

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW082224\
 Data File : VW029993.D
 Acq On : 22 Aug 2024 17:25
 Operator : SY/MD
 Sample : P3673-16
 Misc : 5.62g/10mL/MSVOA_W/SOIL/A
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 DCXZ6

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\SFAMWLM072424SMA.M
 Title : SFAM01.0

Signal : TIC: VW029993.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	72	78	92	rVB	45413	104721	12.42%	1.749%
2	2.899	159	166	181	rVB2	34613	98515	11.68%	1.645%
3	3.387	240	246	255	rBV2	9405	21647	2.57%	0.361%
4	4.021	338	350	360	rBV	80864	258991	30.72%	4.325%
5	4.576	439	441	444	rBV2	123	151	0.02%	0.003%
6	4.606	444	446	449	rVB2	194	181	0.02%	0.003%
7	4.673	449	457	467	rBV2	2962	8612	1.02%	0.144%
8	4.917	488	497	514	rBV3	6043	23391	2.77%	0.391%
9	5.259	551	553	554	rVB	205	112	0.01%	0.002%
10	5.313	561	562	566	rVV2	90	113	0.01%	0.002%
11	5.563	601	603	606	rBV2	107	121	0.01%	0.002%
12	5.618	610	612	614	rVB	153	143	0.02%	0.002%
13	5.679	619	622	625	rVB2	98	125	0.01%	0.002%
14	5.710	625	627	628	rBV2	144	153	0.02%	0.003%
15	5.789	632	640	641	rBV4	1085	2205	0.26%	0.037%
16	5.856	649	651	654	rBV2	184	164	0.02%	0.003%
17	5.941	656	665	676	rVB2	3656	10431	1.24%	0.174%
18	6.021	676	678	684	rVB	182	168	0.02%	0.003%
19	6.094	686	690	692	rBV2	227	348	0.04%	0.006%
20	6.173	700	703	706	rBV3	140	151	0.02%	0.003%
21	6.252	714	716	717	rVB	207	126	0.01%	0.002%
22	6.265	717	718	720	rBV2	214	193	0.02%	0.003%
23	6.557	763	766	769	rBV2	261	323	0.04%	0.005%
24	6.850	811	814	815	rBV2	96	116	0.01%	0.002%
25	6.911	819	824	827	rBV3	583	1099	0.13%	0.018%
26	7.075	842	851	866	rBV	29091	95426	11.32%	1.594%
27	7.350	895	896	898	rVB2	270	175	0.02%	0.003%
28	7.386	901	902	904	rVB	274	122	0.01%	0.002%
29	7.423	906	908	913	rBV2	214	345	0.04%	0.006%
30	7.514	919	923	925	rBV	294	333	0.04%	0.006%
31	7.648	935	945	960	rBV	151275	378949	44.95%	6.328%
32	7.764	962	964	969	rVB4	559	539	0.06%	0.009%
33	7.923	988	990	992	rVB	204	179	0.02%	0.003%
34	8.276	1038	1048	1066	rVV2	277841	843129	100.00%	14.079%
35	8.618	1101	1104	1105	rVB2	327	256	0.03%	0.004%
36	8.703	1111	1118	1126	rBV2	8636	19172	2.27%	0.320%

