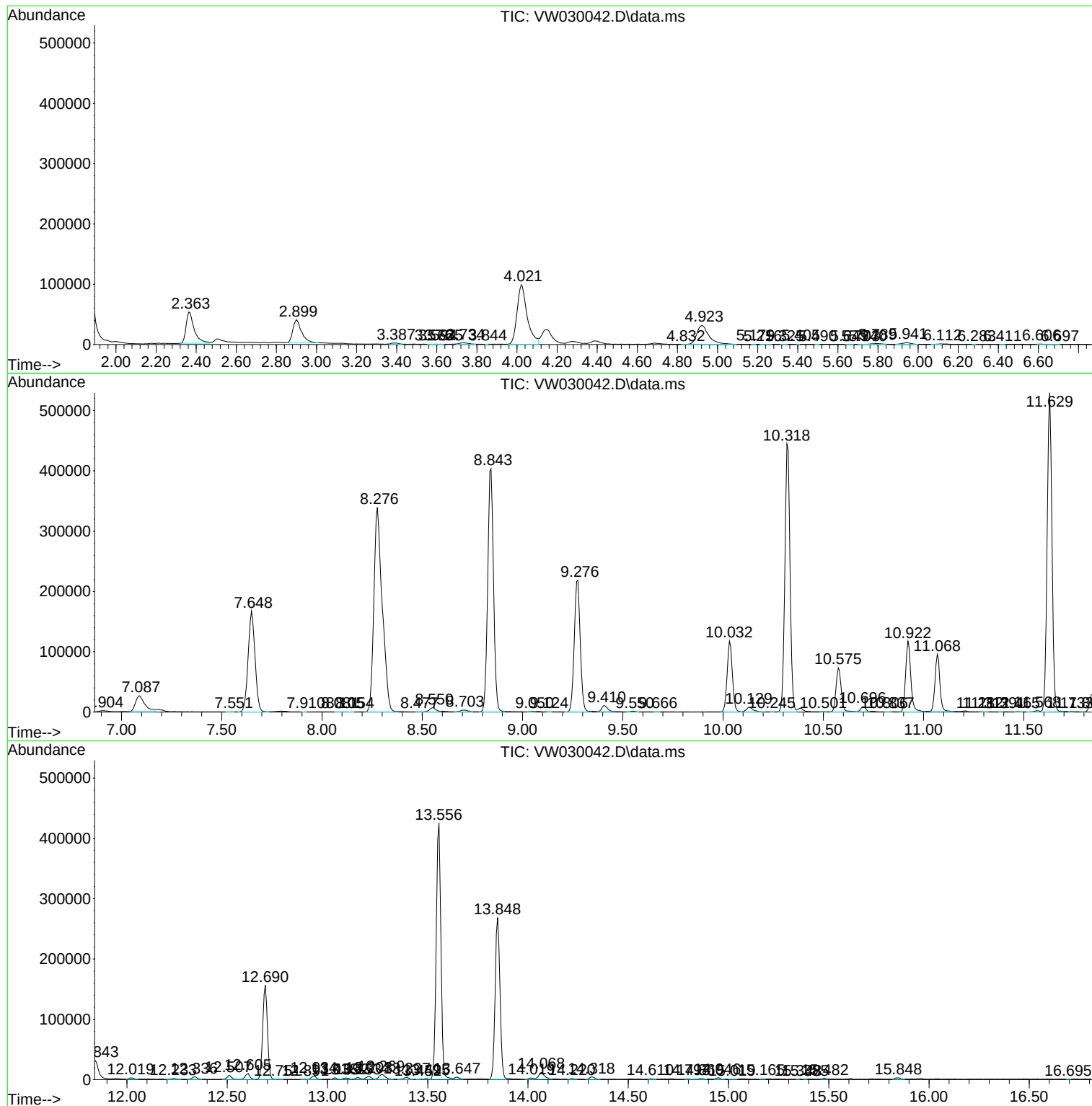
Sum of corrected areas: 7565758

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM082624SMA.M
Quant Title : SFAM01.0

