

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092222\
 Data File : VU050910.D
 Acq On : 22 Sep 2022 19:59
 Operator : JC/MD
 Sample : N4747-10
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 E45A7

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_U\Method\SFAMULM092022WMA.M

Title : VOC Analysis

Signal : TIC: VU050910.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.601	74	81	94	rVB2	245372	293279	17.35%	2.182%
2	1.906	169	176	194	rVB	173614	235372	13.93%	1.751%
3	2.565	368	381	394	rBV	343934	566687	33.53%	4.216%
4	3.038	524	528	530	rBV4	1484	1340	0.08%	0.010%
5	3.179	564	572	580	rBV5	1998	3714	0.22%	0.028%
6	3.353	617	626	643	rVB2	9211	17507	1.04%	0.130%
7	3.465	658	661	663	rBV	351	197	0.01%	0.001%
8	3.504	669	673	677	rVB	484	481	0.03%	0.004%
9	3.539	677	684	690	rBV2	441	709	0.04%	0.005%
10	3.594	698	701	702	rBV	322	133	0.01%	0.001%
11	3.626	708	711	715	rBV	255	170	0.01%	0.001%
12	3.690	729	731	734	rBV2	636	500	0.03%	0.004%
13	3.735	743	745	748	rVB	285	135	0.01%	0.001%
14	3.809	766	768	770	rBV2	181	96	0.01%	0.001%
15	3.871	770	787	802	rVV3	23500	54907	3.25%	0.408%
16	3.973	817	819	825	rVB	284	163	0.01%	0.001%
17	3.996	825	826	827	rVB	143	28	0.00%	0.000%
18	4.092	853	856	860	rBV	374	318	0.02%	0.002%
19	4.166	877	879	884	rVB	404	230	0.01%	0.002%
20	4.189	884	886	890	rVB	406	152	0.01%	0.001%
21	4.221	890	896	898	rBV	245	225	0.01%	0.002%
22	4.237	898	901	903	rBV	210	141	0.01%	0.001%
23	4.330	929	930	934	rVB	175	52	0.00%	0.000%
24	4.366	934	941	943	rBV2	246	309	0.02%	0.002%
25	4.436	959	963	964	rBV	438	244	0.01%	0.002%
26	4.616	1008	1019	1026	rBV	200346	428610	25.36%	3.188%
27	5.060	1141	1157	1181	rBV	305722	672848	39.81%	5.005%
28	5.346	1243	1246	1248	rBV2	486	349	0.02%	0.003%
29	5.452	1277	1279	1280	rBV	139	60	0.00%	0.000%
30	5.552	1305	1310	1317	rBV3	386	412	0.02%	0.003%
31	5.587	1317	1321	1322	rBV2	116	83	0.00%	0.001%
32	5.597	1322	1324	1328	rVB	250	107	0.01%	0.001%
33	5.623	1329	1332	1335	rVB2	326	204	0.01%	0.002%
34	5.639	1335	1337	1340	rVB2	102	51	0.00%	0.000%
35	5.723	1341	1363	1395	rBV2	617169	1690005	100.00%	12.572%
36	6.073	1470	1472	1477	rVB3	505	368	0.02%	0.003%

