LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU072318\
Data File : VU025601.D
Acq On : 23 Jul 2018 14:48
Operator : MD/SY
Sample : PB111343ZHE#07
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : PB111343ZHE#07

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\SOMULM072018WMA.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	0.799	60	65	69	rVB2	239	252	0.02%	0.003%
2	0.822	69	72	76	rBV2	372	373	0.04%	0.004%
3	0.924	99	104	108	rBV2	318	297	0.03%	0.003%
4	0.995	121	126	131	rVB2	258	349	0.03%	0.004%
5	1.088	138	155	168	rBV	167838	189998	18.20%	1.950%
6	1.400	244	252	263	rBV	104270	112494	10.77%	1.155%
7	1.683	332	340	351	rVB	89853	111240	10.65%	1.142%
8	2.275	514	524	533	rBV	201485	301815	28.90%	3.098%
9	2.442	570	576	586	rBV2	3833	6337	0.61%	0.065%
10	2.539	603	606	607	rBV	568	321	0.03%	0.003%
11	2.571	614	616	620	rBV2	421	285	0.03%	0.003%
12	2.622	623	632	643	rVB3	3841	7239	0.69%	0.074%
13	2.706	648	658	673	rVV3	9412	17005	1.63%	0.175%
14	2.764	674	676	681	rVB3	470	309	0.03%	0.003%
15	2.815	688	692	693	rBV2	406	235	0.02%	0.002%
16	2.831	693	697	698	rBV3	1020	577	0.06%	0.006%
17	2.957	732	736	739	rVB	466	282	0.03%	0.003%
18	3.182	804	806	812	rVV3	366	326	0.03%	0.003%
19	3.294	838	841	845	rVB3	619	348	0.03%	0.004%
20	3.320	845	849	851	rBV3	255	235	0.02%	0.002%
21	3.404	869	875	888	rVV6	1130	2638	0.25%	0.027%
22	3.519	908	911	914	rBV	373	279	0.03%	0.003%
23	3.535	914	916	921	rVV2	307	268	0.03%	0.003%
24	3.741	977	980	982	rBV	482	256	0.02%	0.003%
25	3.850	1009	1014	1021	rBV3	265	373	0.04%	0.004%
26	4.108	1090	1094	1100	rBV2	473	578	0.06%	0.006%
27	4.178	1100	1116	1134	rBV	100000	256165	24.53%	2.630%
28	4.458	1201	1203	1207	rBV3	512	319	0.03%	0.003%
29	4.500	1211	1216	1220	rBV4	490	466	0.04%	0.005%
30	4.651	1245	1263	1288	rBV	193230	461542	44.20%	4.738%
31	4.744	1288	1292	1295	rBV4	428	400	0.04%	0.004%
32	4.844	1321	1323	1328	rVB2	579	377	0.04%	0.004%
33	4.886	1328	1336	1339	rBV5	1153	1338	0.13%	0.014%
34	4.934	1347	1351	1353	rBV	343	286	0.03%	0.003%

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ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : PB111343ZHE#07

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\SOMULM072018WMA.M
Title : VOC Analysis

