

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW080521\
 Data File : VW019683.D
 Acq On : 05 Aug 2021 15:14
 Operator : SY/VA
 Sample : M3264-04
 Misc : 6.90g/10mL/MSVOA_W/SOIL
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 GB643

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\SFAMWLM070921SMA.M

Title : SFAM01.0

Signal : TIC: VW019683.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.355	68	74	85	rVB	127822	252037	12.63%	1.575%
2	2.507	93	99	106	rBV	18965	47065	2.36%	0.294%
3	2.891	155	162	177	rVB	102216	241017	12.08%	1.506%
4	3.294	223	228	229	rBV2	1093	1649	0.08%	0.010%
5	3.391	238	244	253	rVB3	3049	7657	0.38%	0.048%
6	4.025	333	348	363	rBV	211651	659672	33.07%	4.122%
7	4.153	364	369	381	rVV	6774	20740	1.04%	0.130%
8	4.269	383	388	399	rVB5	1763	5182	0.26%	0.032%
9	4.373	402	405	406	rBV2	591	649	0.03%	0.004%
10	4.922	480	495	511	rBV2	41869	151096	7.57%	0.944%
11	5.123	526	528	538	rVB3	873	1211	0.06%	0.008%
12	5.379	564	570	572	rBV3	539	1084	0.05%	0.007%
13	5.543	584	597	620	rVV	8936	51893	2.60%	0.324%
14	5.818	640	642	646	rVB2	785	687	0.03%	0.004%
15	5.952	654	664	674	rVB3	9537	27421	1.37%	0.171%
16	6.123	689	692	694	rBV2	394	589	0.03%	0.004%
17	6.903	812	820	833	rBV3	11457	33753	1.69%	0.211%
18	6.994	833	835	839	rVB2	727	798	0.04%	0.005%
19	7.092	841	851	867	rBV	54317	167444	8.39%	1.046%
20	7.653	931	943	957	rBV	335702	818362	41.03%	5.113%
21	7.775	959	963	969	rVB5	679	1364	0.07%	0.009%
22	7.878	976	980	986	rBV4	680	1400	0.07%	0.009%
23	7.958	986	993	1003	rVB5	1978	4778	0.24%	0.030%
24	8.159	1023	1026	1029	rVB4	434	556	0.03%	0.003%
25	8.275	1035	1045	1061	rBV2	657311	1994779	100.00%	12.464%
26	8.391	1061	1064	1067	rVV3	786	897	0.04%	0.006%
27	8.555	1084	1091	1098	rVB7	2599	6976	0.35%	0.044%
28	8.622	1098	1102	1108	rVB3	588	1187	0.06%	0.007%
29	8.695	1108	1114	1121	rBV5	3551	8289	0.42%	0.052%
30	8.842	1129	1138	1150	rBV	662272	1292518	64.80%	8.076%
31	9.073	1169	1176	1183	rBV7	2309	5633	0.28%	0.035%
32	9.274	1200	1209	1219	rBV	464849	928476	46.55%	5.802%
33	9.409	1225	1231	1242	rVB	56106	112122	5.62%	0.701%
34	9.561	1253	1256	1260	rVB4	313	507	0.03%	0.003%
35	9.665	1268	1273	1279	rVB6	1673	3510	0.18%	0.022%
36	10.037	1326	1334	1344	rBV	260859	458082	22.96%	2.862%