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 Title : SFAM01.0

37	8.843	1132	1141	1152	rBV	376220	738994	87.65%	12.340%
38	9.045	1170	1174	1176	rBV2	722	1118	0.13%	0.019%
39	9.270	1202	1211	1222	rBV	203832	409966	48.62%	6.846%
40	9.416	1228	1235	1239	rBV3	3720	7487	0.89%	0.125%
41	9.490	1246	1247	1249	rVB2	441	226	0.03%	0.004%
42	9.538	1253	1255	1258	rVV2	213	168	0.02%	0.003%
43	9.611	1266	1267	1269	rVB2	239	123	0.01%	0.002%
44	9.666	1272	1276	1279	rBV4	833	1286	0.15%	0.021%
45	9.868	1306	1309	1312	rBV	162	230	0.03%	0.004%
46	9.953	1322	1323	1326	rVB2	219	142	0.02%	0.002%
47	10.032	1328	1336	1348	rBV	93071	171296	20.32%	2.860%
48	10.319	1370	1383	1391	rBV	348696	619468	73.47%	10.344%
49	10.508	1409	1414	1419	rVB4	1700	2697	0.32%	0.045%
50	10.575	1419	1425	1434	rBV	61503	109070	12.94%	1.821%
51	10.697	1440	1445	1450	rBV	15516	27772	3.29%	0.464%
52	10.922	1475	1482	1497	rBV	118150	205324	24.35%	3.429%
53	11.069	1500	1506	1517	rVB	45162	78128	9.27%	1.305%
54	11.410	1558	1562	1565	rBV2	218	333	0.04%	0.006%
55	11.471	1568	1572	1574	rBV3	202	329	0.04%	0.005%
56	11.562	1583	1587	1590	rBV4	1011	1412	0.17%	0.024%
57	11.629	1590	1598	1608	rVV	419050	695516	82.49%	11.614%
58	11.788	1622	1624	1627	rBV2	217	237	0.03%	0.004%
59	11.837	1627	1632	1644	rBV	6364	13827	1.64%	0.231%
60	12.014	1656	1661	1672	rBV	24435	41864	4.97%	0.699%
61	12.239	1695	1698	1701	rVB2	981	1259	0.15%	0.021%
62	12.337	1709	1714	1721	rVB2	4296	7463	0.89%	0.125%
63	12.410	1725	1726	1727	rVB	309	113	0.01%	0.002%
64	12.428	1727	1729	1732	rBV	327	328	0.04%	0.005%
65	12.459	1732	1734	1738	rBV3	189	189	0.02%	0.003%
66	12.501	1738	1741	1746	rBV3	675	1207	0.14%	0.020%
67	12.599	1751	1757	1765	rVB2	12235	20870	2.48%	0.349%
68	12.690	1765	1772	1779	rBV	155983	255154	30.26%	4.261%
69	12.812	1790	1792	1793	rBV	285	237	0.03%	0.004%
70	12.861	1797	1800	1801	rBV3	236	180	0.02%	0.003%
71	12.928	1805	1811	1818	rVB5	3106	6227	0.74%	0.104%
72	13.044	1823	1830	1832	rBV3	1578	2232	0.26%	0.037%
73	13.093	1832	1838	1844	rBV5	2880	6724	0.80%	0.112%
74	13.147	1844	1847	1852	rBV5	2023	3049	0.36%	0.051%
75	13.208	1852	1857	1862	rBV2	4766	7248	0.86%	0.121%
76	13.391	1881	1887	1892	rVB3	5208	8777	1.04%	0.147%

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 Title : SFAM01.0

77	13.495	1900	1904	1906	rBV3	815	1140	0.14%	0.019%
78	13.556	1906	1914	1925	rBV	220242	363080	43.06%	6.063%
79	13.751	1944	1946	1950	rVB3	656	632	0.07%	0.011%
80	13.849	1955	1962	1976	rVB	156273	257564	30.55%	4.301%
81	14.013	1984	1989	1993	rBV3	2406	4077	0.48%	0.068%
82	14.068	1993	1998	2008	rVB3	9460	17989	2.13%	0.300%
83	14.214	2019	2022	2026	rBV4	450	766	0.09%	0.013%
84	14.318	2034	2039	2045	rBV3	5712	9901	1.17%	0.165%
85	14.373	2045	2048	2050	rBV2	253	332	0.04%	0.006%
86	14.470	2063	2064	2065	rBV	325	151	0.02%	0.003%
87	14.507	2068	2070	2071	rBV2	375	366	0.04%	0.006%
88	14.556	2076	2078	2079	rBV2	229	121	0.01%	0.002%
89	14.604	2084	2086	2089	rBV3	416	548	0.06%	0.009%
90	14.678	2096	2098	2099	rBV2	326	221	0.03%	0.004%
91	14.708	2101	2103	2109	rVB5	888	1308	0.16%	0.022%
92	14.751	2109	2110	2111	rBV	285	138	0.02%	0.002%
93	14.775	2113	2114	2116	rVB	371	169	0.02%	0.003%
94	14.946	2137	2142	2148	rVB4	1936	3364	0.40%	0.056%
95	15.330	2203	2205	2207	rVB2	345	256	0.03%	0.004%
96	15.476	2226	2229	2234	rVB3	1343	2092	0.25%	0.035%
97	15.842	2287	2289	2297	rVB5	1827	2427	0.29%	0.041%
98	15.958	2305	2308	2314	rVB4	809	1203	0.14%	0.020%
99	16.080	2324	2328	2332	rBV3	648	1103	0.13%	0.018%
100	16.586	2410	2411	2412	rBV	479	245	0.03%	0.004%

