LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051421\
Data File : VU043746.D
Acq On : 14 May 2021 11:18
Operator : SY/MD
Sample : M2350-01DL 20X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 59 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG6L4DL

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\SFAMULM051421WMA.M
Title : VOC Analysis

Signal : TIC: VU043746.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.604	74	82	99	rVB	245367	269042	14.82%	1.714%
2	1.912	169	178	194	rVB	170511	228522	12.59%	1.456%
3	2.571	370	383	402	rBV2	388644	654161	36.03%	4.168%
4	2.764	433	443	448	rBV6	1517	2289	0.13%	0.015%
5	2.948	495	500	501	rBV2	353	279	0.02%	0.002%
6	2.964	502	505	509	rVB2	427	345	0.02%	0.002%
7	3.050	523	532	545	rVB4	3989	7772	0.43%	0.050%
8	3.192	561	576	593	rVB2	13288	31947	1.76%	0.204%
9	3.256	593	596	602	rVB2	360	299	0.02%	0.002%
10	3.346	620	624	627	rBV2	405	374	0.02%	0.002%
11	3.366	627	630	637	rVB4	517	524	0.03%	0.003%
12	3.607	702	705	708	rBV2	282	220	0.01%	0.001%
13	3.880	769	790	810	rBV	103653	242738	13.37%	1.547%
14	4.005	816	829	841	rBV3	2800	6444	0.35%	0.041%
15	4.134	866	869	875	rVB2	213	200	0.01%	0.001%
16	4.185	882	885	889	rVB2	258	201	0.01%	0.001%
17	4.414	952	956	960	rBV2	219	254	0.01%	0.002%
18	4.504	982	984	986	rBV	319	158	0.01%	0.001%
19	4.626	1007	1022	1055	rBV	205368	500074	27.55%	3.186%
20	4.993	1133	1136	1138	rBV3	293	194	0.01%	0.001%
21	5.073	1143	1161	1184	rVV	316179	690982	38.06%	4.402%
22	5.221	1203	1207	1213	rVB4	574	703	0.04%	0.004%
23	5.324	1221	1239	1270	rBV	476513	1071143	59.00%	6.825%
24	5.468	1280	1284	1288	rVB3	312	291	0.02%	0.002%
25	5.491	1288	1291	1294	rVB2	297	203	0.01%	0.001%
26	5.526	1294	1302	1304	rBV	429	459	0.03%	0.003%
27	5.735	1342	1367	1397	rBV2	674666	1815352	100.00%	11.566%
28	6.047	1460	1464	1471	rVB4	813	1030	0.06%	0.007%
29	6.115	1482	1485	1493	rBV4	609	641	0.04%	0.004%
30	6.256	1513	1529	1547	rBV	565570	1065744	58.71%	6.790%
31	6.536	1607	1616	1626	rBV7	2903	5849	0.32%	0.037%
32	6.600	1630	1636	1638	rBV3	247	237	0.01%	0.002%
33	6.697	1648	1666	1687	rBV	418690	813922	44.84%	5.186%
34	6.803	1696	1699	1701	rBV2	686	474	0.03%	0.003%
35	6.851	1712	1714	1719	rBV3	280	180	0.01%	0.001%
36	6.922	1722	1736	1748	rVB	12321	23052	1.27%	0.147%

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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 59 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG6L4DL

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\SFAMULM051421WMA.M
Title : VOC Analysis

