

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW083121\
 Data File : VW019958.D
 Acq On : 31 Aug 2021 15:11
 Operator : SY/VA
 Sample : M3579-14RE
 Misc : 5.07g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 GB6B6RE

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: VW019958.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	84	rVB	90971	175941	18.19%	2.295%
2	2.897	157	163	177	rVB	69449	173944	17.99%	2.269%
3	3.300	227	229	231	rBV3	550	584	0.06%	0.008%
4	3.397	236	245	252	rBV2	5477	13964	1.44%	0.182%
5	3.629	281	283	286	rVB2	604	373	0.04%	0.005%
6	3.690	292	293	297	rVB2	386	260	0.03%	0.003%
7	3.909	323	329	332	rBV4	279	423	0.04%	0.006%
8	4.025	336	348	359	rBV	100100	317707	32.85%	4.145%
9	4.135	361	366	382	rVB	24217	65064	6.73%	0.849%
10	4.336	397	399	400	rBV2	366	316	0.03%	0.004%
11	4.397	400	409	420	rVV2	10307	31702	3.28%	0.414%
12	4.641	444	449	450	rVB2	202	233	0.02%	0.003%
13	4.659	450	452	455	rBV2	226	261	0.03%	0.003%
14	4.751	464	467	471	rVB2	278	494	0.05%	0.006%
15	4.799	471	475	476	rBV2	309	405	0.04%	0.005%
16	4.842	479	482	484	rBV	420	381	0.04%	0.005%
17	4.927	486	496	514	rVV6	6456	26960	2.79%	0.352%
18	5.366	566	568	581	rBV	193	229	0.02%	0.003%
19	5.440	573	580	581	rBV5	859	1595	0.16%	0.021%
20	5.793	630	638	649	rVB4	3346	10505	1.09%	0.137%
21	5.878	649	652	654	rBV2	215	229	0.02%	0.003%
22	5.946	654	663	671	rBV5	2246	7444	0.77%	0.097%
23	6.092	685	687	689	rBV3	357	395	0.04%	0.005%
24	6.110	689	690	691	rBV	502	272	0.03%	0.004%
25	6.311	720	723	725	rVB2	291	278	0.03%	0.004%
26	6.342	725	728	729	rBV2	203	237	0.02%	0.003%
27	6.799	802	803	808	rBV2	156	210	0.02%	0.003%
28	6.903	812	820	828	rBV2	4881	13189	1.36%	0.172%
29	7.079	841	849	861	rBV	38853	117464	12.15%	1.532%
30	7.531	920	923	925	rBV2	460	685	0.07%	0.009%
31	7.653	930	943	957	rVV	173337	422908	43.73%	5.517%
32	7.787	964	965	968	rVB	250	243	0.03%	0.003%
33	8.024	1003	1004	1007	rBV3	296	326	0.03%	0.004%
34	8.159	1020	1026	1032	rBV4	802	1379	0.14%	0.018%
35	8.280	1035	1046	1062	rBV2	312532	967097	100.00%	12.616%
36	8.415	1067	1068	1070	rBV2	420	300	0.03%	0.004%