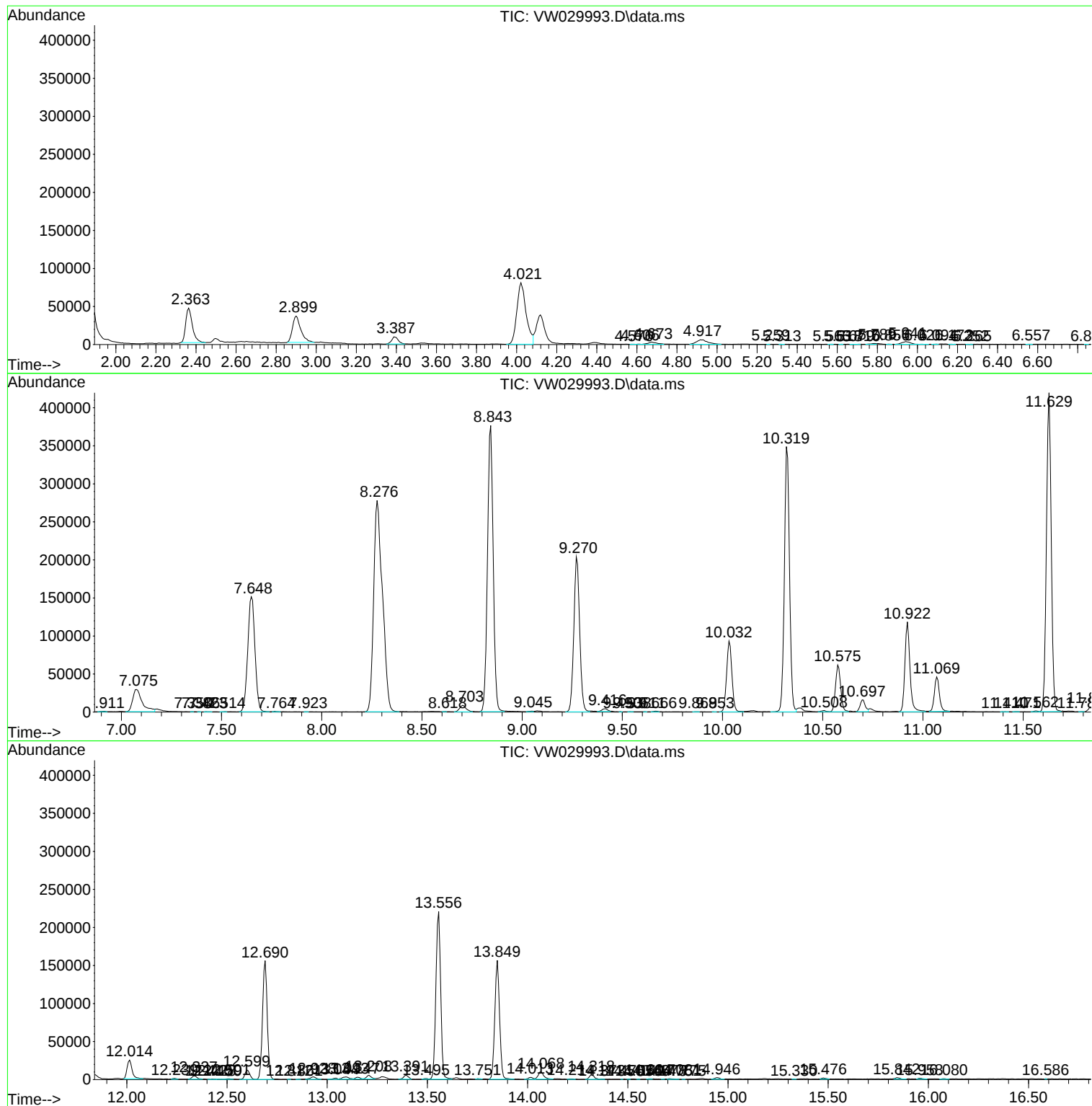
Sum of corrected areas: 5988388

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM072424SMA.M
Quant Title : SFAM01.0