35	4.976	1358	1364	1368	rBV4	776	1021	0.10%	0.010%
36	5.346	1453	1479	1504	rBV2	350548	1044164	100.00%	10.718%
37	5.471	1515	1518	1520	rBV2	527	381	0.04%	0.004%
38	5.551	1529	1543	1564	rBV2	97861	201669	19.31%	2.070%
39	5.667	1576	1579	1582	rVV2	382	223	0.02%	0.002%
40	5.738	1599	1601	1605	rVB3	366	238	0.02%	0.002%
41	5.892	1625	1649	1664	rBV	398817	843965	80.83%	8.663%
42	6.336	1772	1787	1808	rBV	243270	487662	46.70%	5.006%
43	6.532	1843	1848	1855	rBV3	2406	3729	0.36%	0.038%
44	6.709	1890	1903	1924	rBV	148979	262763	25.16%	2.697%
45	7.230	2052	2065	2085	rBV	146353	257065	24.62%	2.639%
46	7.426	2116	2126	2133	rBV2	6428	10405	1.00%	0.107%
47	7.567	2154	2170	2200	rBV	493998	864305	82.77%	8.872%
48	7.741	2218	2224	2226	rBV5	1286	1428	0.14%	0.015%
49	7.853	2247	2259	2275	rBV	105449	177989	17.05%	1.827%
50	8.075	2326	2328	2332	rBV3	523	361	0.03%	0.004%
51	8.117	2339	2341	2344	rVB4	542	331	0.03%	0.003%
52	8.188	2346	2363	2371	rBV4	11143	31234	2.99%	0.321%
53	8.313	2392	2402	2423	rVB	337111	566142	54.22%	5.812%
54	8.419	2426	2435	2450	rVB	74149	117154	11.22%	1.203%
55	8.525	2460	2468	2482	rVB	22822	37846	3.62%	0.388%
56	8.609	2492	2494	2496	rBV2	420	267	0.03%	0.003%
57	8.812	2553	2557	2558	rBV3	429	284	0.03%	0.003%
58	8.908	2576	2587	2602	rBV	83809	131410	12.59%	1.349%
59	8.998	2612	2615	2619	rVB4	803	533	0.05%	0.005%
60	9.091	2627	2644	2661	rBV	533657	890948	85.33%	9.146%
61	9.255	2693	2695	2700	rVB2	656	507	0.05%	0.005%
62	9.281	2700	2703	2707	rVB3	308	226	0.02%	0.002%
63	9.304	2708	2710	2714	rVB2	536	360	0.03%	0.004%
64	9.374	2730	2732	2735	rBV2	574	364	0.03%	0.004%
65	9.554	2786	2788	2791	rVB2	607	366	0.04%	0.004%
66	9.683	2825	2828	2830	rBV	434	264	0.03%	0.003%
67	9.770	2846	2855	2860	rBV5	2276	3621	0.35%	0.037%
68	9.857	2878	2882	2883	rBV2	421	307	0.03%	0.003%
69	9.988	2919	2923	2929	rBV4	577	577	0.06%	0.006%
70	10.075	2946	2950	2953	rBV3	395	406	0.04%	0.004%
71	10.095	2953	2956	2962	rVB2	729	577	0.06%	0.006%

LSC Area Percent Report

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Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0 % of largest Peak
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Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM072018WMA.M
Title : VOC Analysis

72	10.165	2974	2978	2982	rBV2	325	339	0.03%	0.003%
73	10.185	2982	2984	2987	rVB	441	229	0.02%	0.002%
74	10.233	2987	2999	3016	rBV7	3479	6682	0.64%	0.069%
75	10.294	3016	3018	3021	rVB2	465	239	0.02%	0.002%
76	10.435	3049	3062	3080	rVV	353553	557942	53.43%	5.727%
77	10.516	3086	3087	3093	rVB2	622	345	0.03%	0.004%
78	10.619	3110	3119	3128	rVB5	3689	6589	0.63%	0.068%
79	10.670	3132	3135	3138	rBV2	376	234	0.02%	0.002%
80	10.686	3138	3140	3145	rVB2	334	270	0.03%	0.003%
81	10.712	3145	3148	3152	rVB3	456	296	0.03%	0.003%
82	10.744	3152	3158	3160	rBV3	472	465	0.04%	0.005%
83	10.776	3160	3168	3176	rBV5	2599	4137	0.40%	0.042%
84	10.882	3195	3201	3204	rBV4	433	472	0.05%	0.005%
85	10.911	3207	3210	3214	rVB2	506	319	0.03%	0.003%
86	11.059	3252	3256	3258	rBV	310	252	0.02%	0.003%
87	11.152	3283	3285	3289	rBV2	392	269	0.03%	0.003%
88	11.487	3377	3389	3410	rBV	565895	892332	85.46%	9.160%
89	11.744	3464	3469	3472	rBV3	484	555	0.05%	0.006%
90	11.773	3476	3478	3483	rVB3	436	349	0.03%	0.004%
91	11.863	3493	3506	3525	rBV	530678	847648	81.18%	8.701%
92	12.230	3614	3620	3624	rBV3	504	660	0.06%	0.007%
93	12.574	3723	3727	3730	rBV2	609	638	0.06%	0.007%
94	12.625	3740	3743	3744	rBV2	528	266	0.03%	0.003%
95	12.773	3784	3789	3792	rBV3	480	462	0.04%	0.005%
96	12.889	3822	3825	3829	rBV3	369	361	0.03%	0.004%
97	13.059	3875	3878	3881	rBV2	461	375	0.04%	0.004%
98	13.162	3907	3910	3912	rBV	341	222	0.02%	0.002%
99	14.522	4327	4333	4336	rBV3	761	1040	0.10%	0.011%
100	14.602	4352	4358	4362	rBV3	796	1067	0.10%	0.011%

