

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU062219\
 Data File : VU032968.D
 Acq On : 22 Jun 2019 00:27
 Operator : JC/SP
 Sample : K3464-07
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ETF27

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
 Title : VOC Analysis

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.392	88	94	108	rVB	83043	85266	11.93%	1.324%
2	1.466	110	117	134	rBV	264556	298115	41.70%	4.628%
3	1.672	174	181	195	rVB	70514	88570	12.39%	1.375%
4	2.264	354	365	376	rVB	143620	215553	30.15%	3.346%
5	2.392	403	405	411	rVB2	375	329	0.05%	0.005%
6	2.469	423	429	438	rVB2	3634	5489	0.77%	0.085%
7	2.582	456	464	466	rBV2	392	524	0.07%	0.008%
8	2.620	474	476	483	rVB2	496	339	0.05%	0.005%
9	2.682	493	495	500	rVB2	489	318	0.04%	0.005%
10	2.778	522	525	527	rBV2	474	291	0.04%	0.005%
11	2.829	530	541	550	rVV2	3015	5646	0.79%	0.088%
12	2.932	571	573	578	rBV2	374	266	0.04%	0.004%
13	3.058	608	612	615	rVB2	334	301	0.04%	0.005%
14	3.077	615	618	624	rVB	390	311	0.04%	0.005%
15	3.106	624	627	629	rBV	347	241	0.03%	0.004%
16	3.128	629	634	640	rVB4	305	393	0.05%	0.006%
17	3.170	644	647	648	rBV2	723	449	0.06%	0.007%
18	3.292	679	685	690	rVB5	406	481	0.07%	0.007%
19	3.492	742	747	751	rBV2	431	422	0.06%	0.007%
20	3.620	783	787	790	rVV3	489	444	0.06%	0.007%
21	3.665	799	801	808	rVB3	334	273	0.04%	0.004%
22	3.707	811	814	818	rVB2	438	262	0.04%	0.004%
23	3.749	823	827	830	rBV3	338	281	0.04%	0.004%
24	3.778	832	836	839	rVB3	384	331	0.05%	0.005%
25	3.910	873	877	881	rVB2	354	262	0.04%	0.004%
26	4.000	894	905	916	rBV5	1970	4602	0.64%	0.071%
27	4.080	927	930	938	rVB2	512	456	0.06%	0.007%
28	4.119	938	942	945	rBV3	315	251	0.04%	0.004%
29	4.170	945	958	984	rBV	89282	239645	33.52%	3.720%
30	4.386	1022	1025	1028	rBV2	533	376	0.05%	0.006%
31	4.402	1028	1030	1036	rVB	412	339	0.05%	0.005%
32	4.524	1065	1068	1071	rVB	513	355	0.05%	0.006%
33	4.569	1078	1082	1085	rVV	448	448	0.06%	0.007%
34	4.640	1088	1104	1126	rVV	125476	291722	40.81%	4.529%