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 Title : VOC Analysis

37	6.099	1477	1480	1481	rBV	296	182	0.01%	0.001%
38	6.186	1506	1507	1508	rBV	116	39	0.00%	0.000%
39	6.247	1510	1526	1556	rBV	492167	931597	55.12%	6.930%
40	6.542	1604	1618	1643	rBV	396580	755413	44.70%	5.620%
41	6.690	1650	1664	1682	rBV	396101	770354	45.58%	5.731%
42	6.854	1712	1715	1717	rBV2	545	364	0.02%	0.003%
43	6.883	1717	1724	1737	rVB7	3120	5526	0.33%	0.041%
44	7.041	1767	1773	1776	rBV3	434	504	0.03%	0.004%
45	7.147	1804	1806	1808	rBV	283	179	0.01%	0.001%
46	7.237	1831	1834	1837	rBV2	238	176	0.01%	0.001%
47	7.263	1840	1842	1845	rVV	213	125	0.01%	0.001%
48	7.279	1845	1847	1849	rVB	253	93	0.01%	0.001%
49	7.298	1849	1853	1857	rBV3	362	349	0.02%	0.003%
50	7.343	1864	1867	1869	rBV2	267	161	0.01%	0.001%
51	7.372	1874	1876	1878	rBV2	219	120	0.01%	0.001%
52	7.414	1888	1889	1890	rBV2	146	39	0.00%	0.000%
53	7.481	1905	1910	1913	rVB3	393	323	0.02%	0.002%
54	7.501	1913	1916	1917	rBV2	198	126	0.01%	0.001%
55	7.565	1923	1936	1957	rBV	195754	344053	20.36%	2.559%
56	7.845	2019	2023	2025	rBV	358	289	0.02%	0.002%
57	7.896	2025	2039	2055	rBV	700987	1199310	70.96%	8.922%
58	8.176	2110	2126	2142	rBV2	154972	309736	18.33%	2.304%
59	8.433	2203	2206	2209	rBV2	436	270	0.02%	0.002%
60	8.449	2209	2211	2213	rBV2	373	209	0.01%	0.002%
61	8.465	2213	2216	2217	rBV	1325	732	0.04%	0.005%
62	8.568	2246	2248	2249	rBV2	304	113	0.01%	0.001%
63	8.632	2253	2268	2305	rBV2	541115	1063805	62.95%	7.914%
64	8.783	2306	2315	2337	rVB	95339	163035	9.65%	1.213%
65	8.941	2361	2364	2366	rBV2	402	259	0.02%	0.002%
66	9.028	2390	2391	2394	rVB	221	69	0.00%	0.001%
67	9.047	2394	2397	2400	rBV2	394	297	0.02%	0.002%
68	9.092	2410	2411	2414	rBV2	201	122	0.01%	0.001%
69	9.140	2424	2426	2429	rVB	565	296	0.02%	0.002%
70	9.166	2430	2434	2436	rVV3	447	266	0.02%	0.002%
71	9.285	2469	2471	2474	rVB2	338	139	0.01%	0.001%
72	9.337	2483	2487	2488	rBV	303	189	0.01%	0.001%
73	9.417	2497	2512	2545	rBV	670473	1118323	66.17%	8.319%
74	9.648	2576	2584	2585	rBV3	683	655	0.04%	0.005%
75	9.735	2607	2611	2613	rBV2	391	278	0.02%	0.002%
76	9.886	2653	2658	2660	rBV2	665	570	0.03%	0.004%

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77	9.938	2671	2674	2676	rBV2	419	222	0.01%	0.002%
78	10.025	2699	2701	2704	rBV	344	253	0.01%	0.002%
79	10.295	2783	2785	2786	rBV	222	79	0.00%	0.001%
80	10.346	2794	2801	2810	rBV7	2706	3657	0.22%	0.027%
81	10.462	2833	2837	2838	rBV	373	232	0.01%	0.002%
82	10.671	2892	2902	2910	rVB4	2472	3810	0.23%	0.028%
83	10.706	2910	2913	2915	rBV	222	169	0.01%	0.001%
84	10.754	2915	2928	2946	rBV	586247	940578	55.66%	6.997%
85	10.886	2965	2969	2979	rVB9	1922	3073	0.18%	0.023%
86	10.928	2980	2982	2984	rVB	370	110	0.01%	0.001%
87	11.304	3091	3099	3104	rBV6	1618	2166	0.13%	0.016%
88	11.468	3136	3150	3159	rBV7	4996	8436	0.50%	0.063%
89	11.520	3164	3166	3168	rBV	257	135	0.01%	0.001%
90	11.555	3173	3177	3179	rVB2	495	338	0.02%	0.003%
91	11.571	3180	3182	3185	rBV3	516	339	0.02%	0.003%
92	11.687	3214	3218	3228	rVB7	2224	3485	0.21%	0.026%
93	11.748	3235	3237	3241	rVB3	688	415	0.02%	0.003%
94	11.809	3244	3256	3275	rBV	526758	832212	49.24%	6.191%
95	12.063	3325	3335	3351	rBV2	24250	47553	2.81%	0.354%
96	12.192	3363	3375	3396	rVB	594088	953009	56.39%	7.089%
97	12.619	3507	3508	3509	rBV	352	97	0.01%	0.001%
98	12.832	3569	3574	3578	rBV3	672	670	0.04%	0.005%
99	12.889	3588	3592	3601	rVB7	1938	2689	0.16%	0.020%