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 Title : SFAM01.0

37	10.323	1373	1381	1388	rVV	970883	1699714	85.21%	10.621%
38	10.390	1388	1392	1403	rVV	27017	49837	2.50%	0.311%
39	10.506	1407	1411	1416	rVV3	4385	7416	0.37%	0.046%
40	10.579	1416	1423	1436	rVB	173701	294935	14.79%	1.843%
41	10.701	1436	1443	1450	rBV	33316	61141	3.07%	0.382%
42	10.866	1463	1470	1474	rBV	39943	70405	3.53%	0.440%
43	10.927	1474	1480	1494	rVV	256032	423242	21.22%	2.645%
44	11.073	1497	1504	1519	rVV	145238	238361	11.95%	1.489%
45	11.408	1558	1559	1564	rVB3	527	596	0.03%	0.004%
46	11.634	1588	1596	1606	rVV	958976	1610165	80.72%	10.061%
47	11.713	1606	1609	1610	rVV2	2374	2990	0.15%	0.019%
48	11.725	1610	1611	1618	rVV3	3445	4229	0.21%	0.026%
49	11.835	1624	1629	1639	rVB2	5259	10767	0.54%	0.067%
50	11.981	1650	1653	1659	rBV3	378	602	0.03%	0.004%
51	12.164	1677	1683	1691	rVB5	5119	10033	0.50%	0.063%
52	12.237	1691	1695	1702	rVB3	2182	3554	0.18%	0.022%
53	12.341	1705	1712	1720	rBV2	33528	56313	2.82%	0.352%
54	12.396	1720	1721	1727	rVB2	921	1152	0.06%	0.007%
55	12.463	1727	1732	1735	rBV4	2045	2897	0.15%	0.018%
56	12.603	1746	1755	1762	rBV2	50312	95641	4.79%	0.598%
57	12.695	1762	1770	1777	rBV	378591	628029	31.48%	3.924%
58	12.756	1777	1780	1790	rVB4	5141	11159	0.56%	0.070%
59	12.896	1794	1803	1805	rBV5	2831	6177	0.31%	0.039%
60	12.938	1806	1810	1820	rVV7	6087	13991	0.70%	0.087%
61	13.006	1820	1821	1828	rVB6	1690	2858	0.14%	0.018%
62	13.085	1828	1834	1838	rBV7	1966	4258	0.21%	0.027%
63	13.195	1847	1852	1856	rVB	7401	11213	0.56%	0.070%
64	13.274	1856	1865	1875	rVB5	7375	25235	1.27%	0.158%
65	13.396	1878	1885	1894	rBV3	36662	64256	3.22%	0.401%
66	13.493	1894	1901	1904	rBV6	3911	9959	0.50%	0.062%
67	13.560	1905	1912	1918	rVV	989784	1624379	81.43%	10.150%
68	13.646	1922	1926	1934	rVB	48399	75317	3.78%	0.471%
69	13.761	1942	1945	1952	rVB4	5501	9068	0.45%	0.057%
70	13.853	1953	1960	1968	rBV	862893	1405192	70.44%	8.780%
71	14.018	1984	1987	1990	rBV4	2140	3087	0.15%	0.019%
72	14.066	1990	1995	2002	rVV	17615	27298	1.37%	0.171%
73	14.182	2012	2014	2017	rBV4	722	822	0.04%	0.005%
74	14.322	2032	2037	2047	rVB3	22537	37745	1.89%	0.236%
75	14.426	2052	2054	2058	rVB5	1092	786	0.04%	0.005%
76	14.493	2061	2065	2067	rBV3	1543	2449	0.12%	0.015%

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 Title : SFAM01.0

77	14.621	2080	2086	2092	rBV4	11051	18218	0.91%	0.114%
78	14.725	2099	2103	2109	rVB6	2019	3368	0.17%	0.021%
79	14.767	2109	2110	2112	rBV	581	481	0.02%	0.003%
80	14.792	2112	2114	2117	rVV4	818	1041	0.05%	0.007%
81	14.822	2117	2119	2123	rVV4	823	984	0.05%	0.006%
82	14.865	2125	2126	2132	rVB3	1006	1210	0.06%	0.008%
83	14.956	2136	2141	2143	rBV4	850	1262	0.06%	0.008%
84	15.005	2148	2149	2153	rVB3	818	620	0.03%	0.004%
85	15.066	2156	2159	2160	rVV3	606	518	0.03%	0.003%
86	15.127	2164	2169	2173	rVV5	5645	9446	0.47%	0.059%
87	15.182	2173	2178	2186	rVV7	3789	8634	0.43%	0.054%
88	15.255	2186	2190	2192	rVB4	1359	1842	0.09%	0.012%
89	15.292	2195	2196	2199	rBV3	551	463	0.02%	0.003%
90	15.359	2203	2207	2212	rBV2	6009	10695	0.54%	0.067%
91	15.401	2212	2214	2219	rVB4	1499	1737	0.09%	0.011%
92	15.487	2223	2228	2233	rVV	3139	5493	0.28%	0.034%
93	15.554	2233	2239	2245	rVB5	5484	10144	0.51%	0.063%
94	15.651	2252	2255	2258	rVB3	595	615	0.03%	0.004%
95	15.682	2258	2260	2263	rBV4	428	609	0.03%	0.004%
96	15.755	2269	2272	2273	rBV2	546	564	0.03%	0.004%
97	15.798	2273	2279	2282	rBV5	998	1739	0.09%	0.011%
98	15.846	2284	2287	2294	rBV7	1854	3687	0.18%	0.023%
99	16.090	2324	2327	2333	rVB7	1036	1833	0.09%	0.011%
100	16.407	2377	2379	2380	rBV2	534	464	0.02%	0.003%