Sum of corrected areas: 9741748

LSC Report - Integrated Chromatogram

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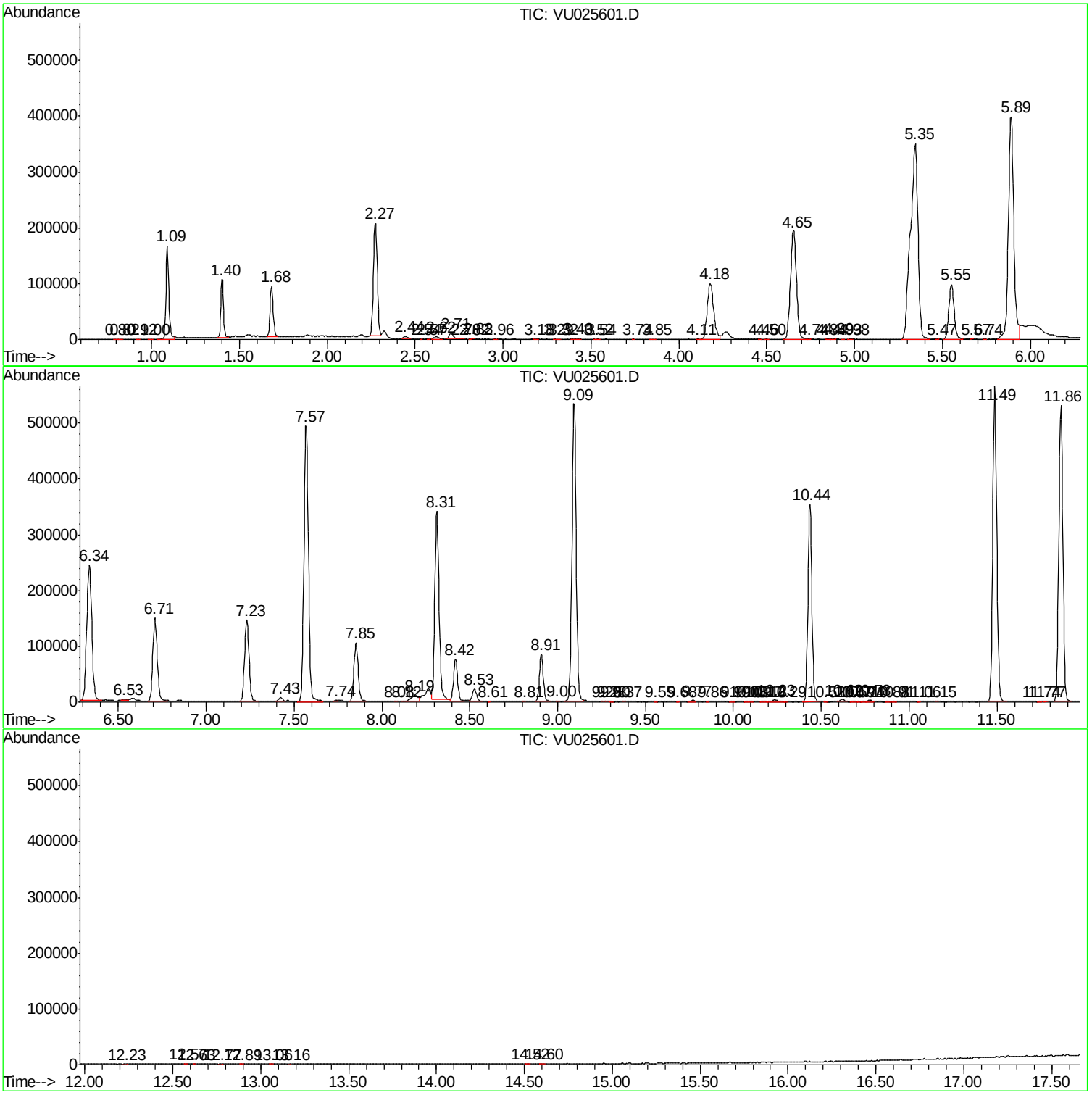
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : PB111343ZHE#07

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM072018WMA.M
Quant Title : VOC Analysis

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



Library Search Compound Report

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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM072018WMA.M
Quant Title : VOC Analysis