37	7.050	1773	1776	1783	rVB4	920	1007	0.06%	0.006%
38	7.169	1805	1813	1815	rBV3	450	435	0.02%	0.003%
39	7.185	1815	1818	1825	rVB4	711	765	0.04%	0.005%
40	7.343	1854	1867	1878	rBV4	5501	9717	0.54%	0.062%
41	7.523	1912	1923	1927	rBV4	10761	17502	0.96%	0.112%
42	7.571	1927	1938	1957	rVV	226558	392433	21.62%	2.500%
43	7.639	1957	1959	1962	rVB3	705	410	0.02%	0.003%
44	7.658	1962	1965	1968	rVB2	373	220	0.01%	0.001%
45	7.719	1971	1984	1996	rVB3	11135	20693	1.14%	0.132%
46	7.793	2004	2007	2012	rVB3	505	372	0.02%	0.002%
47	7.906	2027	2042	2056	rBV	826137	1413229	77.85%	9.004%
48	7.976	2058	2064	2077	rVB	13201	21499	1.18%	0.137%
49	8.185	2116	2129	2152	rBV	157958	263128	14.49%	1.676%
50	8.362	2182	2184	2191	rVB2	398	378	0.02%	0.002%
51	8.481	2218	2221	2224	rVB3	299	198	0.01%	0.001%
52	8.510	2227	2230	2233	rBV3	242	157	0.01%	0.001%
53	8.558	2241	2245	2257	rVB4	550	759	0.04%	0.005%
54	8.639	2257	2270	2305	rBV	559492	1011162	55.70%	6.442%
55	8.877	2342	2344	2348	rVB3	213	156	0.01%	0.001%
56	8.963	2369	2371	2376	rVB	220	161	0.01%	0.001%
57	9.002	2380	2383	2386	rVB2	328	186	0.01%	0.001%
58	9.025	2386	2390	2393	rBV2	420	310	0.02%	0.002%
59	9.137	2422	2425	2428	rBV2	202	175	0.01%	0.001%
60	9.185	2435	2440	2441	rBV2	249	166	0.01%	0.001%
61	9.324	2476	2483	2487	rBV3	488	654	0.04%	0.004%
62	9.423	2499	2514	2538	rBV	793516	1311607	72.25%	8.357%
63	9.571	2556	2560	2564	rBV3	582	472	0.03%	0.003%
64	9.703	2589	2601	2606	rBV5	1228	2344	0.13%	0.015%
65	9.754	2611	2617	2619	rVB3	187	161	0.01%	0.001%
66	9.867	2649	2652	2655	rBV	240	161	0.01%	0.001%
67	10.082	2715	2719	2722	rBV2	182	185	0.01%	0.001%
68	10.105	2722	2726	2731	rBV4	488	565	0.03%	0.004%
69	10.192	2746	2753	2757	rVB2	274	258	0.01%	0.002%
70	10.275	2759	2779	2799	rBV2	69143	150291	8.28%	0.958%
71	10.442	2828	2831	2837	rVB2	282	217	0.01%	0.001%
72	10.555	2857	2866	2885	rBV5	2282	5429	0.30%	0.035%
73	10.677	2893	2904	2912	rVB4	5466	8907	0.49%	0.057%
74	10.761	2916	2930	2949	rBV	590435	941919	51.89%	6.001%
75	10.886	2961	2969	2980	rVV8	2388	4556	0.25%	0.029%
76	10.963	2991	2993	2997	rBV2	284	191	0.01%	0.001%

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Sample : M2350-01DL 20X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 59 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG6L4DL

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\SFAMULM051421WMA.M
Title : VOC Analysis

77	11.037	3004	3016	3033	rVB2	118256	201051	11.08%	1.281%
78	11.124	3035	3043	3049	rVB6	1978	2663	0.15%	0.017%
79	11.195	3063	3065	3068	rBV2	473	328	0.02%	0.002%
80	11.272	3086	3089	3091	rBV2	310	189	0.01%	0.001%
81	11.295	3091	3096	3097	rBV	514	383	0.02%	0.002%
82	11.465	3138	3149	3159	rVB5	3483	6186	0.34%	0.039%
83	11.587	3177	3187	3192	rBV3	820	1218	0.07%	0.008%
84	11.700	3214	3222	3230	rVB3	1859	2973	0.16%	0.019%
85	11.751	3235	3238	3245	rVB4	563	499	0.03%	0.003%
86	11.819	3245	3259	3282	rBV	753849	1199942	66.10%	7.645%
87	11.922	3287	3291	3293	rBV3	634	567	0.03%	0.004%
88	11.979	3305	3309	3316	rVB3	3274	3668	0.20%	0.023%
89	12.102	3339	3347	3356	rVB6	5593	7515	0.41%	0.048%
90	12.198	3357	3377	3396	rBV	769268	1240691	68.34%	7.905%
91	12.336	3416	3420	3428	rVB6	1660	2127	0.12%	0.014%
92	12.397	3432	3439	3440	rBV3	686	613	0.03%	0.004%
93	12.520	3471	3477	3482	rBV3	260	425	0.02%	0.003%
94	12.600	3498	3502	3506	rVB2	479	347	0.02%	0.002%
95	12.642	3511	3515	3523	rVB5	934	947	0.05%	0.006%
96	12.786	3557	3560	3564	rBV3	386	283	0.02%	0.002%
97	13.147	3668	3672	3675	rBV3	598	479	0.03%	0.003%
98	13.372	3739	3742	3744	rBV2	296	206	0.01%	0.001%
99	13.854	3886	3892	3896	rBV2	636	842	0.05%	0.005%
100	14.089	3960	3965	3975	rBV3	1032	1937	0.11%	0.012%