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 Title : SFAM01.0

37	8.482	1077	1079	1080	rBV	262	220	0.02%	0.003%
38	8.561	1080	1092	1098	rVV4	6094	17049	1.76%	0.222%
39	8.707	1109	1116	1129	rBV3	6914	16548	1.71%	0.216%
40	8.847	1130	1139	1150	rVV	348125	690160	71.36%	9.003%
41	9.043	1169	1171	1173	rBV2	461	553	0.06%	0.007%
42	9.091	1173	1179	1186	rVB8	2386	5617	0.58%	0.073%
43	9.152	1187	1189	1190	rBV	472	216	0.02%	0.003%
44	9.274	1200	1209	1218	rBV	229812	468507	48.44%	6.112%
45	9.408	1225	1231	1242	rVB	19051	38890	4.02%	0.507%
46	9.664	1268	1273	1279	rVB3	1160	2221	0.23%	0.029%
47	9.744	1284	1286	1290	rBV2	124	202	0.02%	0.003%
48	9.920	1313	1315	1317	rVB	286	267	0.03%	0.003%
49	9.957	1317	1321	1325	rBV4	537	935	0.10%	0.012%
50	10.036	1327	1334	1342	rBV2	113654	204006	21.09%	2.661%
51	10.207	1360	1362	1370	rVB3	517	803	0.08%	0.010%
52	10.323	1373	1381	1388	rBV	376707	672088	69.50%	8.768%
53	10.390	1389	1392	1399	rVB	14037	22754	2.35%	0.297%
54	10.506	1406	1411	1416	rVB5	1738	2806	0.29%	0.037%
55	10.579	1416	1423	1430	rBV	77583	135420	14.00%	1.767%
56	10.707	1440	1444	1448	rVB3	3416	5328	0.55%	0.070%
57	10.865	1461	1470	1475	rBV	392856	684570	70.79%	8.930%
58	10.926	1475	1480	1497	rVB	139836	239832	24.80%	3.129%
59	11.073	1497	1504	1515	rBV2	143665	238426	24.65%	3.110%
60	11.335	1545	1547	1550	rBV3	433	456	0.05%	0.006%
61	11.402	1555	1558	1559	rBV2	363	414	0.04%	0.005%
62	11.548	1580	1582	1583	rBV2	284	249	0.03%	0.003%
63	11.566	1583	1585	1588	rVV	594	605	0.06%	0.008%
64	11.634	1588	1596	1604	rVV	415142	703495	72.74%	9.177%
65	11.731	1608	1612	1621	rVV2	4934	8526	0.88%	0.111%
66	11.841	1624	1630	1642	rVV4	8709	18144	1.88%	0.237%
67	11.944	1642	1647	1652	rVB5	1967	3494	0.36%	0.046%
68	12.091	1669	1671	1674	rBV2	426	527	0.05%	0.007%
69	12.133	1676	1678	1679	rBV2	368	286	0.03%	0.004%
70	12.164	1679	1683	1689	rVB4	1265	2039	0.21%	0.027%
71	12.237	1691	1695	1702	rVB4	952	1885	0.19%	0.025%
72	12.341	1706	1712	1722	rVB4	8865	15609	1.61%	0.204%
73	12.438	1725	1728	1729	rBV2	267	257	0.03%	0.003%
74	12.566	1747	1749	1750	rVV2	303	274	0.03%	0.004%
75	12.609	1750	1756	1761	rVB6	3249	6103	0.63%	0.080%
76	12.694	1762	1770	1778	rVB	211803	341108	35.27%	4.450%

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 Title : SFAM01.0

77	12.755	1778	1780	1785	rVB3	559	618	0.06%	0.008%
78	12.798	1785	1787	1791	rBV2	363	455	0.05%	0.006%
79	12.865	1794	1798	1799	rBV2	407	457	0.05%	0.006%
80	12.932	1806	1809	1817	rVB4	2772	4528	0.47%	0.059%
81	13.048	1825	1828	1830	rBV4	748	770	0.08%	0.010%
82	13.139	1841	1843	1844	rBV	463	351	0.04%	0.005%
83	13.273	1857	1865	1872	rVB8	2391	6680	0.69%	0.087%
84	13.395	1878	1885	1892	rBV4	6153	10654	1.10%	0.139%
85	13.469	1893	1897	1901	rVV3	636	1033	0.11%	0.013%
86	13.511	1901	1904	1905	rVV3	672	743	0.08%	0.010%
87	13.560	1905	1912	1920	rVV	240935	398309	41.19%	5.196%
88	13.645	1922	1926	1935	rVB2	6354	10525	1.09%	0.137%
89	13.853	1953	1960	1968	rBV	185507	308843	31.94%	4.029%
90	14.017	1985	1987	1990	rVB3	811	807	0.08%	0.011%
91	14.066	1991	1995	2003	rVB6	2700	5268	0.54%	0.069%
92	14.206	2016	2018	2020	rBV2	246	229	0.02%	0.003%
93	14.322	2032	2037	2043	rBV4	4764	8156	0.84%	0.106%
94	14.694	2096	2098	2100	rVB3	455	275	0.03%	0.004%
95	14.755	2107	2108	2112	rBV2	459	395	0.04%	0.005%
96	14.871	2124	2127	2131	rVB3	363	481	0.05%	0.006%
97	15.322	2200	2201	2202	rBV	445	212	0.02%	0.003%
98	15.438	2218	2220	2221	rVB	489	276	0.03%	0.004%
99	15.456	2221	2223	2224	rBV	335	229	0.02%	0.003%
100	16.566	2401	2405	2408	rBV2	354	442	0.05%	0.006%