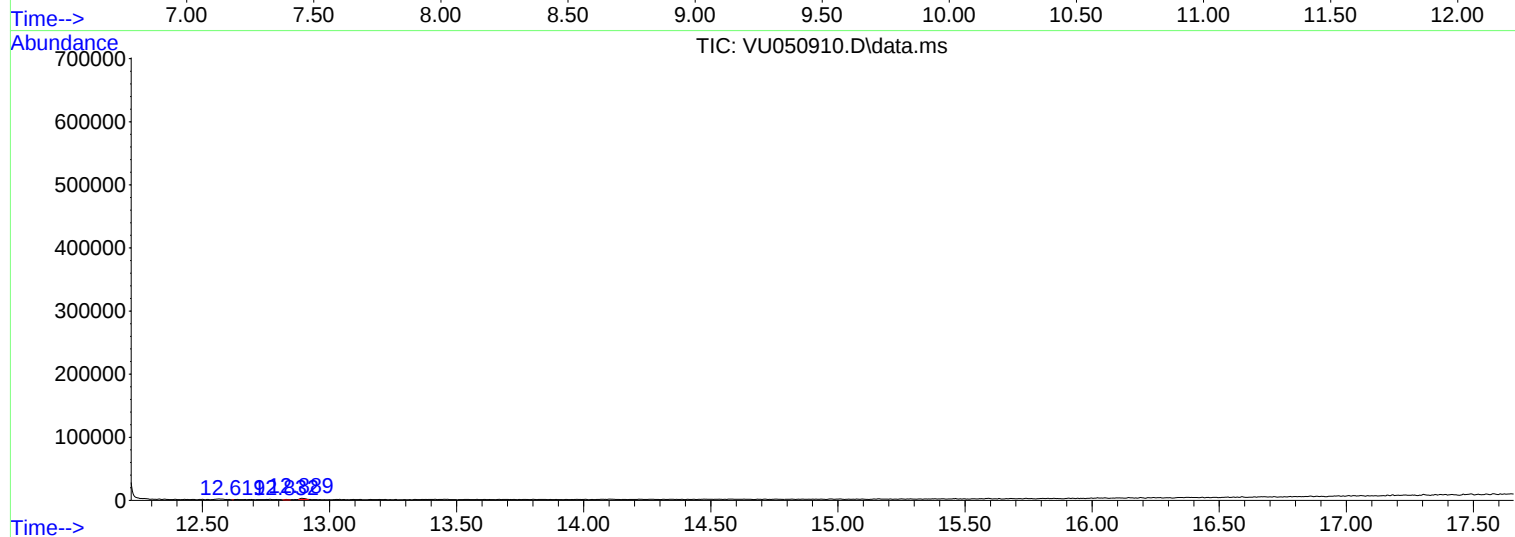
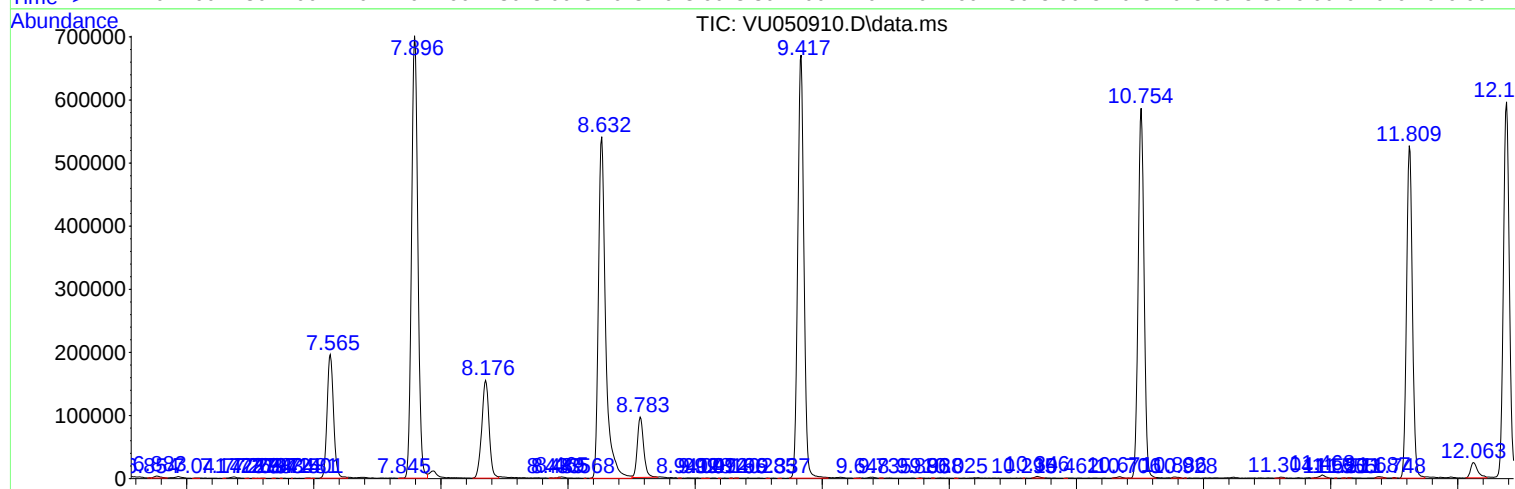