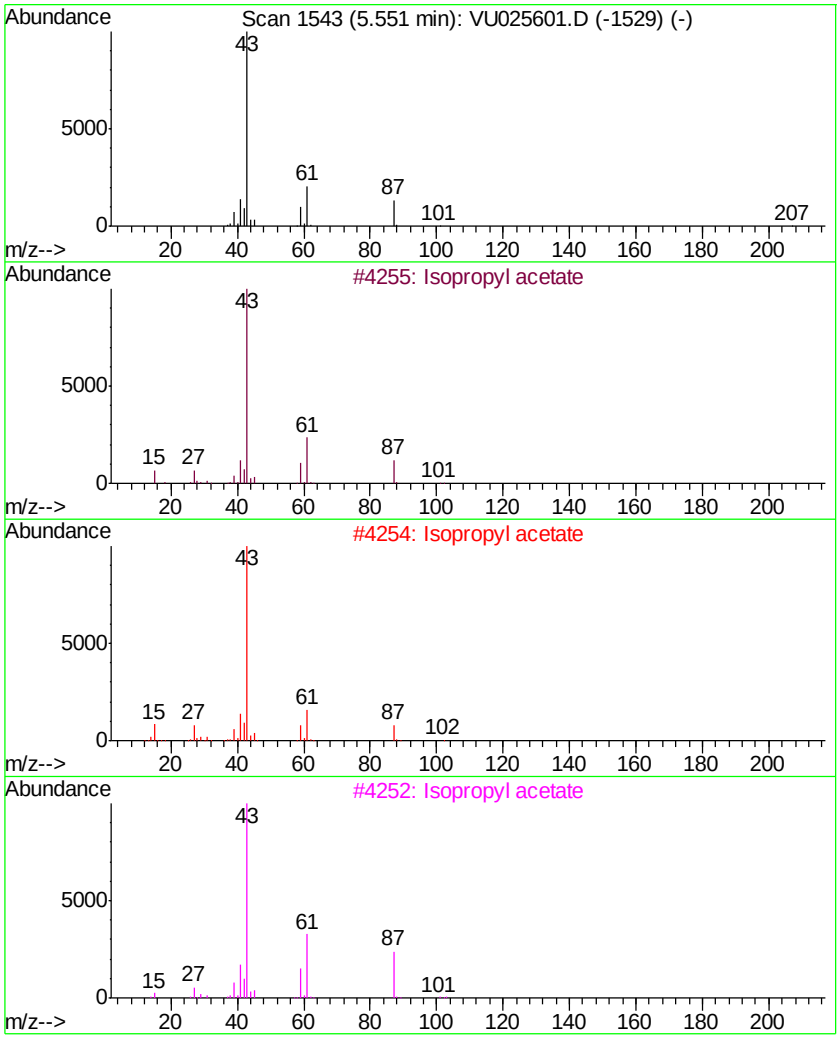
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

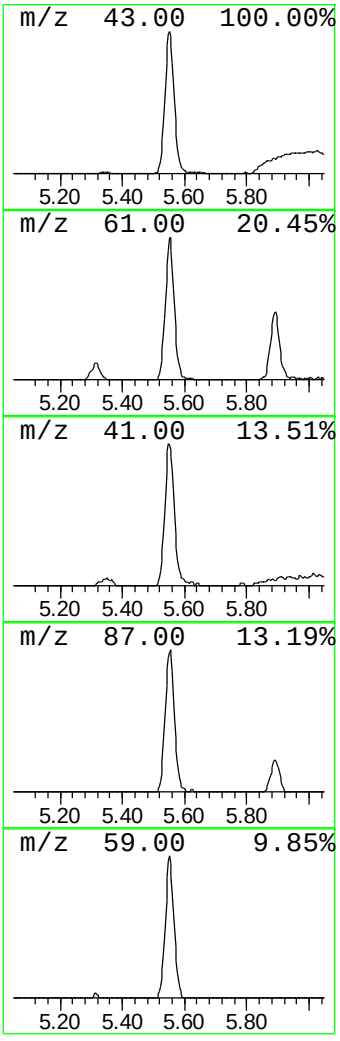
****

Peak Number 2 Isopropyl acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.55	11.95 ug/L	201669	1,4-Difluorobenzene	5.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl acetate	102	C5H10O2	000108-21-4	83
2	Isopropyl acetate	102	C5H10O2	000108-21-4	72
3	Isopropyl acetate	102	C5H10O2	000108-21-4	64
4	Acetaldehyde, O-ethyloxime-	87	C4H9NO	1000288-34-6	16
5	sec-Butyl acetate	116	C6H12O2	000105-46-4	9





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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM072018WMA.M
Quant Title : VOC Analysis