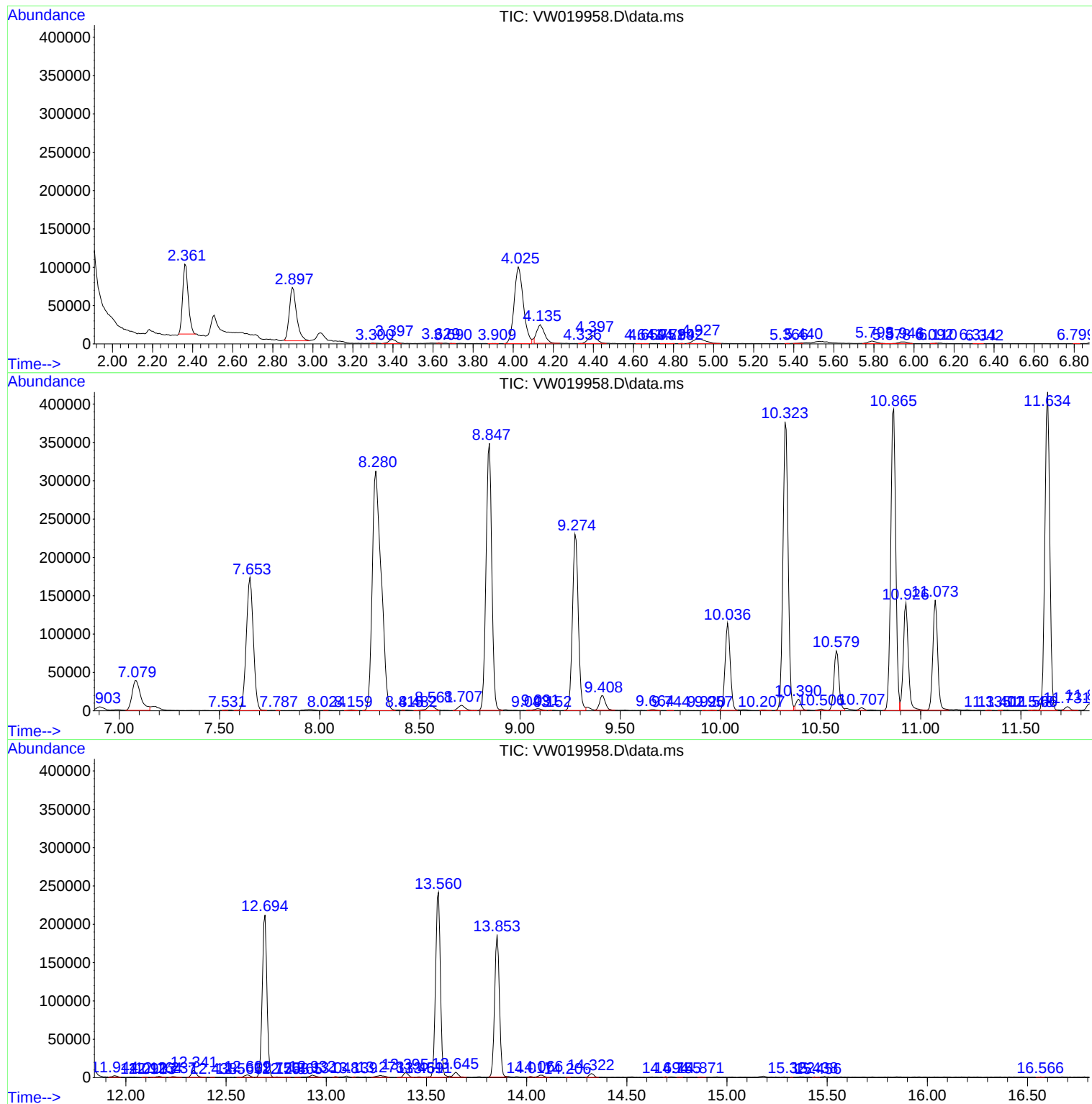
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Quant Title : SFAM01.0