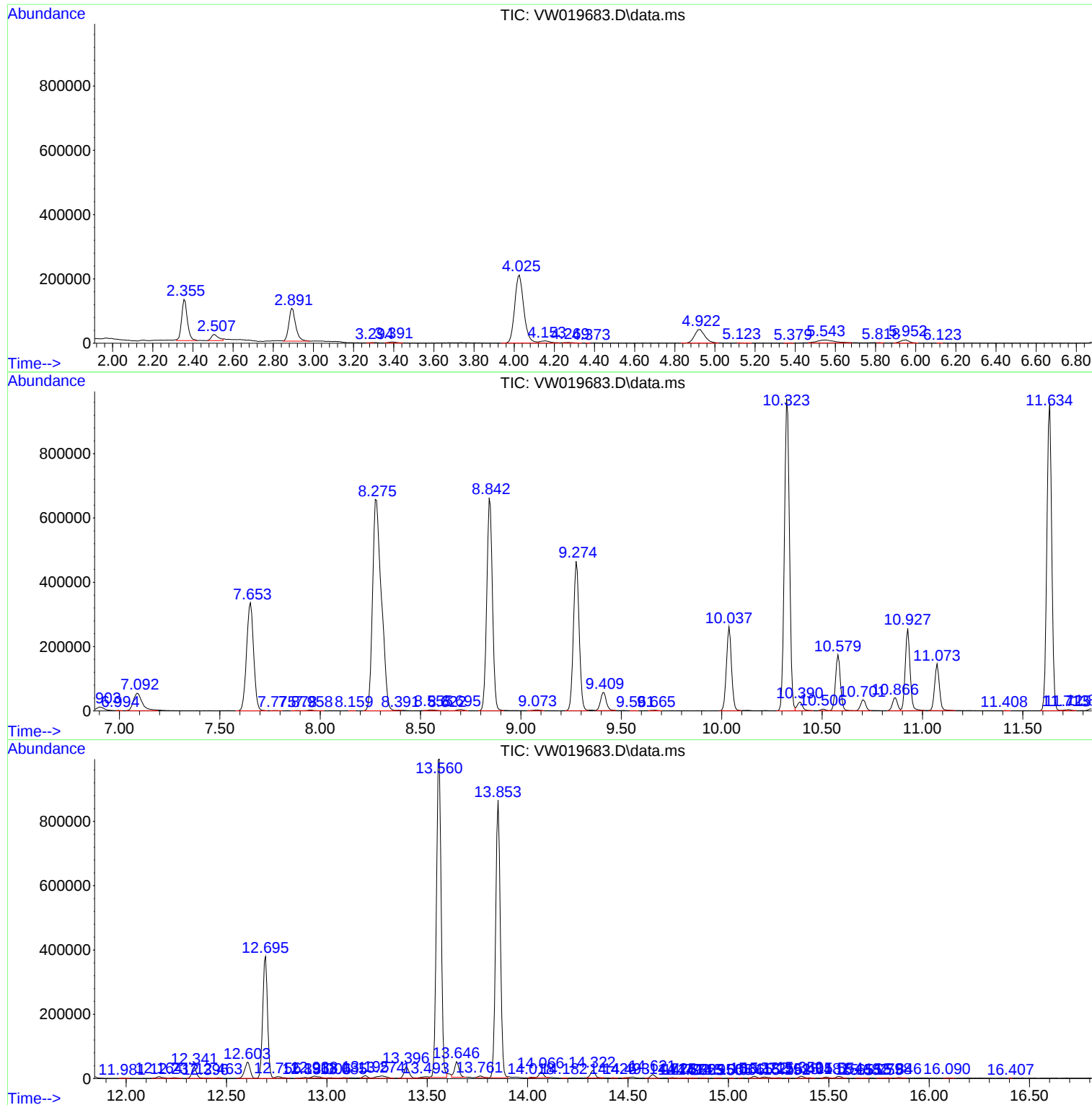
Sum of corrected areas: 16004015

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM070921SMA.M
Quant Title : SFAM01.0

