LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU080918\
Data File : VU026006.D
Acq On : 09 Aug 2018 19:14
Operator : MD/SY
Sample : J4361-07
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 30 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : A4ZB4

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\SOMULM080918WMA.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	0.780	56	59	62	rVV2	367	298	0.02%	0.003%
2	0.902	94	97	102	rBV2	410	398	0.03%	0.004%
3	0.960	111	115	118	rVB3	360	324	0.02%	0.003%
4	1.085	141	154	174	rBV	237677	291021	18.85%	2.611%
5	1.400	244	252	267	rBV	141785	147843	9.57%	1.327%
6	1.471	270	274	282	rVB	7601	8584	0.56%	0.077%
7	1.680	331	339	355	rVB	107791	145017	9.39%	1.301%
8	2.191	493	498	506	rVB5	2410	3375	0.22%	0.030%
9	2.272	512	523	532	rBV	249577	382371	24.76%	3.431%
10	2.320	532	538	562	rVB	97048	155897	10.10%	1.399%
11	2.445	571	577	586	rVB5	1367	2069	0.13%	0.019%
12	2.616	627	630	632	rVV2	724	543	0.04%	0.005%
13	2.680	644	650	653	rBV2	348	461	0.03%	0.004%
14	2.699	653	656	658	rBV3	510	358	0.02%	0.003%
15	2.815	686	692	695	rBV3	499	589	0.04%	0.005%
16	2.934	723	729	732	rBV2	276	298	0.02%	0.003%
17	3.143	787	794	799	rBV3	391	593	0.04%	0.005%
18	3.172	799	803	804	rBV2	538	330	0.02%	0.003%
19	3.185	804	807	815	rVB3	1072	1360	0.09%	0.012%
20	3.387	866	870	874	rVV2	453	495	0.03%	0.004%
21	3.445	878	888	901	rVB	5696	12351	0.80%	0.111%
22	3.834	1006	1009	1013	rVB	470	354	0.02%	0.003%
23	3.889	1021	1026	1028	rBV2	483	398	0.03%	0.004%
24	3.944	1039	1043	1047	rVB	432	304	0.02%	0.003%
25	3.985	1047	1056	1061	rBV5	1157	1824	0.12%	0.016%
26	4.178	1099	1116	1134	rBV	107064	278604	18.04%	2.500%
27	4.522	1220	1223	1226	rVB3	425	304	0.02%	0.003%
28	4.651	1243	1263	1284	rBV	214635	507869	32.89%	4.557%
29	4.915	1329	1345	1362	rBV3	18277	43951	2.85%	0.394%
30	5.095	1396	1401	1403	rBV	316	330	0.02%	0.003%
31	5.233	1435	1444	1448	rBV2	454	712	0.05%	0.006%
32	5.342	1453	1478	1503	rBV3	413584	1245965	80.68%	11.180%
33	5.596	1552	1557	1566	rVB4	1379	2403	0.16%	0.022%
34	5.680	1579	1583	1588	rVB4	387	350	0.02%	0.003%

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ALS Vial : 30 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : A4ZB4

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

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Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM080918WMA.M
Title : VOC Analysis

