

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW082024\
 Data File : VW029961.D
 Acq On : 20 Aug 2024 16:08
 Operator : SY/MD
 Sample : P3626-19
 Misc : 4.68g/10mL/MSVOA_W/SOIL/A
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 DCYB0

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: VW029961.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.155	42	44	46	rBV2	943	936	0.13%	0.016%
2	2.363	70	78	90	rBV	43974	105828	14.15%	1.778%
3	2.497	97	100	109	rVB2	4194	9865	1.32%	0.166%
4	2.899	158	166	185	rBV	34055	103154	13.79%	1.733%
5	3.393	241	247	254	rVV2	4971	11228	1.50%	0.189%
6	3.753	304	306	309	rVV2	862	904	0.12%	0.015%
7	4.021	337	350	361	rBV	77426	250149	33.45%	4.202%
8	4.125	362	367	376	rVV	16261	45907	6.14%	0.771%
9	4.216	380	382	385	rVB3	853	739	0.10%	0.012%
10	4.545	434	436	439	rVB3	575	630	0.08%	0.011%
11	4.673	452	457	461	rBV5	1267	2519	0.34%	0.042%
12	4.917	486	497	509	rBV2	6211	22798	3.05%	0.383%
13	5.143	529	534	536	rBV2	490	940	0.13%	0.016%
14	5.716	625	628	631	rVB2	474	534	0.07%	0.009%
15	5.777	631	638	641	rBV5	1861	4249	0.57%	0.071%
16	5.947	659	666	672	rVV8	1149	3468	0.46%	0.058%
17	6.898	816	822	834	rBV3	4221	11598	1.55%	0.195%
18	7.081	843	852	860	rBV	18727	55708	7.45%	0.936%
19	7.545	924	928	931	rBV4	426	765	0.10%	0.013%
20	7.648	934	945	958	rBV	139528	343131	45.88%	5.764%
21	7.770	962	965	968	rBV5	643	1093	0.15%	0.018%
22	8.276	1038	1048	1063	rBV2	256056	747917	100.00%	12.563%
23	8.471	1076	1080	1082	rVB3	624	707	0.09%	0.012%
24	8.557	1084	1094	1099	rBV4	3770	9036	1.21%	0.152%
25	8.709	1110	1119	1127	rBV6	4159	10116	1.35%	0.170%
26	8.843	1131	1141	1156	rBV	362080	705833	94.37%	11.856%
27	9.032	1168	1172	1174	rBV4	846	1264	0.17%	0.021%
28	9.063	1174	1177	1179	rBV3	672	875	0.12%	0.015%
29	9.270	1202	1211	1221	rBV	181356	374209	50.03%	6.286%
30	9.404	1227	1233	1243	rBV	25844	51577	6.90%	0.866%
31	9.660	1270	1275	1277	rBV4	547	898	0.12%	0.015%
32	9.758	1289	1291	1294	rBV2	532	534	0.07%	0.009%
33	9.898	1309	1314	1317	rVB7	894	1662	0.22%	0.028%
34	10.032	1328	1336	1346	rBV	84952	157303	21.03%	2.642%
35	10.245	1367	1371	1374	rVV7	917	1557	0.21%	0.026%
36	10.319	1374	1383	1391	rVV	312248	576126	77.03%	9.677%