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 Title : VOC Analysis

35	4.717	1126	1128	1134	rVB3	405	341	0.05%	0.005%
36	4.865	1171	1174	1177	rVV4	414	319	0.04%	0.005%
37	4.884	1177	1180	1186	rVV3	679	672	0.09%	0.010%
38	4.981	1205	1210	1213	rBV2	559	485	0.07%	0.008%
39	5.331	1296	1319	1345	rBV2	238917	714836	100.00%	11.097%
40	5.489	1365	1368	1372	rVB2	323	254	0.04%	0.004%
41	5.524	1377	1379	1383	rVB3	446	256	0.04%	0.004%
42	5.640	1410	1415	1418	rVB2	543	489	0.07%	0.008%
43	5.665	1418	1423	1425	rBV	327	241	0.03%	0.004%
44	5.694	1428	1432	1435	rVB2	421	353	0.05%	0.005%
45	5.768	1452	1455	1459	rBV2	411	369	0.05%	0.006%
46	5.881	1476	1490	1513	rBV	238747	469318	65.65%	7.286%
47	6.074	1545	1550	1556	rBV3	416	551	0.08%	0.009%
48	6.167	1572	1579	1580	rBV2	1570	1415	0.20%	0.022%
49	6.273	1608	1612	1615	rBV3	360	306	0.04%	0.005%
50	6.324	1615	1628	1647	rBV	165238	332225	46.48%	5.158%
51	6.447	1662	1666	1671	rVV3	533	538	0.08%	0.008%
52	6.530	1682	1692	1717	rBV3	10295	22670	3.17%	0.352%
53	6.643	1724	1727	1731	rVB2	466	384	0.05%	0.006%
54	6.861	1789	1795	1797	rVV3	466	451	0.06%	0.007%
55	6.878	1797	1800	1802	rVB2	547	292	0.04%	0.005%
56	6.932	1811	1817	1818	rBV3	383	323	0.05%	0.005%
57	7.019	1840	1844	1848	rBV2	315	338	0.05%	0.005%
58	7.222	1895	1907	1930	rBV	90448	163003	22.80%	2.531%
59	7.360	1947	1950	1956	rVB4	370	346	0.05%	0.005%
60	7.559	1996	2012	2030	rBV	312129	539502	75.47%	8.375%
61	7.765	2071	2076	2084	rVB5	329	446	0.06%	0.007%
62	7.842	2090	2100	2117	rBV	63277	110668	15.48%	1.718%
63	8.135	2187	2191	2193	rBV	311	241	0.03%	0.004%
64	8.157	2193	2198	2199	rBV2	597	448	0.06%	0.007%
65	8.222	2213	2218	2219	rBV2	678	530	0.07%	0.008%
66	8.305	2233	2244	2280	rVV	260638	467062	65.34%	7.251%
67	8.459	2282	2292	2315	rVB2	72570	124066	17.36%	1.926%
68	8.591	2332	2333	2336	rVB2	692	241	0.03%	0.004%
69	8.826	2400	2406	2409	rBV2	419	503	0.07%	0.008%
70	9.083	2473	2486	2505	rBV	357986	591658	82.77%	9.185%
71	9.263	2540	2542	2546	rBV3	307	287	0.04%	0.004%

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 Title : VOC Analysis

72	9.440	2591	2597	2603	rBV3	365	429	0.06%	0.007%
73	9.521	2612	2622	2625	rBV3	438	573	0.08%	0.009%
74	9.540	2625	2628	2630	rBV	346	257	0.04%	0.004%
75	9.582	2635	2641	2649	rVV4	524	935	0.13%	0.015%
76	9.704	2674	2679	2681	rBV2	830	829	0.12%	0.013%
77	9.980	2759	2765	2766	rBV3	456	380	0.05%	0.006%
78	10.022	2768	2778	2803	rVB2	59499	97963	13.70%	1.521%
79	10.189	2827	2830	2835	rBV4	353	373	0.05%	0.006%
80	10.363	2881	2884	2886	rVV3	471	334	0.05%	0.005%
81	10.424	2891	2903	2925	rVV	259703	417269	58.37%	6.478%
82	10.607	2950	2960	2969	rVV3	1454	2239	0.31%	0.035%
83	10.691	2980	2986	2988	rBV2	475	521	0.07%	0.008%
84	10.945	3059	3065	3070	rVB3	868	1102	0.15%	0.017%
85	10.983	3070	3077	3083	rVB5	746	1039	0.15%	0.016%
86	11.209	3134	3147	3160	rBV5	5577	9349	1.31%	0.145%
87	11.331	3181	3185	3187	rBV3	372	297	0.04%	0.005%
88	11.366	3187	3196	3210	rVV5	13266	22169	3.10%	0.344%
89	11.479	3219	3231	3252	rBV	361977	565493	79.11%	8.779%
90	11.855	3334	3348	3369	rBV	323618	526173	73.61%	8.169%
91	12.016	3394	3398	3401	rVB5	543	485	0.07%	0.008%
92	12.154	3433	3441	3443	rBV2	534	557	0.08%	0.009%
93	12.241	3463	3468	3469	rBV2	824	690	0.10%	0.011%
94	12.456	3533	3535	3537	rBV	534	268	0.04%	0.004%
95	12.839	3652	3654	3655	rBV2	532	245	0.03%	0.004%
96	13.083	3727	3730	3733	rBV3	484	374	0.05%	0.006%
97	13.392	3821	3826	3829	rBV2	282	301	0.04%	0.005%
98	13.424	3833	3836	3837	rBV	633	384	0.05%	0.006%
99	14.221	4082	4084	4088	rVB3	532	348	0.05%	0.005%
100	14.964	4312	4315	4316	rBV2	570	290	0.04%	0.005%