Sum of corrected areas: 15695513

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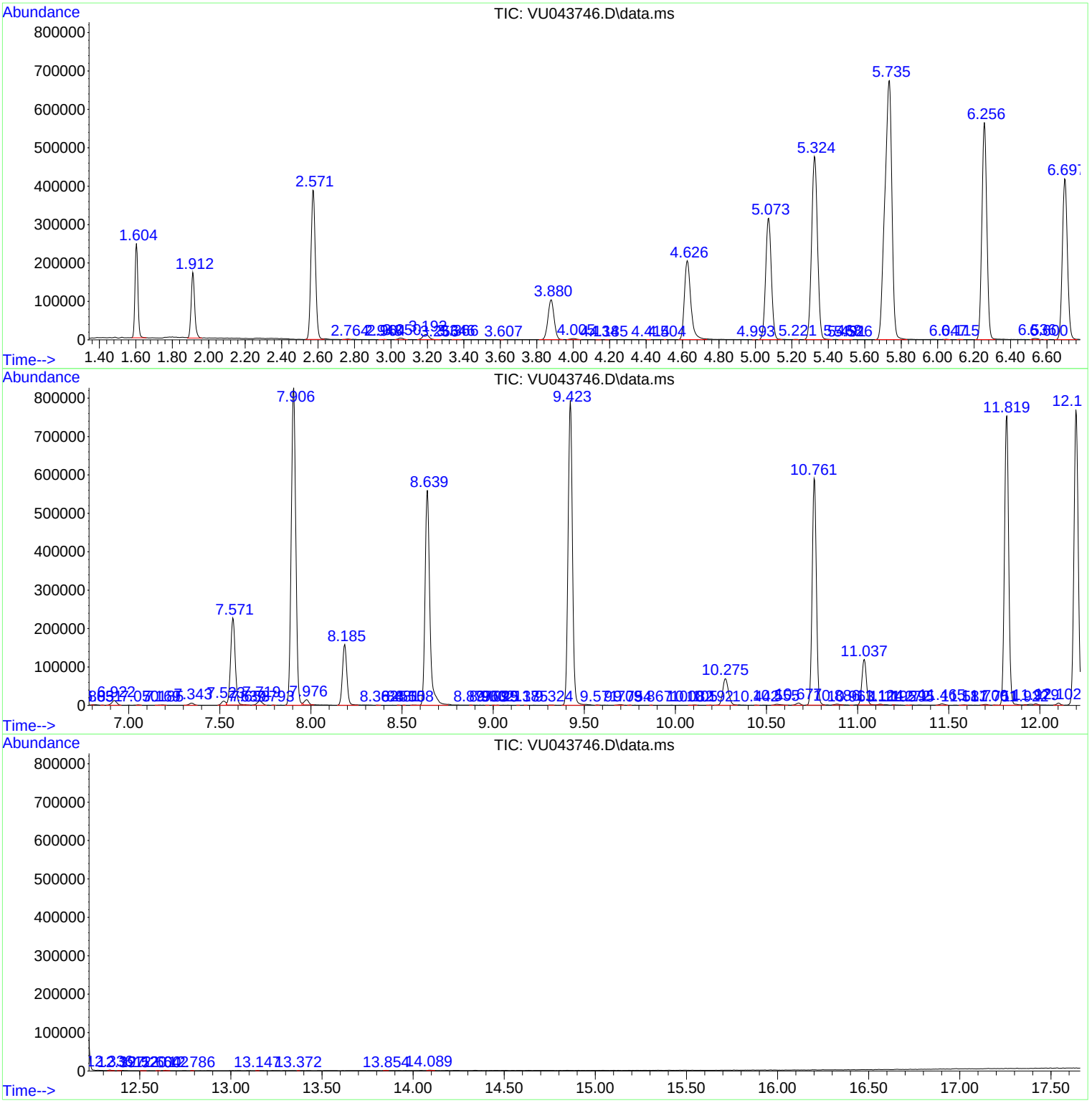
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 59 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BG6L4DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051421WMA.M
Quant Title : VOC Analysis