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 Title : SFAM01.0

37	10.386	1391	1394	1407	rVB2	10459	20939	2.80%	0.352%
38	10.495	1407	1412	1416	rBV5	2082	3927	0.53%	0.066%
39	10.575	1419	1425	1434	rVV	52794	95960	12.83%	1.612%
40	10.696	1438	1445	1450	rBV2	9679	17574	2.35%	0.295%
41	10.739	1450	1452	1456	rVB3	704	1008	0.13%	0.017%
42	10.843	1465	1469	1472	rBV4	1315	2287	0.31%	0.038%
43	10.922	1476	1482	1494	rVV	72337	131524	17.59%	2.209%
44	11.068	1499	1506	1522	rVV	210608	343010	45.86%	5.762%
45	11.178	1522	1524	1527	rVB4	985	787	0.11%	0.013%
46	11.373	1554	1556	1559	rBV5	596	883	0.12%	0.015%
47	11.574	1584	1589	1591	rBV5	930	1462	0.20%	0.025%
48	11.629	1591	1598	1606	rBV	431411	709992	94.93%	11.926%
49	11.721	1611	1613	1618	rVB3	1072	1691	0.23%	0.028%
50	11.843	1628	1633	1645	rVB2	6033	13896	1.86%	0.233%
51	11.952	1648	1651	1655	rVB4	1083	1639	0.22%	0.028%
52	12.019	1655	1662	1667	rBV4	2221	5108	0.68%	0.086%
53	12.166	1684	1686	1688	rBV	694	842	0.11%	0.014%
54	12.245	1692	1699	1702	rBV3	1082	2237	0.30%	0.038%
55	12.336	1708	1714	1721	rBV3	9515	17503	2.34%	0.294%
56	12.464	1733	1735	1738	rVB2	731	779	0.10%	0.013%
57	12.513	1738	1743	1748	rBV4	1977	3188	0.43%	0.054%
58	12.599	1753	1757	1764	rVV2	9101	15152	2.03%	0.255%
59	12.690	1764	1772	1782	rVB	114613	188558	25.21%	3.167%
60	12.806	1788	1791	1796	rVB4	754	1084	0.14%	0.018%
61	12.891	1803	1805	1808	rBV3	712	853	0.11%	0.014%
62	12.934	1808	1812	1819	rVB8	2313	4697	0.63%	0.079%
63	13.031	1825	1828	1833	rBV6	1157	1984	0.27%	0.033%
64	13.098	1834	1839	1845	rVV7	2459	5001	0.67%	0.084%
65	13.153	1845	1848	1853	rVV5	1472	2540	0.34%	0.043%
66	13.208	1853	1857	1860	rVV4	993	1319	0.18%	0.022%
67	13.275	1863	1868	1874	rVB7	1561	3750	0.50%	0.063%
68	13.391	1879	1887	1893	rBV4	8161	14511	1.94%	0.244%
69	13.495	1899	1904	1907	rVV4	4527	8194	1.10%	0.138%
70	13.556	1907	1914	1924	rVV	236373	390734	52.24%	6.563%
71	13.647	1925	1929	1934	rVV5	4018	6625	0.89%	0.111%
72	13.751	1942	1946	1949	rBV5	759	1093	0.15%	0.018%
73	13.848	1955	1962	1969	rBV	149434	244103	32.64%	4.100%
74	14.013	1986	1989	1991	rBV3	875	1021	0.14%	0.017%
75	14.068	1992	1998	2005	rVB3	8260	15973	2.14%	0.268%
76	14.318	2032	2039	2047	rBV5	8185	14779	1.98%	0.248%

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 Title : SFAM01.0

77	14.415	2053	2055	2059	rBV4	624	732	0.10%	0.012%
78	14.519	2067	2072	2076	rVB6	2123	3720	0.50%	0.062%
79	14.617	2086	2088	2091	rVV3	707	752	0.10%	0.013%
80	14.684	2097	2099	2102	rBV4	544	633	0.08%	0.011%
81	14.714	2102	2104	2110	rVB5	1571	2295	0.31%	0.039%
82	14.848	2122	2126	2131	rBV6	2491	3799	0.51%	0.064%
83	14.952	2138	2143	2147	rBV8	1339	2335	0.31%	0.039%
84	15.068	2159	2162	2164	rBV4	622	594	0.08%	0.010%
85	15.183	2175	2181	2182	rBV4	1690	2625	0.35%	0.044%
86	15.238	2187	2190	2197	rVB5	1944	3405	0.46%	0.057%
87	15.366	2209	2211	2215	rBV5	546	933	0.12%	0.016%
88	15.427	2220	2221	2225	rVB3	535	558	0.07%	0.009%
89	15.482	2225	2230	2233	rBV3	1105	2259	0.30%	0.038%
90	15.549	2239	2241	2244	rVB4	697	603	0.08%	0.010%
91	15.671	2259	2261	2265	rBV3	678	822	0.11%	0.014%
92	15.787	2278	2280	2283	rVB2	981	1080	0.14%	0.018%
93	15.836	2283	2288	2296	rBV5	1914	4567	0.61%	0.077%
94	15.958	2304	2308	2314	rVB5	1303	2980	0.40%	0.050%
95	16.013	2314	2317	2318	rBV	745	759	0.10%	0.013%
96	16.074	2324	2327	2330	rBV2	823	1021	0.14%	0.017%
97	16.336	2368	2370	2373	rVB2	609	638	0.09%	0.011%
98	16.378	2373	2377	2382	rVB7	592	1119	0.15%	0.019%
99	16.482	2391	2394	2396	rBV4	479	556	0.07%	0.009%
100	16.573	2403	2409	2412	rBV6	354	653	0.09%	0.011%