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



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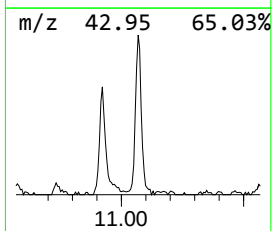
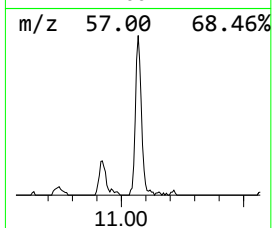
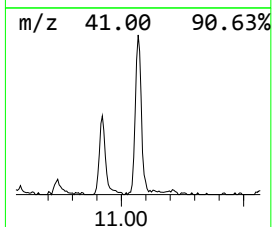
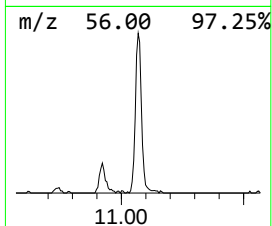
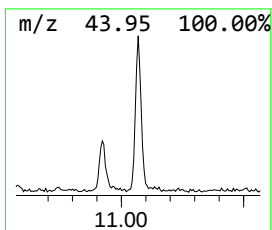
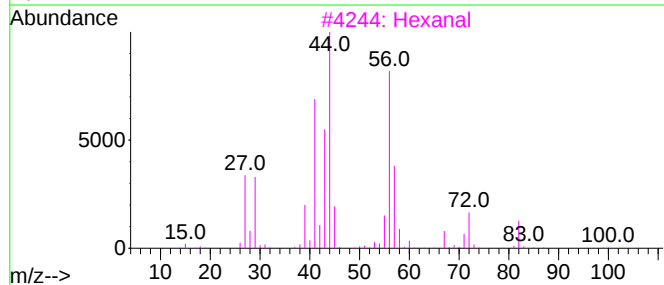
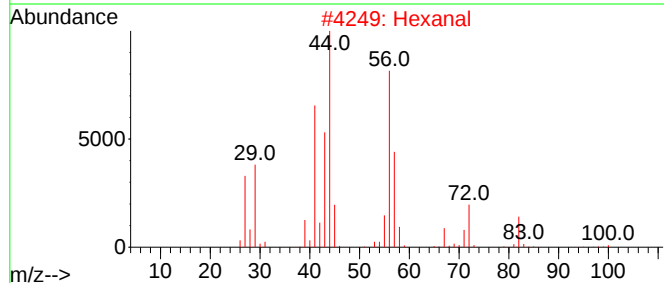
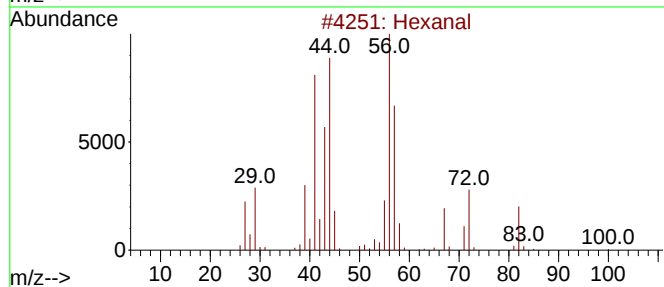
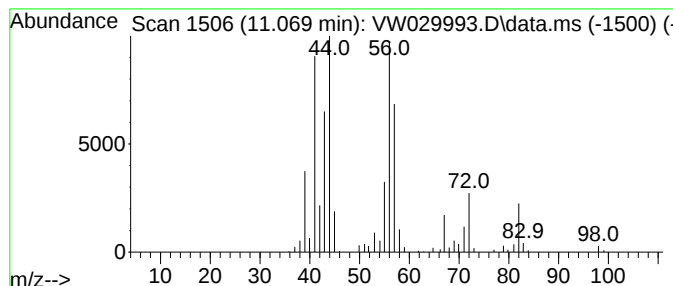
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM072424SMA.M
Quant Title : SFAM01.0

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.
11.069	2.81 ug/L	78128	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	78
3	Hexanal			100	C6H12O	000066-25-1	78
4	Hexanal			100	C6H12O	000066-25-1	72
5	Hexanal			100	C6H12O	000066-25-1	64