35	5.763	1607	1609	1611	rBV	483	283	0.02%	0.003%
36	5.789	1611	1617	1618	rBV3	1289	1329	0.09%	0.012%
37	5.889	1632	1648	1674	rBV	350479	688004	44.55%	6.173%
38	6.188	1734	1741	1744	rBV5	1622	1912	0.12%	0.017%
39	6.333	1771	1786	1808	rVV	282666	564728	36.57%	5.067%
40	6.506	1836	1840	1842	rBV4	447	268	0.02%	0.002%
41	6.538	1842	1850	1859	rVV5	2409	4267	0.28%	0.038%
42	6.596	1865	1868	1870	rBV2	530	307	0.02%	0.003%
43	6.670	1885	1891	1893	rBV	313	284	0.02%	0.003%
44	6.706	1899	1902	1904	rBV3	429	289	0.02%	0.003%
45	6.821	1933	1938	1941	rBV3	441	455	0.03%	0.004%
46	6.860	1941	1950	1959	rVV5	1303	2352	0.15%	0.021%
47	6.956	1976	1980	1983	rBV	404	311	0.02%	0.003%
48	7.001	1991	1994	1997	rBV2	431	305	0.02%	0.003%
49	7.024	1997	2001	2005	rVV2	361	424	0.03%	0.004%
50	7.143	2033	2038	2039	rBV	333	291	0.02%	0.003%
51	7.152	2039	2041	2047	rVB2	447	271	0.02%	0.002%
52	7.230	2053	2065	2084	rBV	158503	281425	18.22%	2.525%
53	7.374	2104	2110	2112	rBV3	893	964	0.06%	0.009%
54	7.471	2131	2140	2146	rVB5	1517	2093	0.14%	0.019%
55	7.567	2153	2170	2184	rBV	558742	957954	62.03%	8.596%
56	7.641	2185	2193	2207	rVB	37662	66969	4.34%	0.601%
57	7.850	2246	2258	2279	rBV	115033	196190	12.70%	1.760%
58	8.185	2349	2362	2380	rBV	41881	102808	6.66%	0.922%
59	8.313	2391	2402	2433	rVB	354320	610647	39.54%	5.479%
60	8.468	2440	2450	2465	rVB2	35727	60045	3.89%	0.539%
61	8.673	2511	2514	2521	rBV2	207	264	0.02%	0.002%
62	9.017	2617	2621	2625	rBV2	380	312	0.02%	0.003%
63	9.091	2631	2644	2666	rBV	496833	832469	53.91%	7.470%
64	9.214	2680	2682	2687	rVB3	431	266	0.02%	0.002%
65	9.287	2694	2705	2708	rBV2	805	1009	0.07%	0.009%
66	9.381	2731	2734	2742	rBV3	732	980	0.06%	0.009%
67	9.490	2764	2768	2773	rVB3	294	320	0.02%	0.003%
68	9.580	2792	2796	2801	rVB2	405	389	0.03%	0.003%
69	9.609	2801	2805	2809	rVB3	791	696	0.05%	0.006%
70	9.760	2848	2852	2855	rBV3	418	455	0.03%	0.004%
71	9.779	2855	2858	2863	rVB4	487	483	0.03%	0.004%

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ALS Vial : 30 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : A4ZB4

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\SOMULM080918WMA.M
Title : VOC Analysis

72	9.821	2863	2871	2876	rBV3	1865	2463	0.16%	0.022%
73	9.927	2892	2904	2918	rBV3	7164	11798	0.76%	0.106%
74	10.033	2927	2937	2945	rBV5	2858	4795	0.31%	0.043%
75	10.313	3021	3024	3026	rBV2	601	376	0.02%	0.003%
76	10.435	3049	3062	3084	rVV	406616	644915	41.76%	5.787%
77	10.612	3106	3117	3132	rVV3	18621	33410	2.16%	0.300%
78	10.667	3132	3134	3139	rVB3	486	297	0.02%	0.003%
79	10.731	3151	3154	3162	rVB5	1289	1609	0.10%	0.014%
80	10.805	3172	3177	3181	rBV2	1005	969	0.06%	0.009%
81	10.927	3212	3215	3219	rVB	480	359	0.02%	0.003%
82	10.953	3219	3223	3226	rBV	562	510	0.03%	0.005%
83	11.059	3250	3256	3257	rBV2	409	323	0.02%	0.003%
84	11.069	3257	3259	3264	rVB2	391	286	0.02%	0.003%
85	11.143	3274	3282	3293	rVB7	3722	6673	0.43%	0.060%
86	11.258	3310	3318	3330	rVB4	2714	4114	0.27%	0.037%
87	11.336	3335	3342	3343	rBV3	830	828	0.05%	0.007%
88	11.374	3350	3354	3360	rVB6	1763	2065	0.13%	0.019%
89	11.419	3362	3368	3376	rVV4	6222	8613	0.56%	0.077%
90	11.487	3377	3389	3410	rVB2	465344	890987	57.70%	7.995%
91	11.686	3448	3451	3454	rBV2	463	285	0.02%	0.003%
92	11.750	3459	3471	3493	rBV2	155582	321517	20.82%	2.885%
93	11.866	3495	3507	3527	rVB2	674577	1544235	100.00%	13.856%
94	12.352	3656	3658	3660	rBV2	468	281	0.02%	0.003%
95	12.577	3721	3728	3729	rBV4	6661	7241	0.47%	0.065%
96	13.509	4009	4018	4029	rBV3	19084	28388	1.84%	0.255%
97	13.930	4147	4149	4155	rBV4	415	404	0.03%	0.004%
98	13.991	4162	4168	4178	rVB3	3623	5169	0.33%	0.046%
99	14.503	4323	4327	4328	rBV2	476	365	0.02%	0.003%
100	15.001	4479	4482	4486	rBV	757	535	0.03%	0.005%