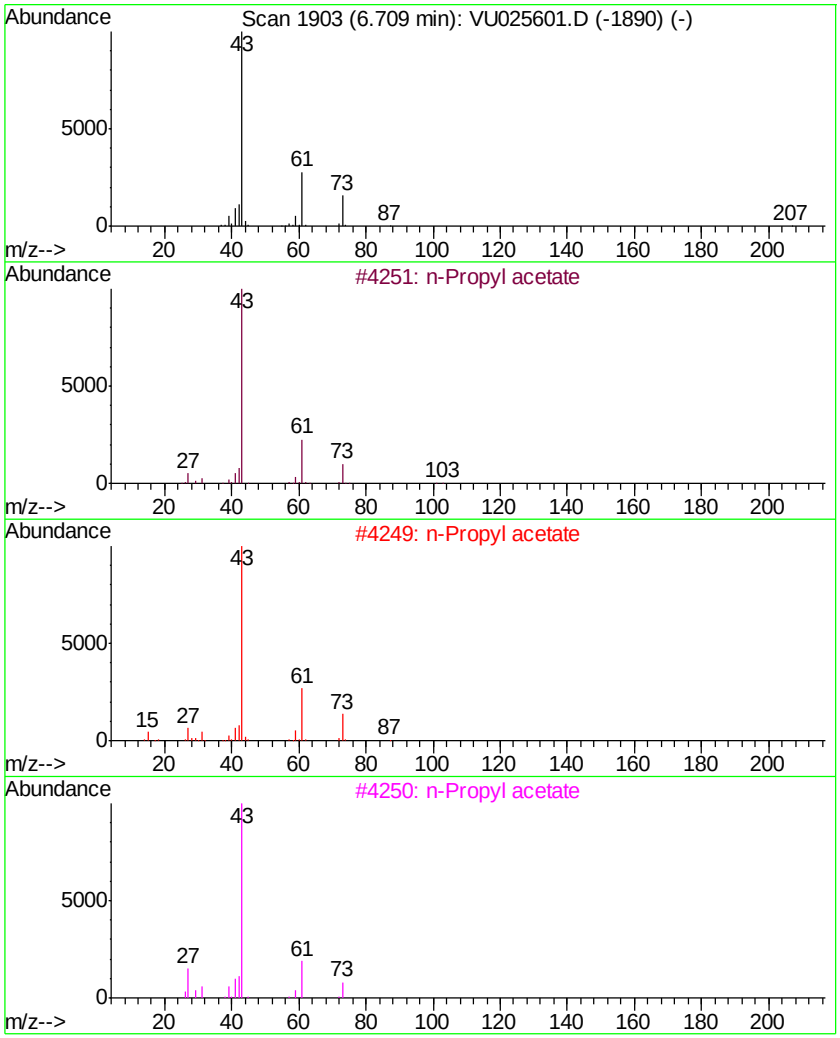
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

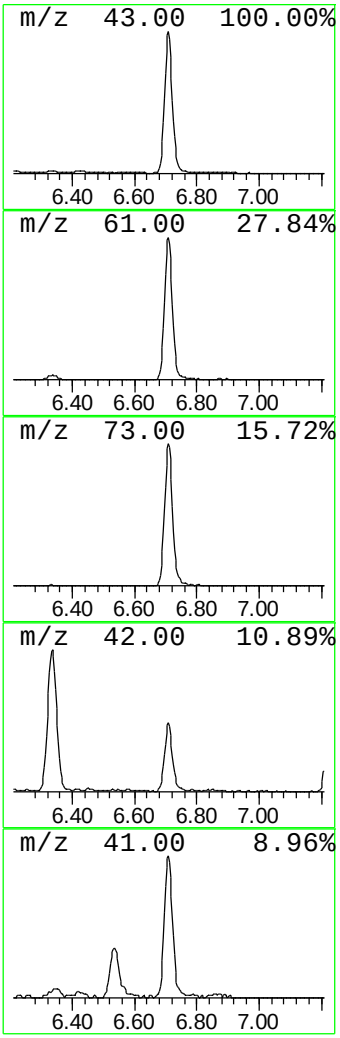
****

Peak Number 3 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.71	15.57 ug/L	262763	1,4-Difluorobenzene	5.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2	n-Propyl acetate	102	C5H10O2	000109-60-4	78
3	n-Propyl acetate	102	C5H10O2	000109-60-4	64
4	Isopropyl acetate	102	C5H10O2	000108-21-4	36
5	Isobutylamine	73	C4H11N	000078-81-9	9