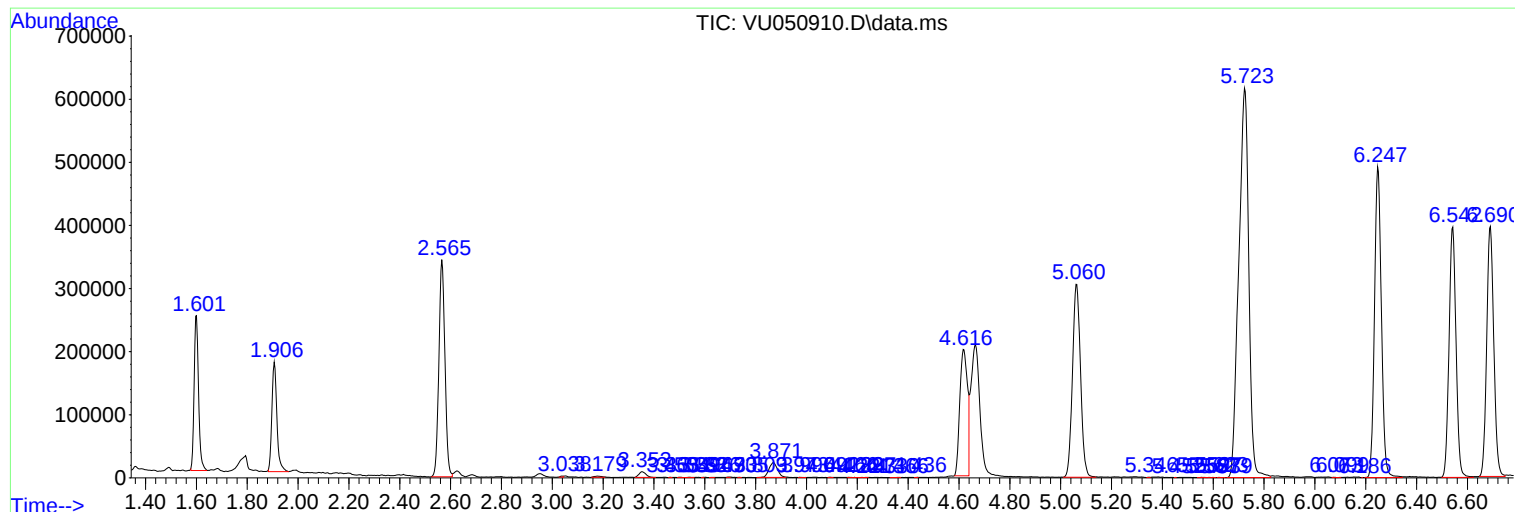
Sum of corrected areas: 13442598