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



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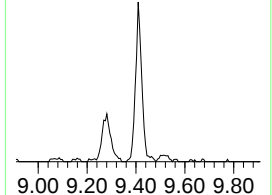
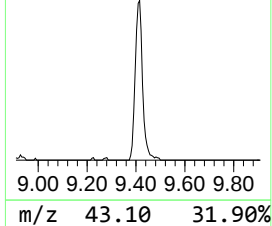
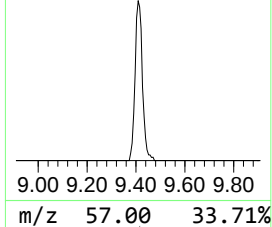
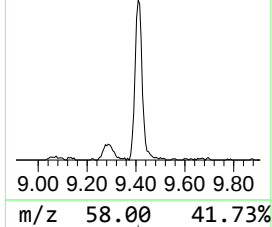
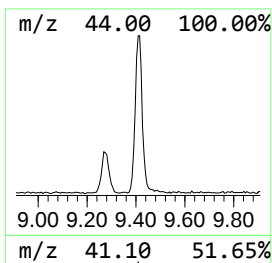
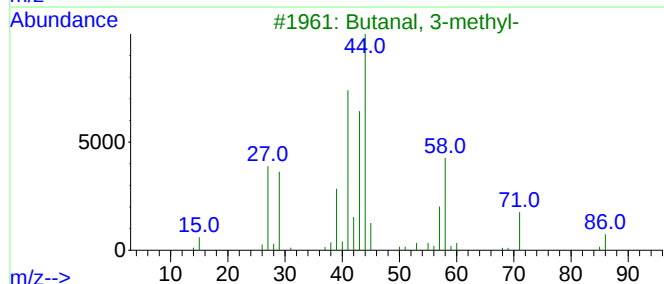
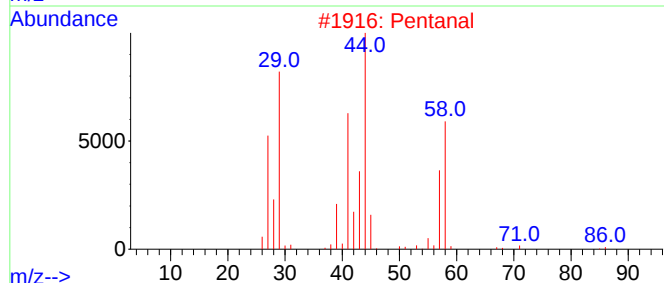
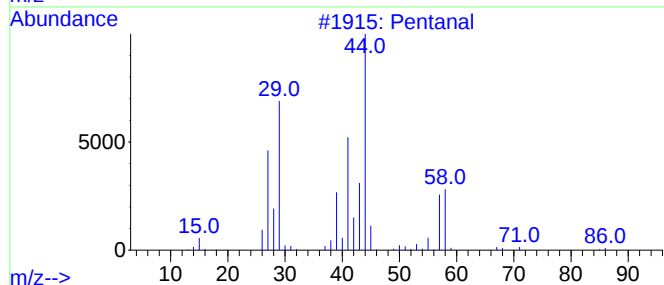
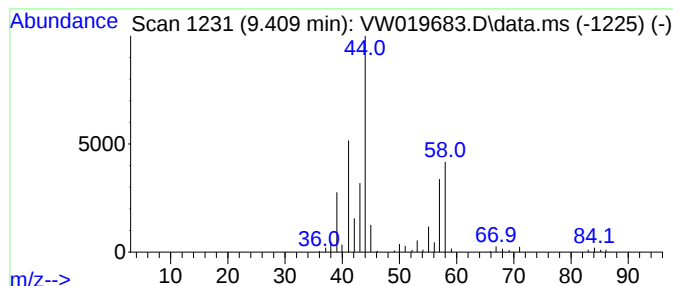
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM070921SMA.M
Quant Title : SFAM01.0

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

Peak Number 1 Pentanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.409	2.17 ug/L	112122	1,4-Difluorobenzene	8.842

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanal			86	C5H10O	000110-62-3	90
2	Pentanal			86	C5H10O	000110-62-3	87
3	Butanal, 3-methyl-			86	C5H10O	000590-86-3	74
4	Pentanal			86	C5H10O	000110-62-3	74
5	Butanal, 3-methyl-			86	C5H10O	000590-86-3	74