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



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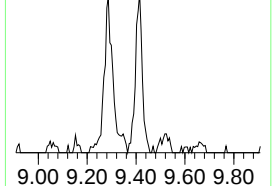
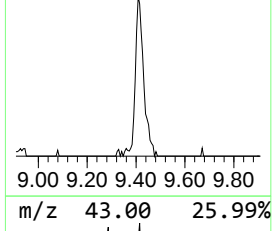
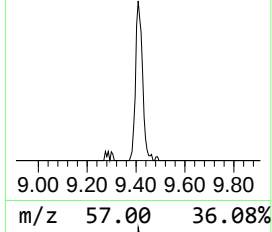
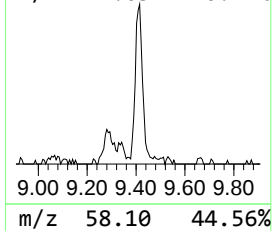
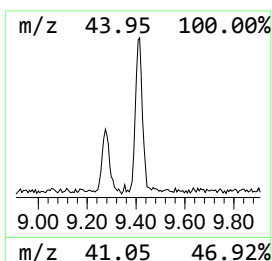
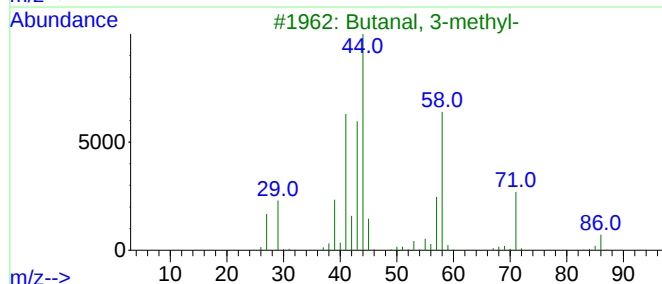
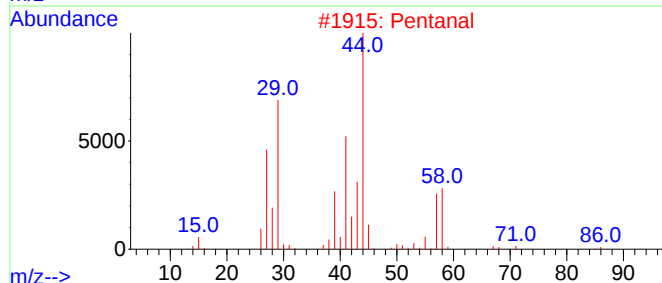
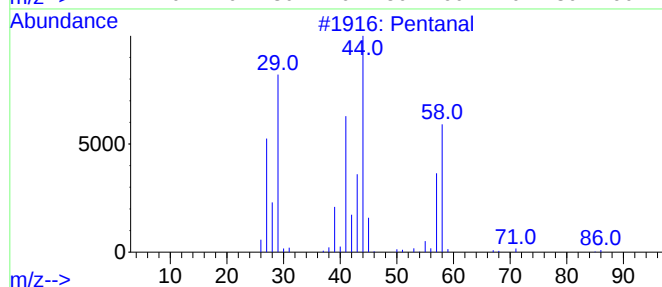
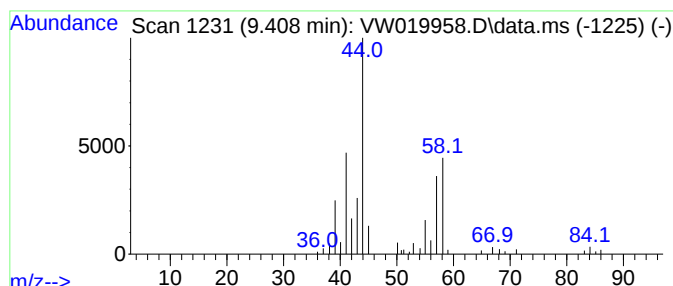
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM081821SMA.M
Quant Title : SFAM01.0

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

Peak Number 1 Pentanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.408	1.41 ug/L	38890	1,4-Difluorobenzene	8.847

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanal			86	C5H10O	000110-62-3	78
2	Pentanal			86	C5H10O	000110-62-3	78
3	Butanal, 3-methyl-			86	C5H10O	000590-86-3	74
4	Pentanal			86	C5H10O	000110-62-3	72
5	Pentanal			86	C5H10O	000110-62-3	43