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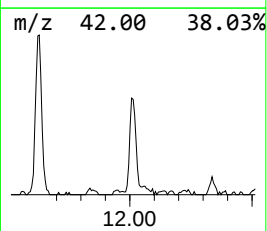
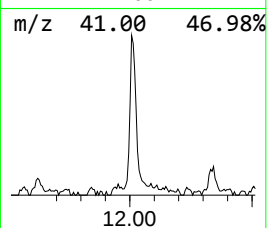
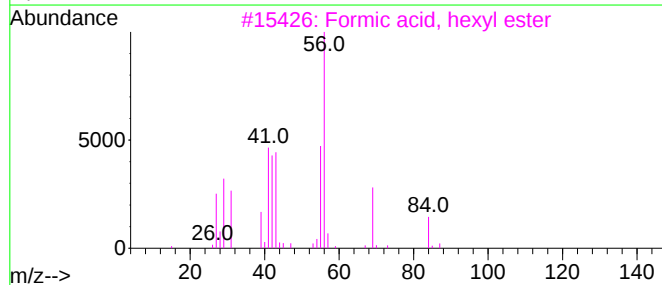
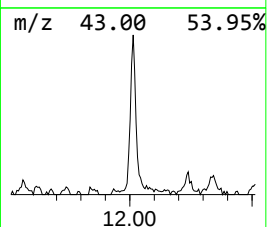
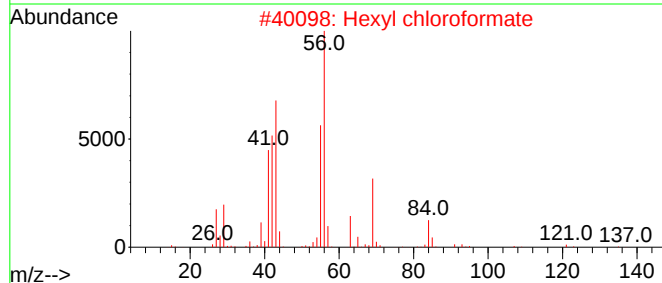
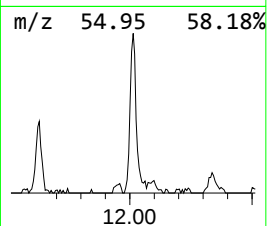
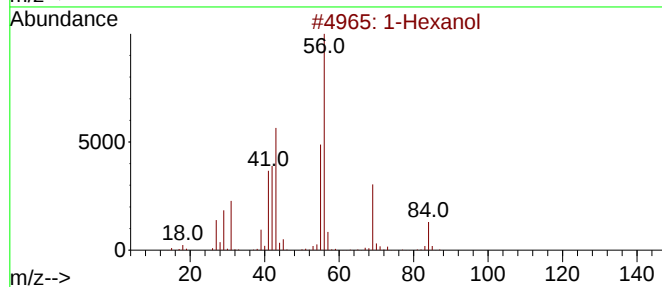
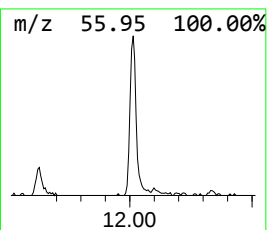
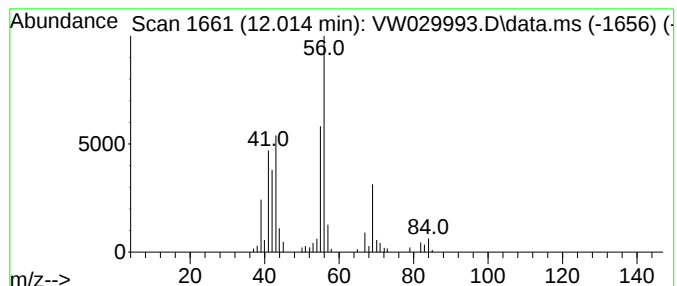
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Quant Title : SFAM01.0

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

Peak Number 3 1-Hexanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.014	1.50 ug/L	41864	Chlorobenzene-d5	11.629

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol			102	C6H14O	000111-27-3	80
2	Hexyl chloroformate			164	C7H13ClO2	006092-54-2	78
3	Formic acid, hexyl ester			130	C7H14O2	000629-33-4	72
4	1-Hexanol			102	C6H14O	000111-27-3	72
5	1-Hexanol			102	C6H14O	000111-27-3	72



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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	11.069	2.8	ug/L	78128	2	11.629	695516	25.0
1-Hexanol	12.014	1.5	ug/L	41864	2	11.629	695516	25.0