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092022WMA.M
Quant Title : VOC Analysis

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



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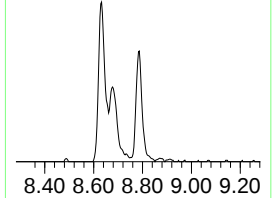
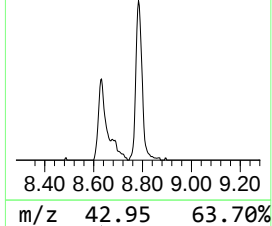
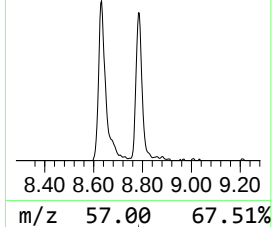
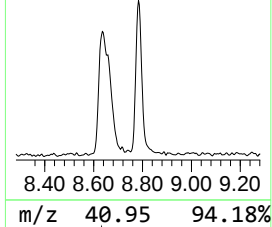
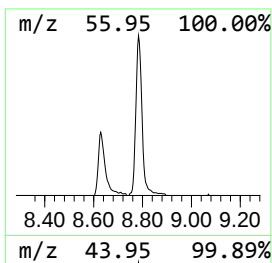
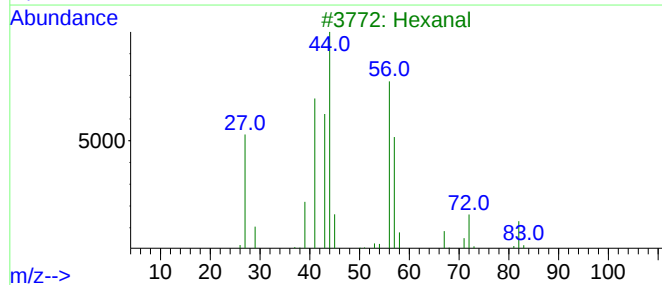
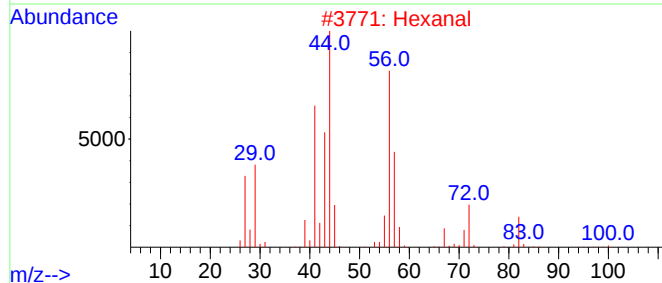
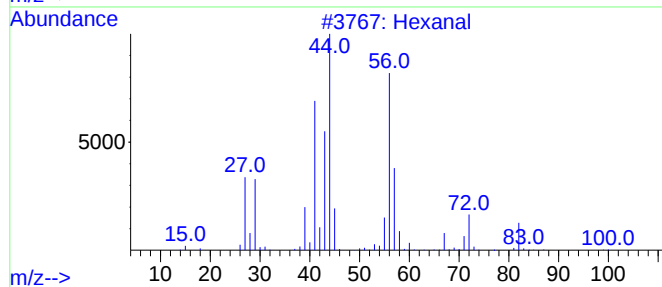
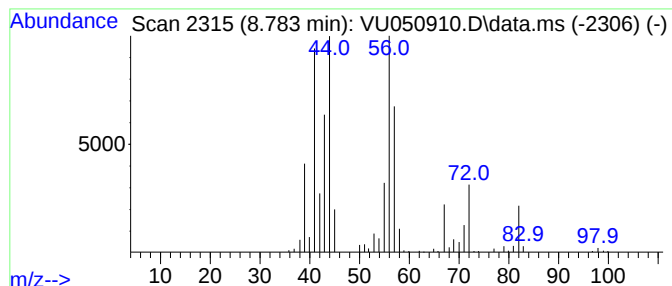
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092022WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Hexanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.783	7.29 ug/L	163035	Chlorobenzene-d5	9.417

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	81
2	Hexanal			100	C6H12O	000066-25-1	64
3	Hexanal			100	C6H12O	000066-25-1	64
4	Hexanal			100	C6H12O	000066-25-1	50
5	2-Hexen-1-ol, (E)-			100	C6H12O	000928-95-0	27