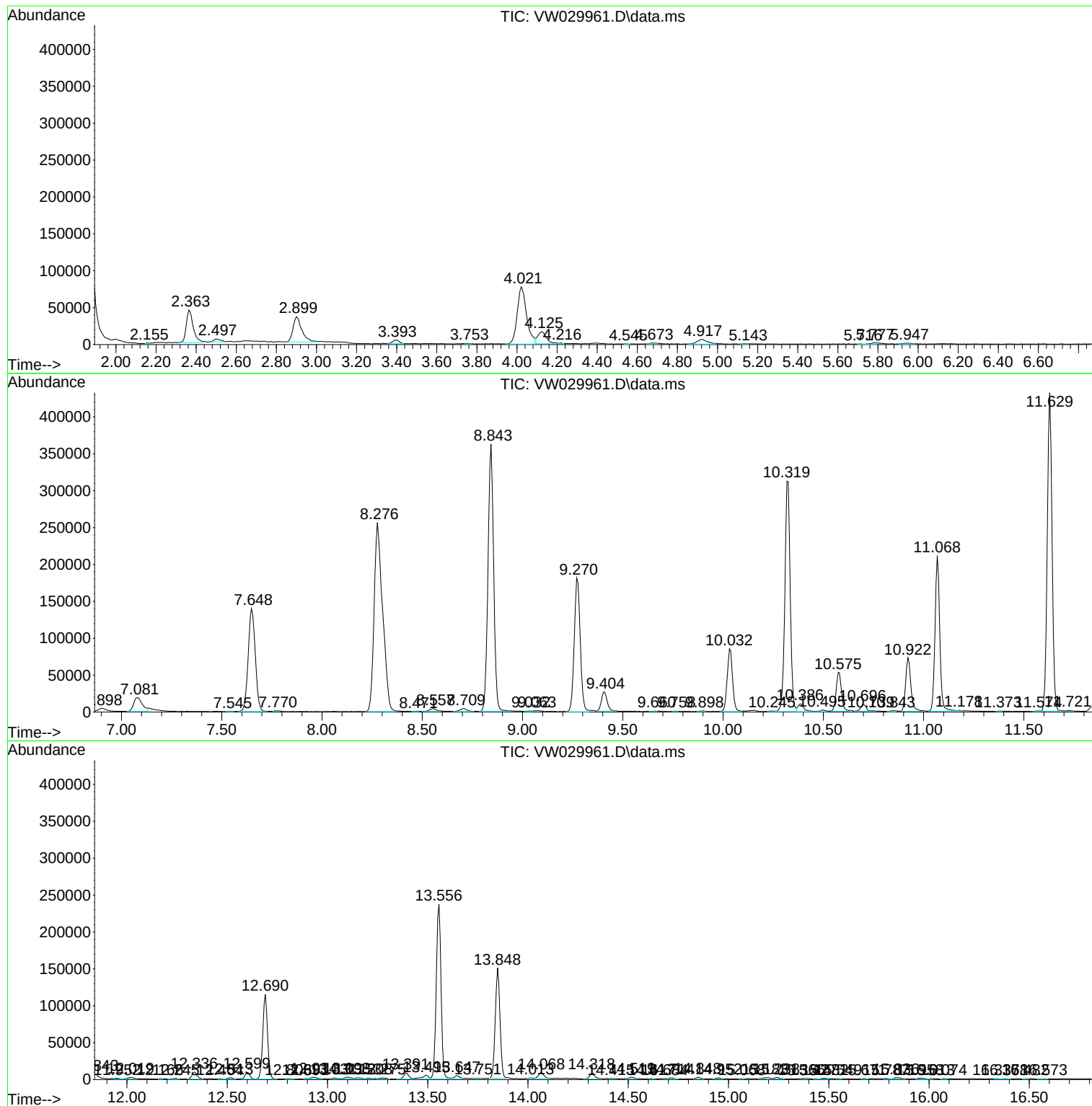
Sum of corrected areas: 5953402

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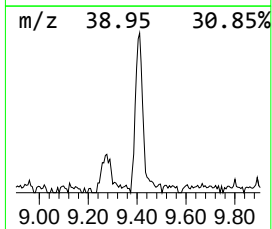
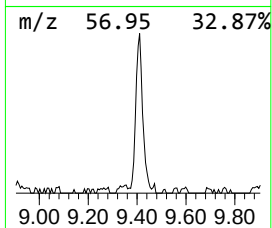
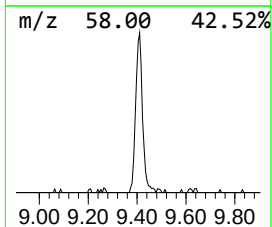
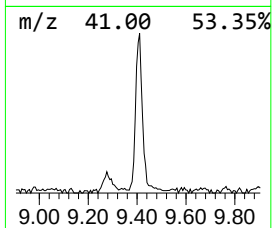
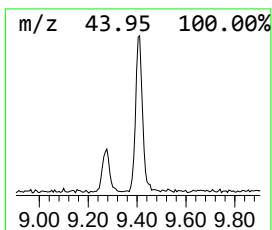
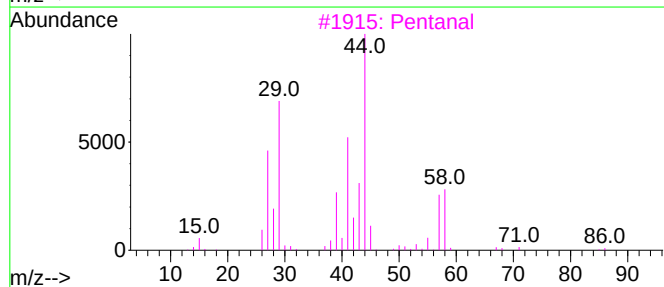
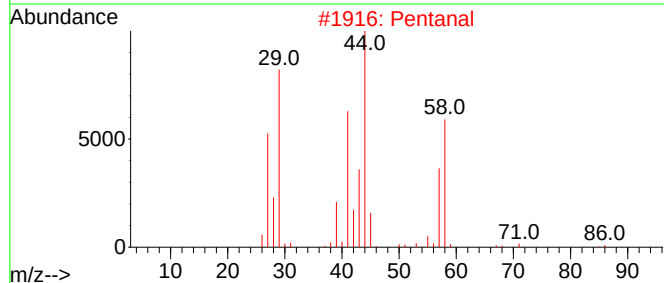
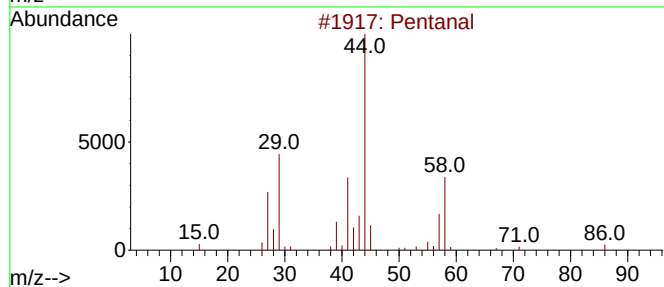
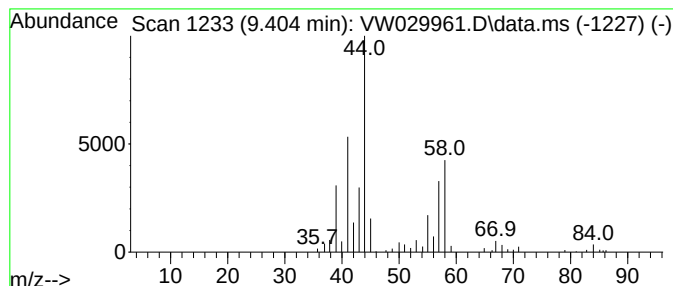
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM072424SMA.M
Quant Title : SFAM01.0

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

Peak Number 1 Pentanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.404	1.83 ug/L	51577	1,4-Difluorobenzene	8.843

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanal			86	C5H10O	000110-62-3	86
2	Pentanal			86	C5H10O	000110-62-3	72
3	Pentanal			86	C5H10O	000110-62-3	59
4	Butanal, 3-methyl-			86	C5H10O	000590-86-3	56
5	Cyclopropyl carbinol			72	C4H8O	002516-33-8	50