Sum of corrected areas: 11144571

LSC Report - Integrated Chromatogram

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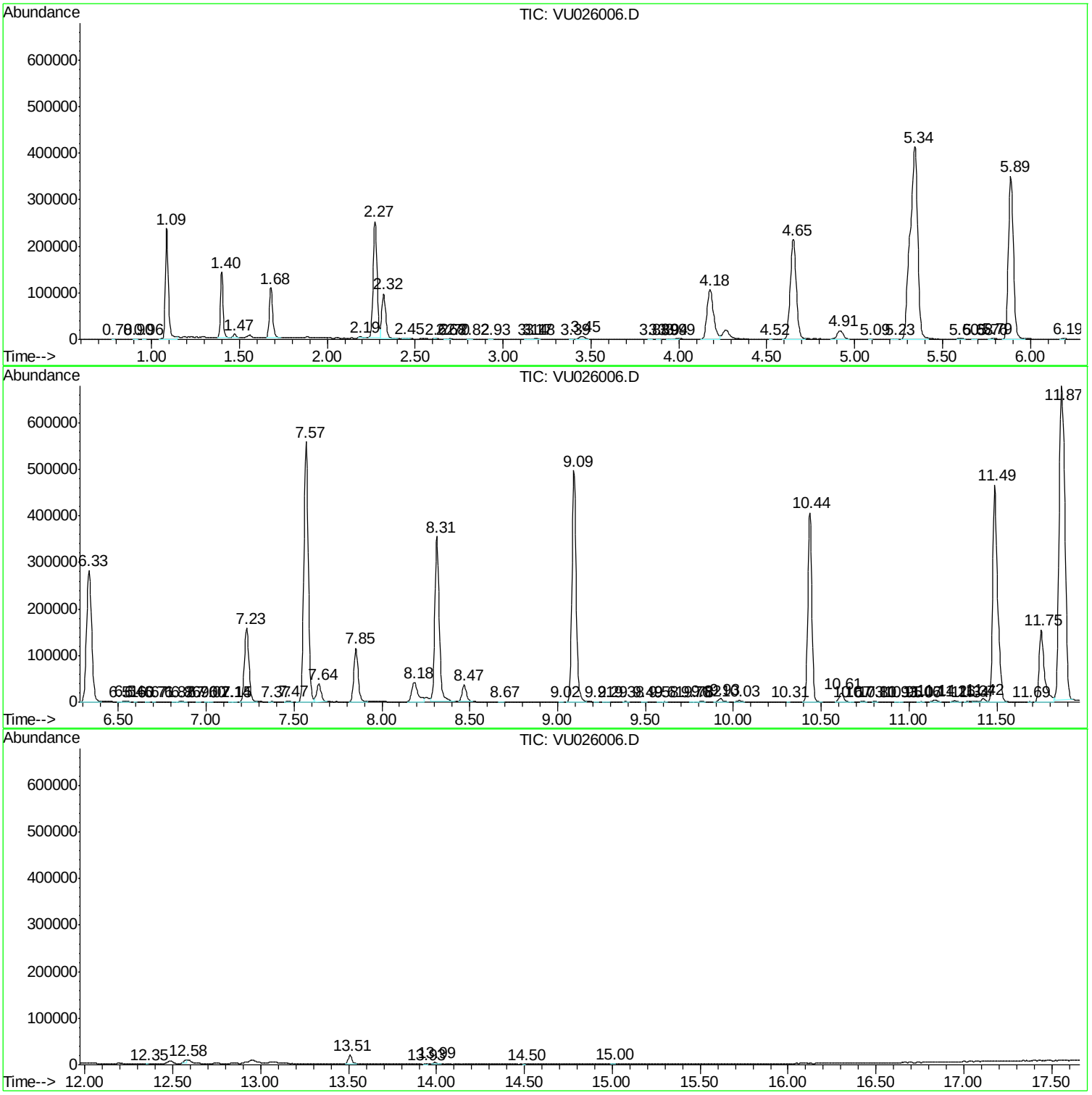
Sample : J4361-07
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 30 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : A4ZB4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM080918WMA.M
Quant Title : VOC Analysis

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU080918\
Data File : VU026006.D
Acq On : 09 Aug 2018 19:14
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Sample : J4361-07
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 30 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : A4ZB4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM080918WMA.M
Quant Title : VOC Analysis