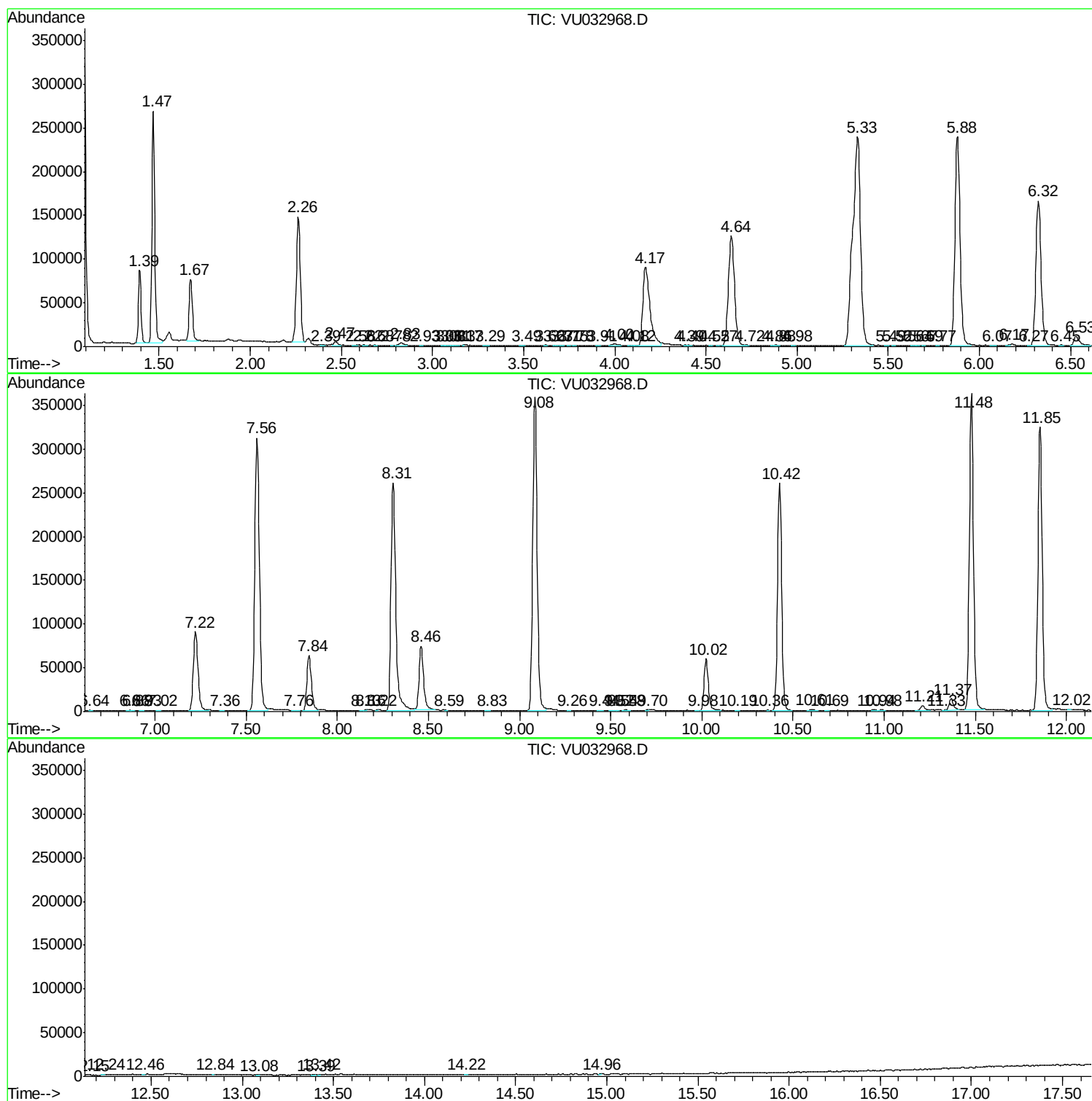
Sum of corrected areas: 6441444

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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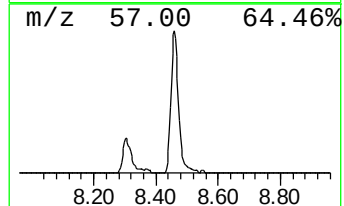
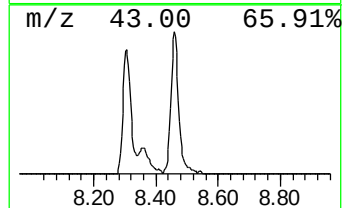
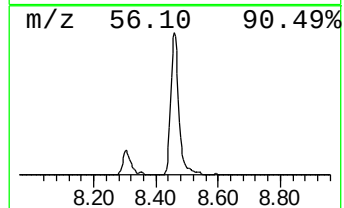
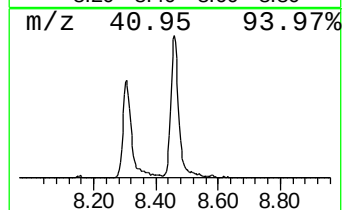
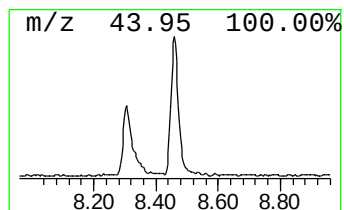
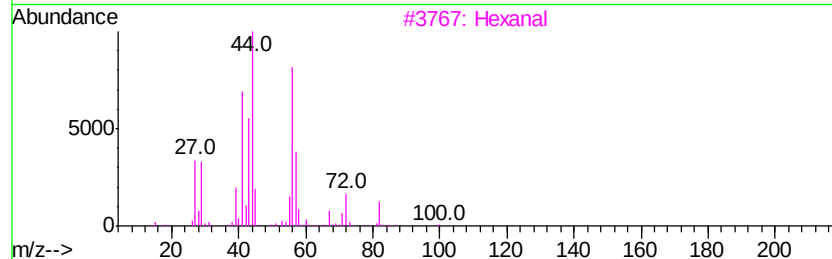
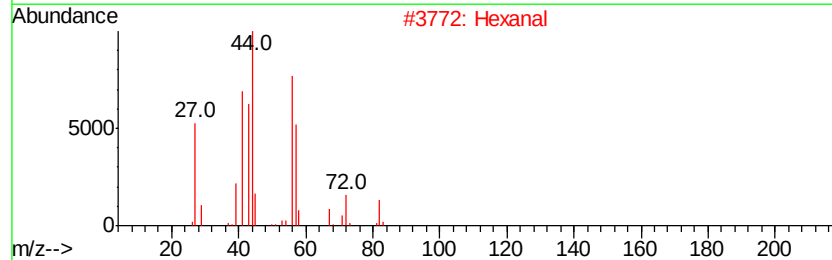