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



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ClientSampleId : BG6L4DL

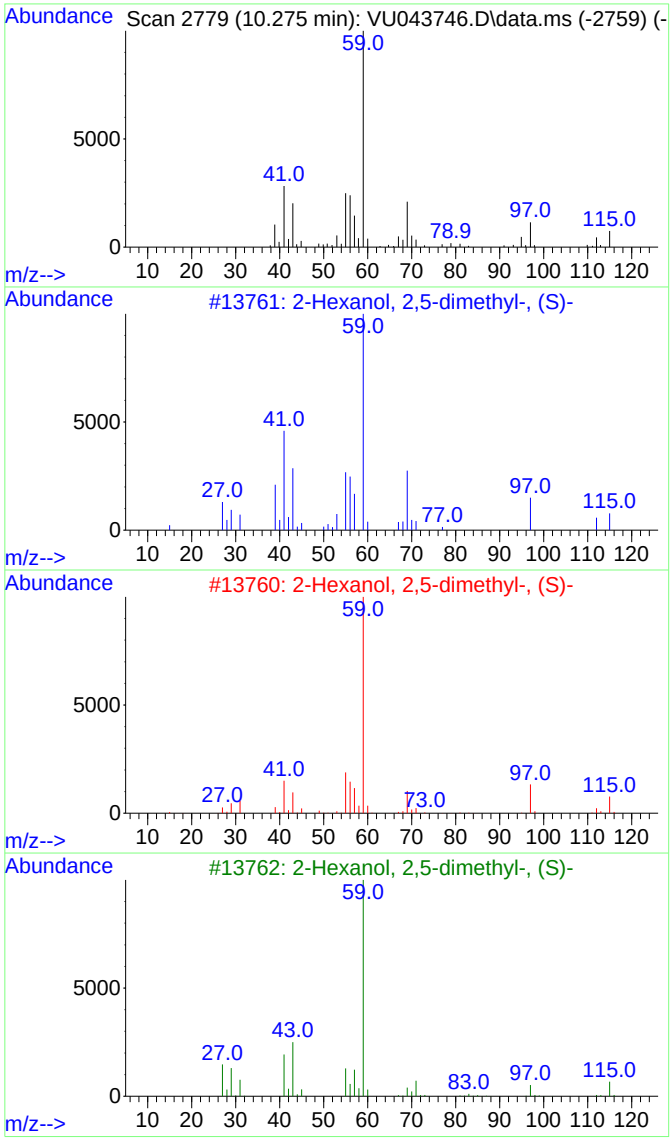
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051421WMA.M
Quant Title : VOC Analysis

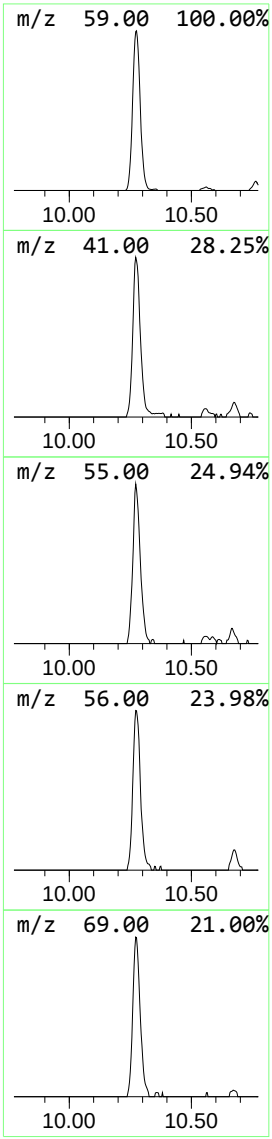
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Hexanol, 2,5-dimethyl-, (S)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.275	5.73 ug/L	150291	Chlorobenzene-d5	9.423

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	86
2	2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	72
3	2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	50
4	Oxetane, 2,2,4-trimethyl-	100	C6H12O	023120-44-7	50
5	Butanamide, 3,3-dimethyl-	115	C6H13NO	000926-04-5	47





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Misc : 5.0mL/MSVOA_U/WATER
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Instrument : MSVOA_U
ClientSampleId : BG6L4DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051421WMA.M
Quant Title : VOC Analysis