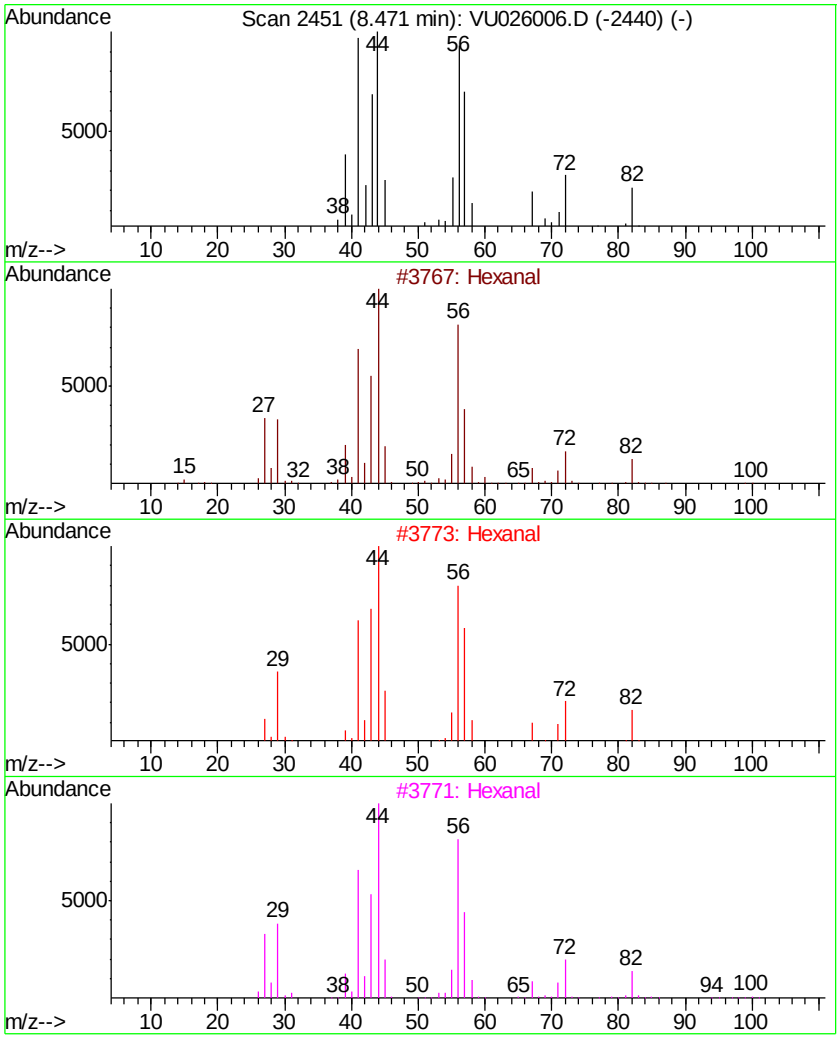
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

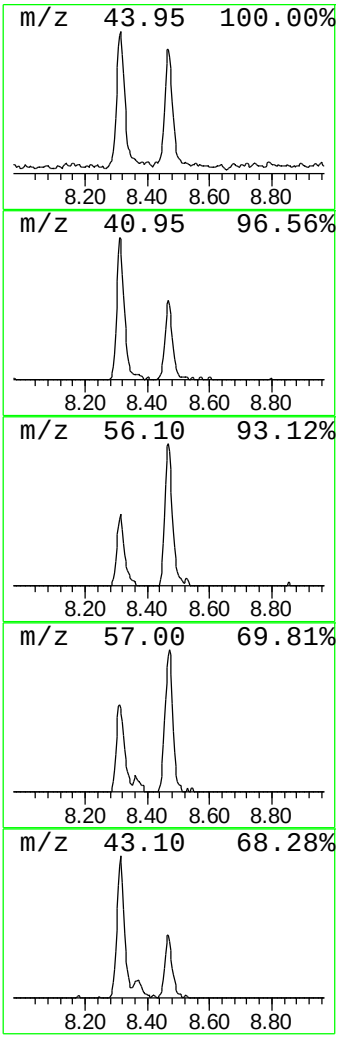
****

Peak Number 4 Hexanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.47	3.61 ug/L	60045	Chlorobenzene-d5	9.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal	100	C6H12O	000066-25-1	64
2	Hexanal	100	C6H12O	000066-25-1	64
3	Hexanal	100	C6H12O	000066-25-1	64
4	Hexanal	100	C6H12O	000066-25-1	59
5	2,2-Dimethyl-3-hydroxypropionald...	102	C5H10O2	000597-31-9	32