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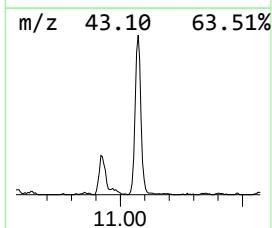
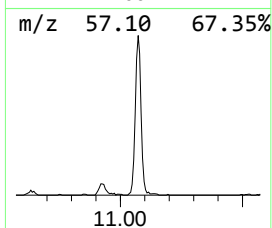
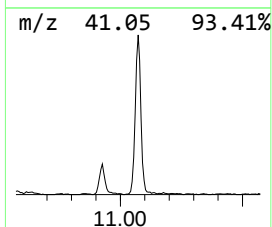
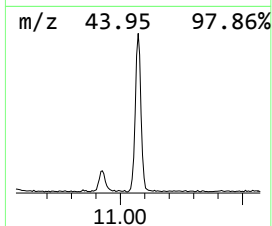
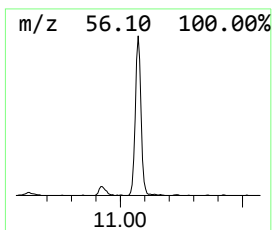
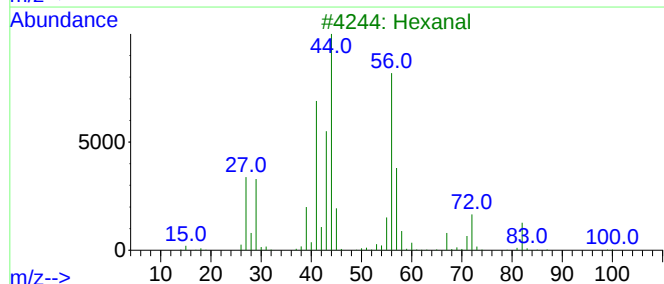
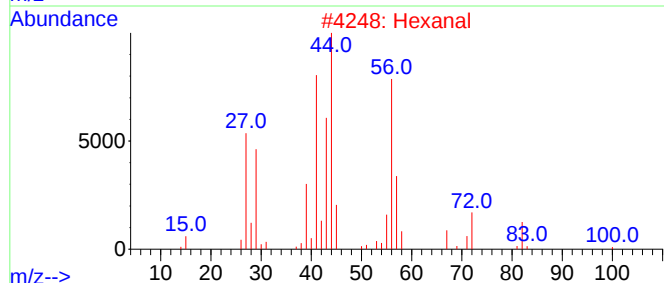
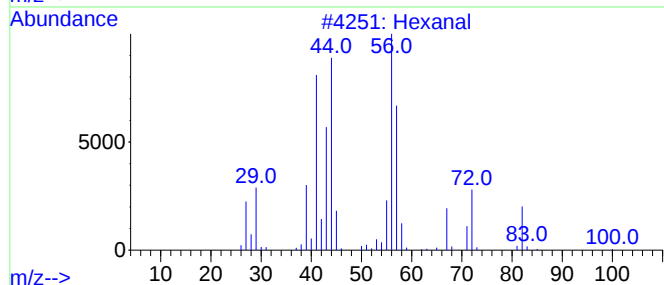
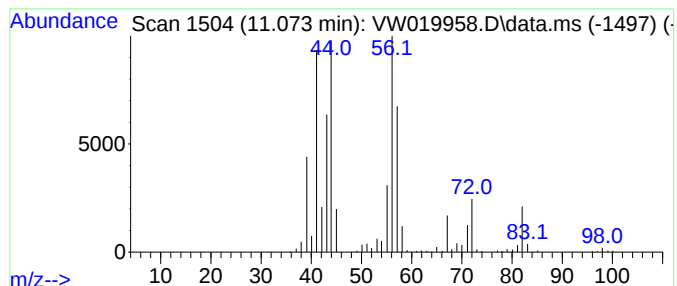
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Hexanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.073	8.47 ug/L	238426	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	81
4	Hexanal			100	C6H12O	000066-25-1	64
5	Hexanal			100	C6H12O	000066-25-1	43



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pentanal	9.408	1.4	ug/L	38890	1	8.847	690160	25.0
Hexanal	11.073	8.5	ug/L	238426	2	11.634	703495	25.0