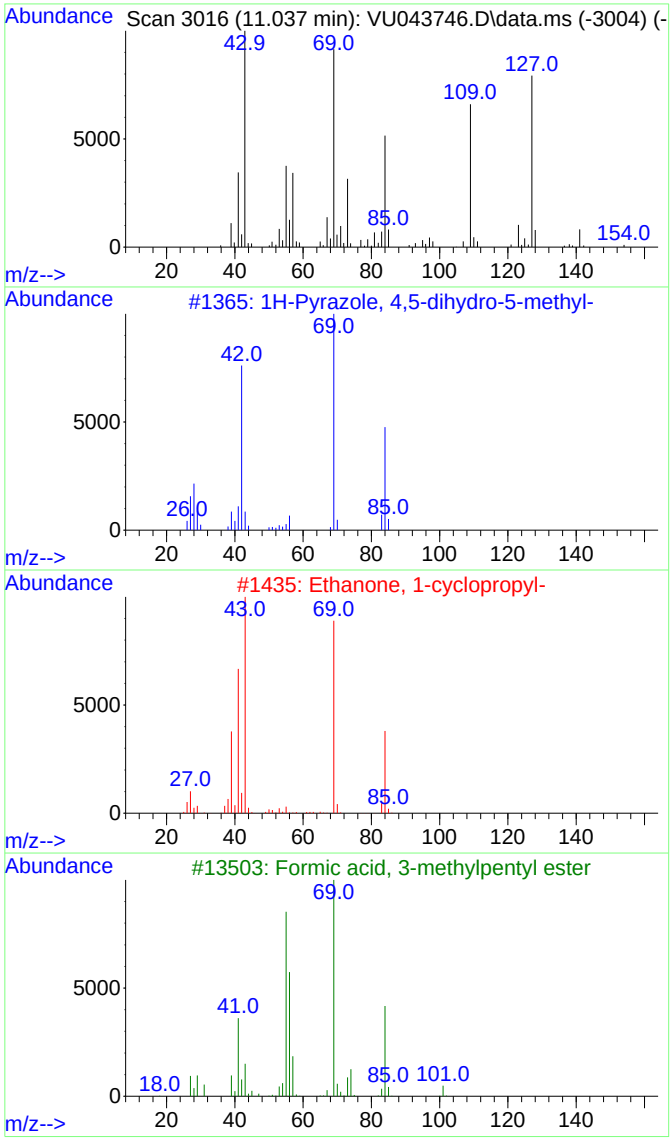
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

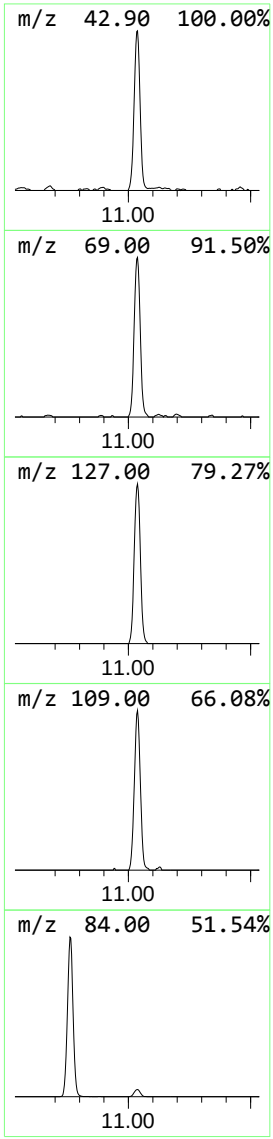
****

Peak Number 3 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.037	8.38 ug/L	201051	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Pyrazole, 4,5-dihydro-5-methyl-	84	C4H8N2	001568-20-3	30
2	Ethanone, 1-cyclopropyl-	84	C5H8O	000765-43-5	27
3	Formic acid, 3-methylpentyl ester	130	C7H14O2	1000368-21-3	27
4	Cyclopropane, (1,2-dimethylpropyl)-	112	C8H16	006976-27-8	27
5	Pentane, 2-chloro-4-methyl-	120	C6H13Cl	025346-32-1	27





Tentatively Identified Compound (LSC) summary

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Quant Title : VOC Analysis

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TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Hexanol, 2,5-...	10.275	5.7	ug/L	150291	2	9.423	1311610	50.0
unknown-01	11.037	8.4	ug/L	201051	3	11.819	1199940	50.0