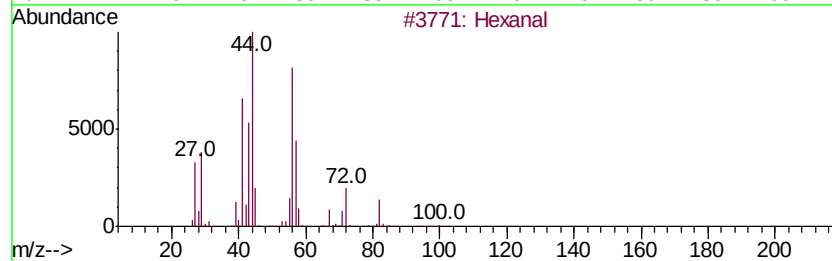
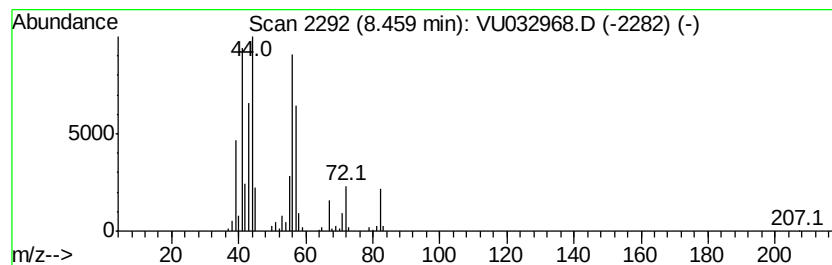
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Hexanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.46	10.48 ug/L	124066	Chlorobenzene-d5	9.08

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal		100	C6H12O	000066-25-1	72
2	Hexanal		100	C6H12O	000066-25-1	64
3	Hexanal		100	C6H12O	000066-25-1	64
4	Hexanal		100	C6H12O	000066-25-1	64
5	Cyclobutanol, 2-ethyl-		100	C6H12O	035301-43-0	42