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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM080918WMA.M
Quant Title : VOC Analysis

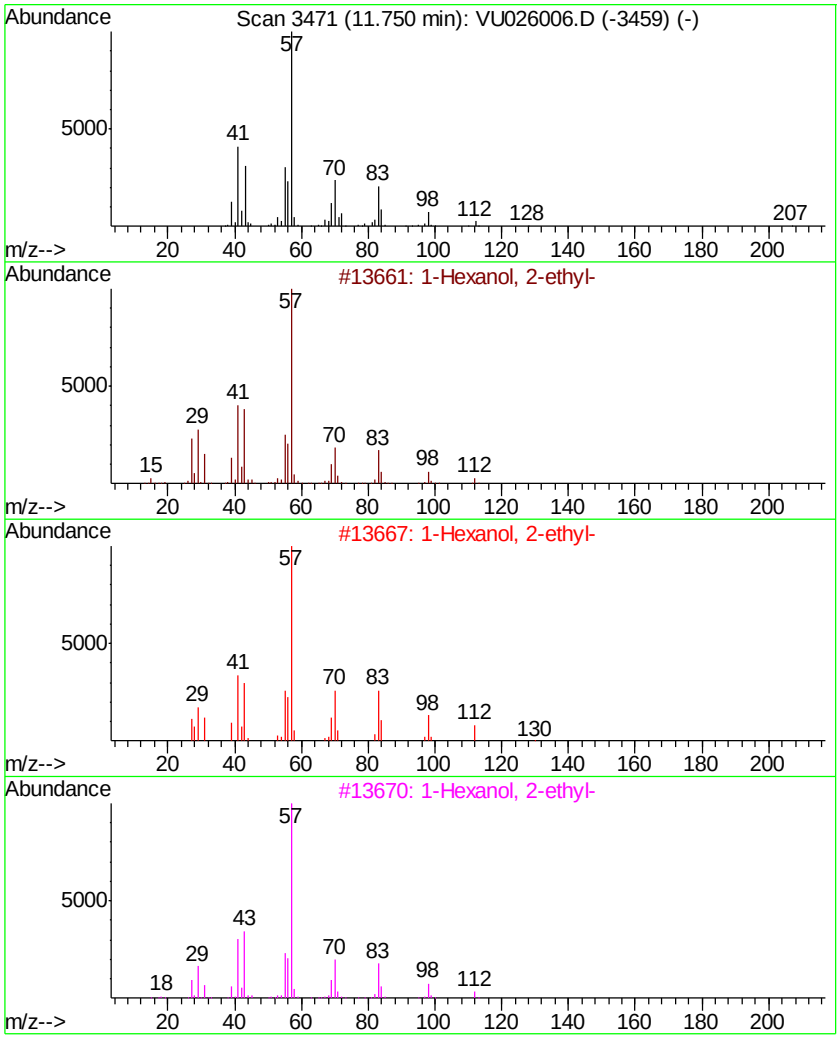
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

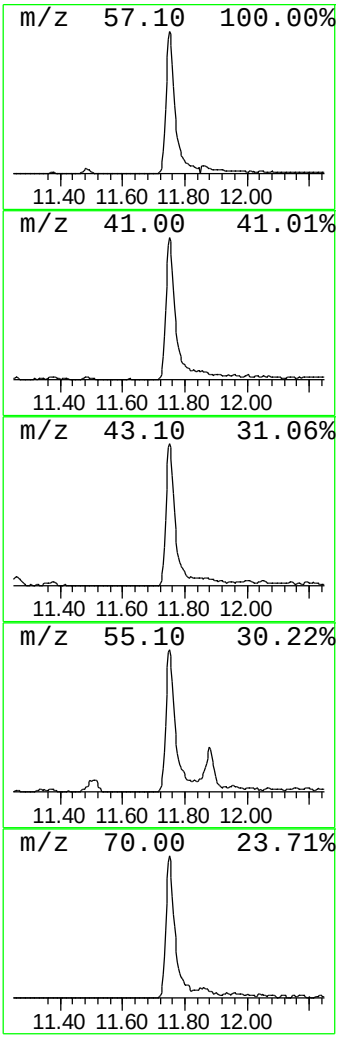
****

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.75	18.04 ug/L	321517	1,4-Dichlorobenzene-d4	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
3	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
4	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
5	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Hexanal	8.47	3.6	ug/L	60045	2	9.09	832469	50.0
1-Hexanol, 2-ethyl-	11.75	18.0	ug/L	321517	3	11.49	890987	50.0