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



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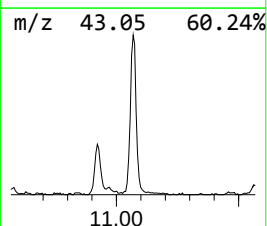
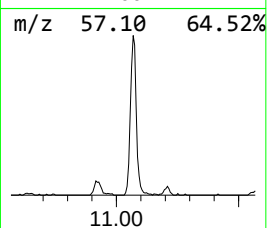
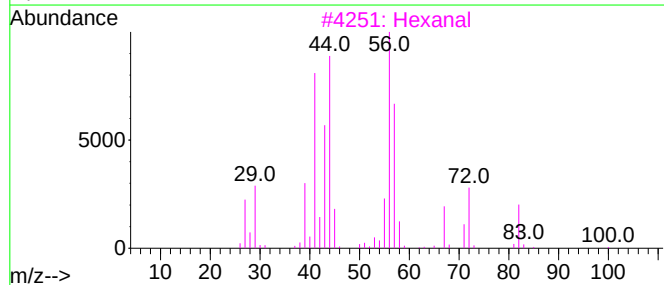
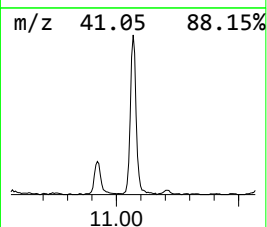
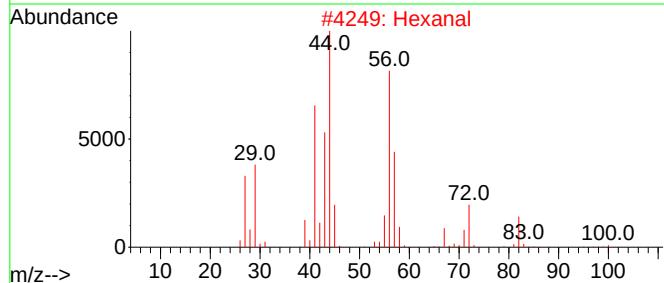
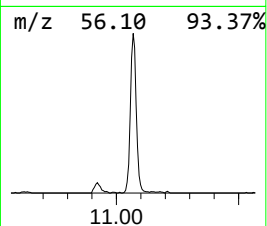
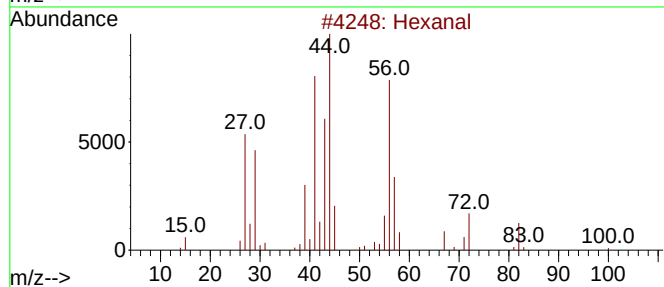
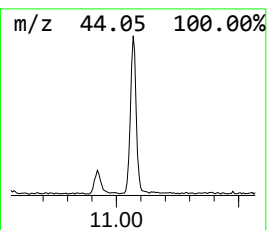
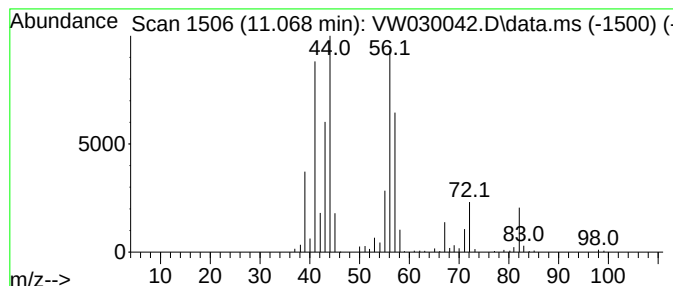
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM082624SMA.M
Quant Title : SFAM01.0

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

Peak Number 2 Hexanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.068	4.51 ug/L	158641	Chlorobenzene-d5	11.629

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	90
2	Hexanal			100	C6H12O	000066-25-1	83
3	Hexanal			100	C6H12O	000066-25-1	83
4	Hexanal			100	C6H12O	000066-25-1	78
5	Hexanal			100	C6H12O	000066-25-1	78