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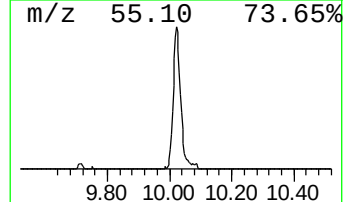
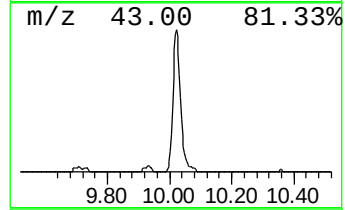
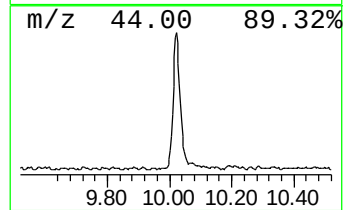
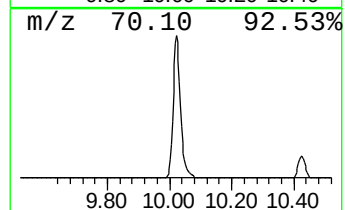
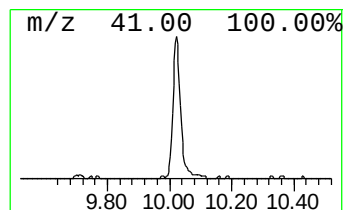
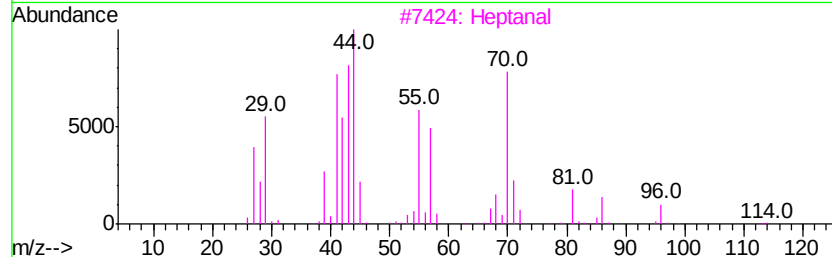
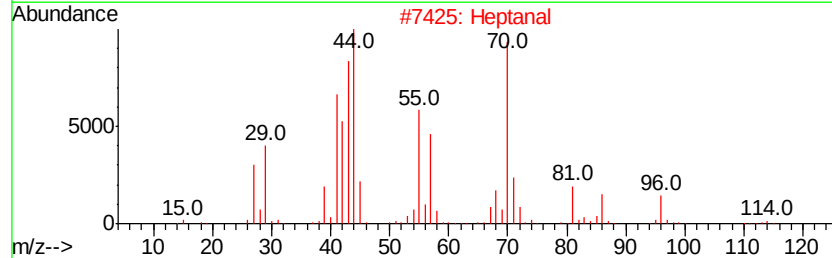
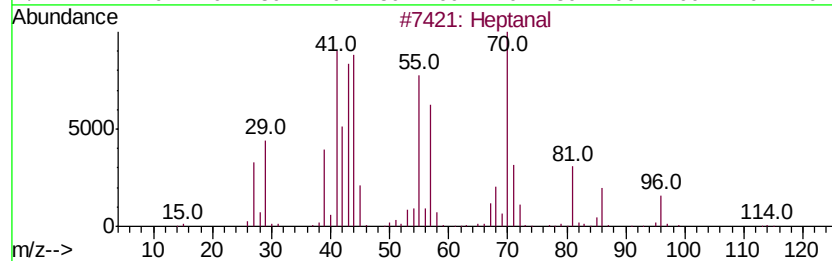
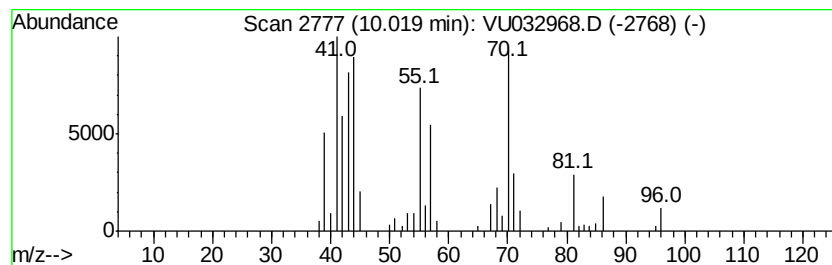
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Heptanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.02	8.28 ug/L	97963	Chlorobenzene-d5	9.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptanal	114	C7H14O	000111-71-7	91
2		Heptanal	114	C7H14O	000111-71-7	90
3		Heptanal	114	C7H14O	000111-71-7	90
4		Heptanal	114	C7H14O	000111-71-7	83
5		Heptanal	114	C7H14O	000111-71-7	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexanal	8.46	10.5	ug/L	124066	2	9.08	591658	50.0
Heptanal	10.02	8.3	ug/L	97963	2	9.08	591658	50.0