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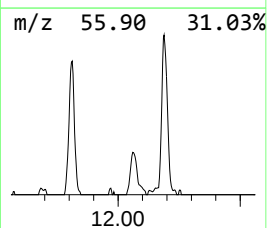
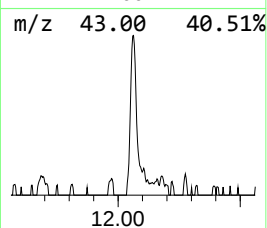
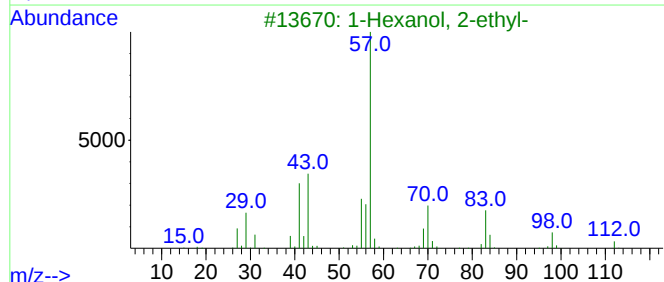
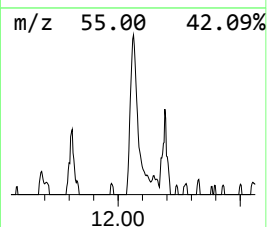
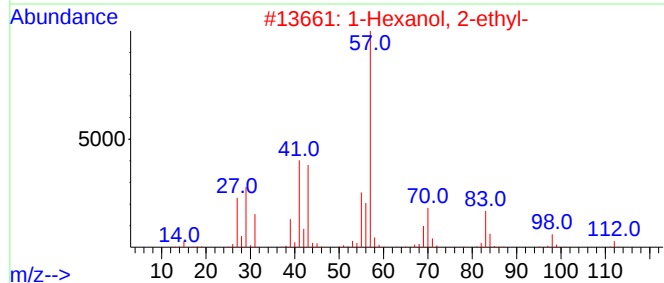
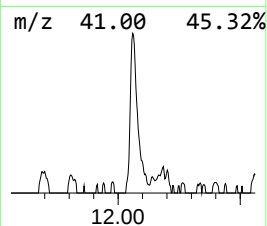
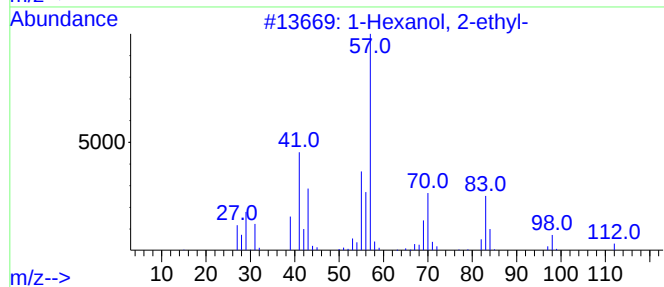
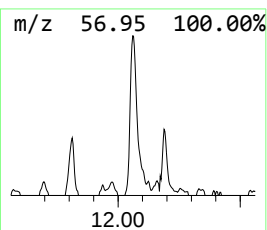
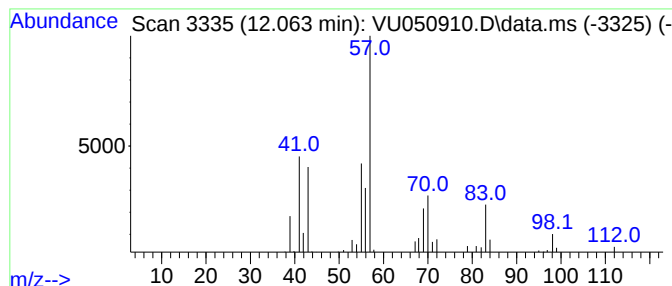
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.063	2.86 ug/L	47553	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	72
2	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	72
3	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	64
4	2-Propyl-1-pentanol			130	C8H18O	058175-57-8	50
5	Oxirane, [(2-ethylhexyl)oxy]met...			186	C11H22O2	002461-15-6	42



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexanal	8.783	7.3	ug/L	163035	2	9.417	1118320	50.0
1-Hexanol, 2-et...	12.063	2.9	ug/L	47553	3	11.809	832212	50.0