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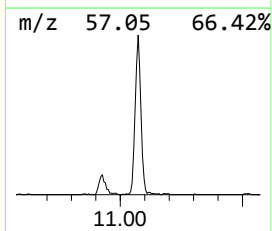
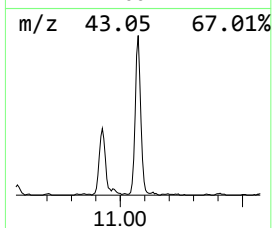
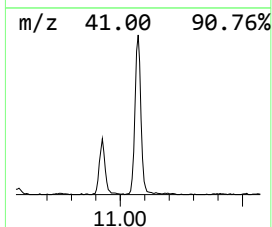
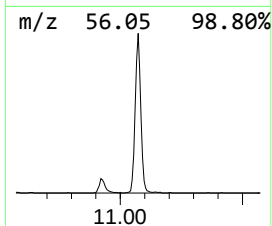
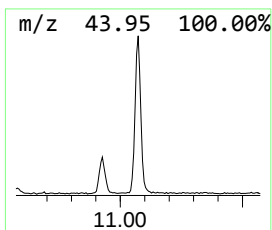
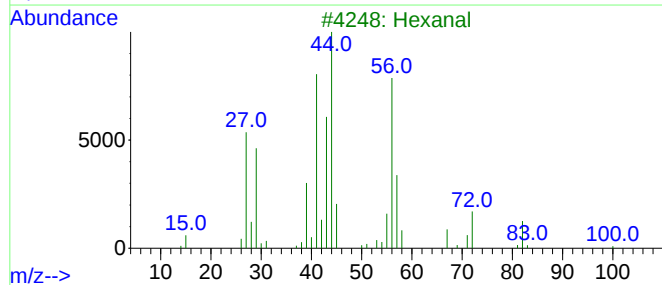
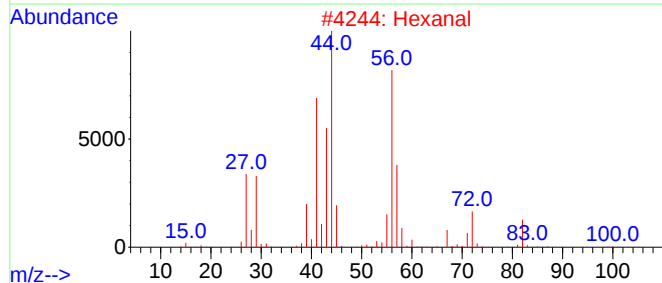
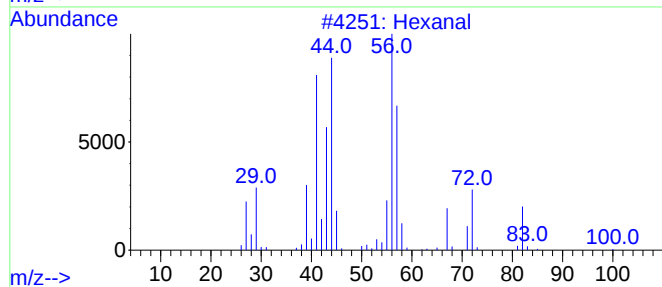
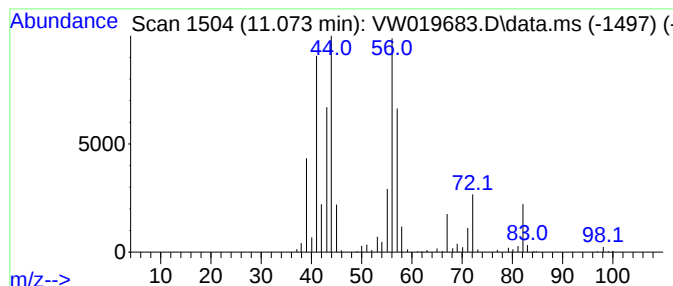
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Quant Title : SFAM01.0

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

Peak Number 3 Hexanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.073	3.70 ug/L	238361	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	72
4	Hexanal			100	C6H12O	000066-25-1	64
5	Hexanal			100	C6H12O	000066-25-1	64



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pentanal	9.409	2.2	ug/L	112122	1	8.842	1292520	25.0
Hexanal	11.073	3.7	ug/L	238361	2	11.634	1610170	25.0