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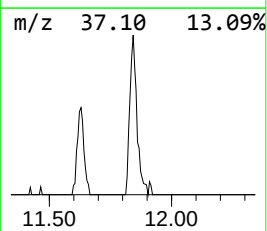
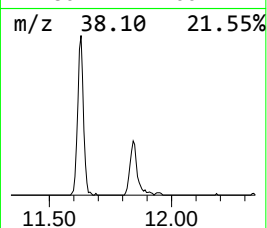
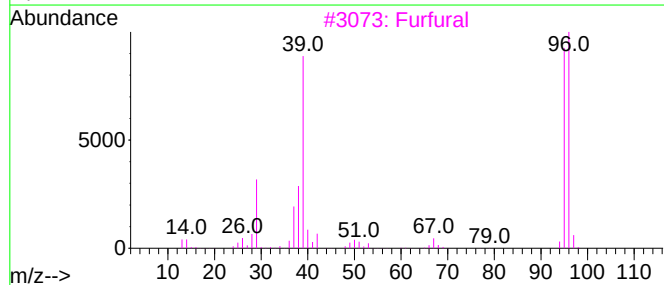
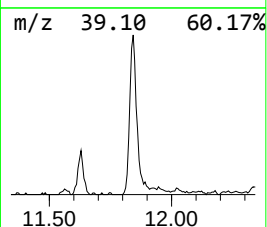
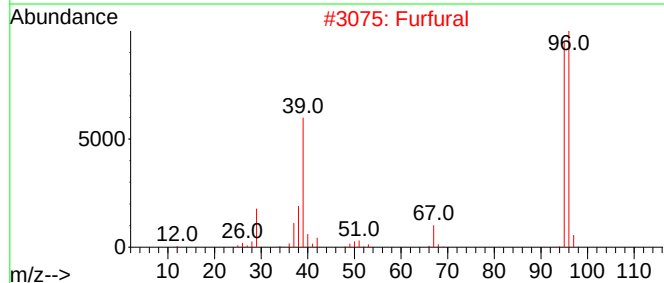
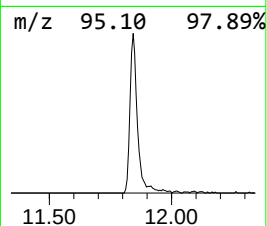
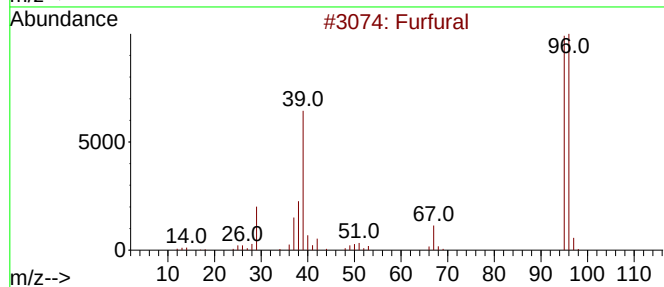
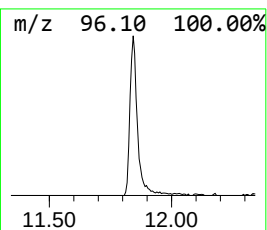
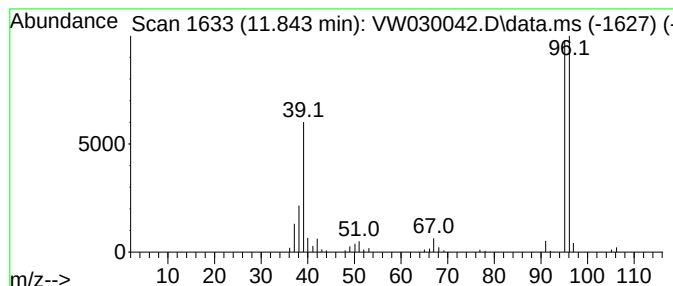
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM082624SMA.M
Quant Title : SFAM01.0

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

Peak Number 3 Furfural Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.843	1.83 ug/L	64353	Chlorobenzene-d5	11.629

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furfural			96	C5H4O2	000098-01-1	94
2	Furfural			96	C5H4O2	000098-01-1	94
3	Furfural			96	C5H4O2	000098-01-1	91
4	3-Furaldehyde			96	C5H4O2	000498-60-2	90
5	Furfural			96	C5H4O2	000098-01-1	76



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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	11.068	4.5	ug/L	158641	2	11.629	878938	25.0
Furfural	11.843	1.8	ug/L	64353	2	11.629	878938	25.0