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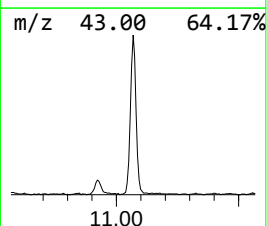
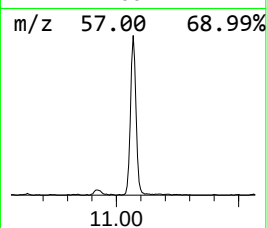
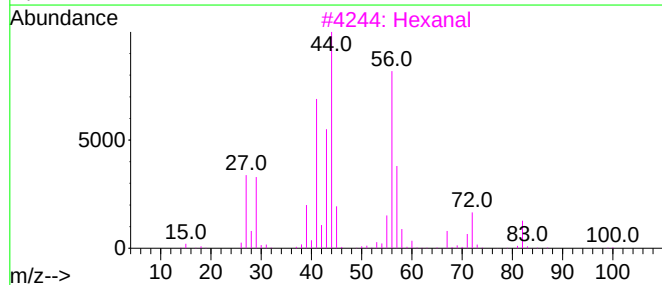
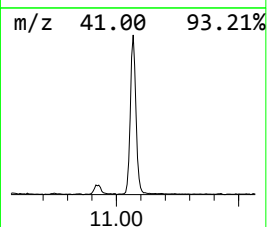
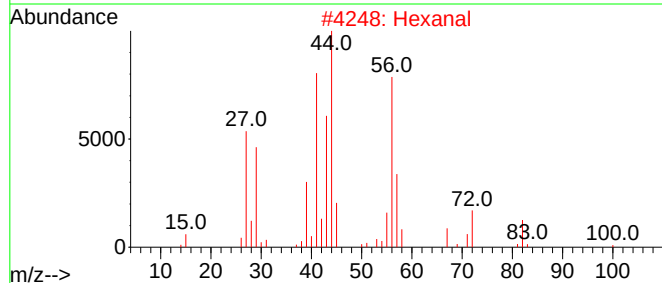
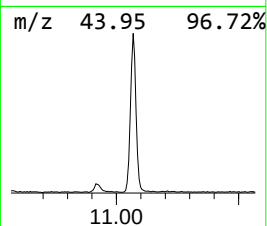
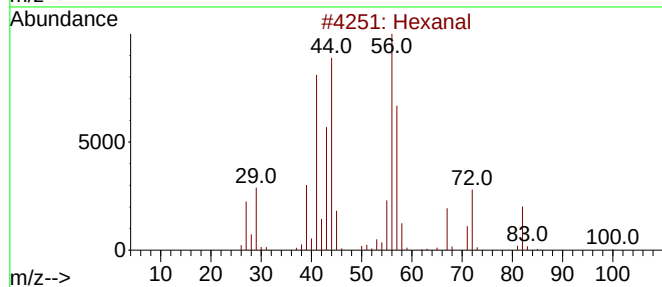
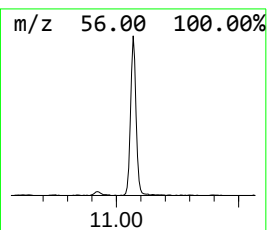
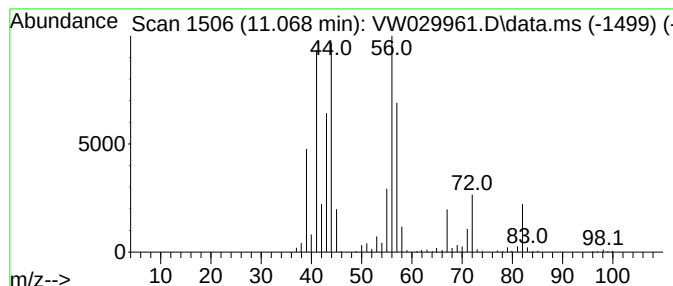
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Hexanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.068	12.08 ug/L	343010	Chlorobenzene-d5	11.629

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	68
5	Hexanal			100	C6H12O	000066-25-1	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pentanal	9.404	1.8	ug/L	51577	1	8.843	705833	25.0
Hexanal	11.068	12.1	ug/L	343010	2	11.629	709992	25.0