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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM072018WMA.M
Quant Title : VOC Analysis

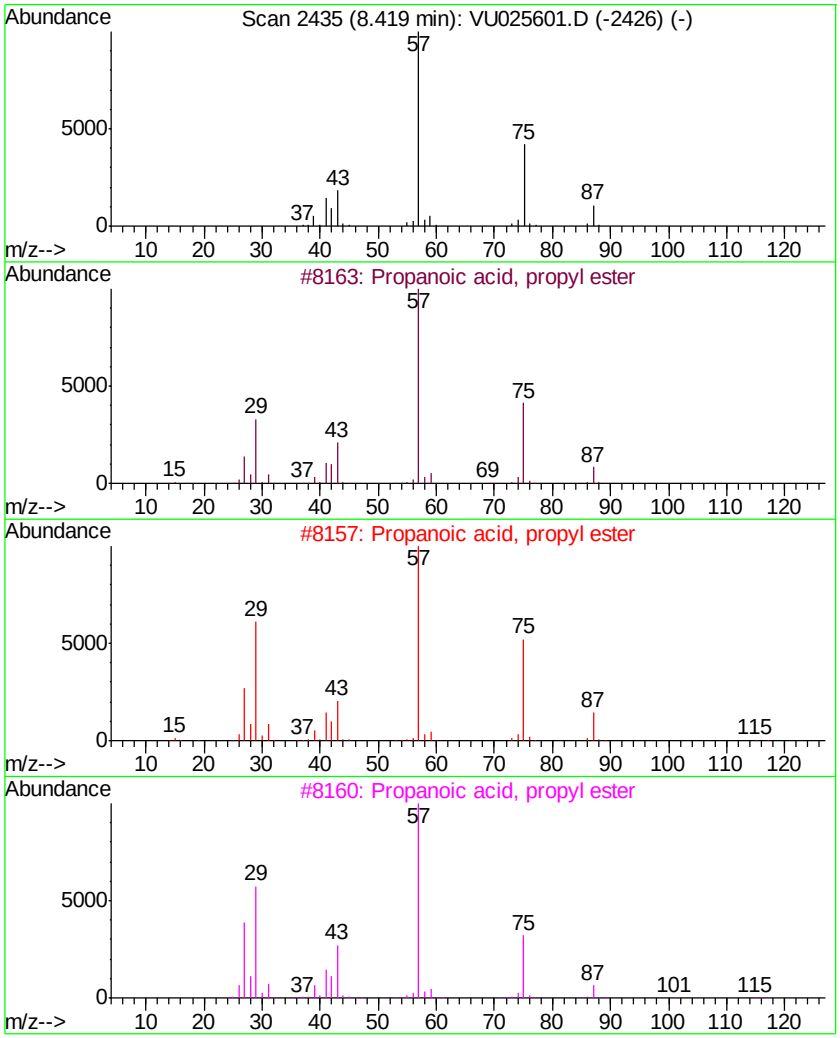
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

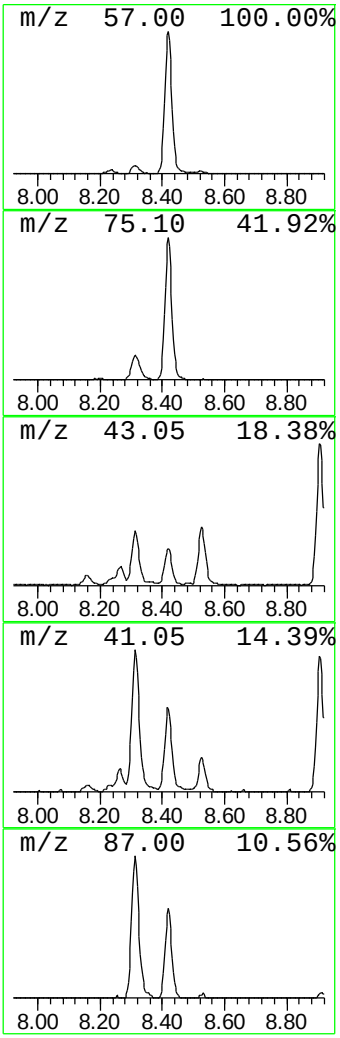
****

Peak Number 5 Propanoic acid, propyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.42	6.57 ug/L	117154	Chlorobenzene-d5	9.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
2	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
3	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
4	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	78
5	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	38





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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM072018WMA.M
Quant Title : VOC Analysis

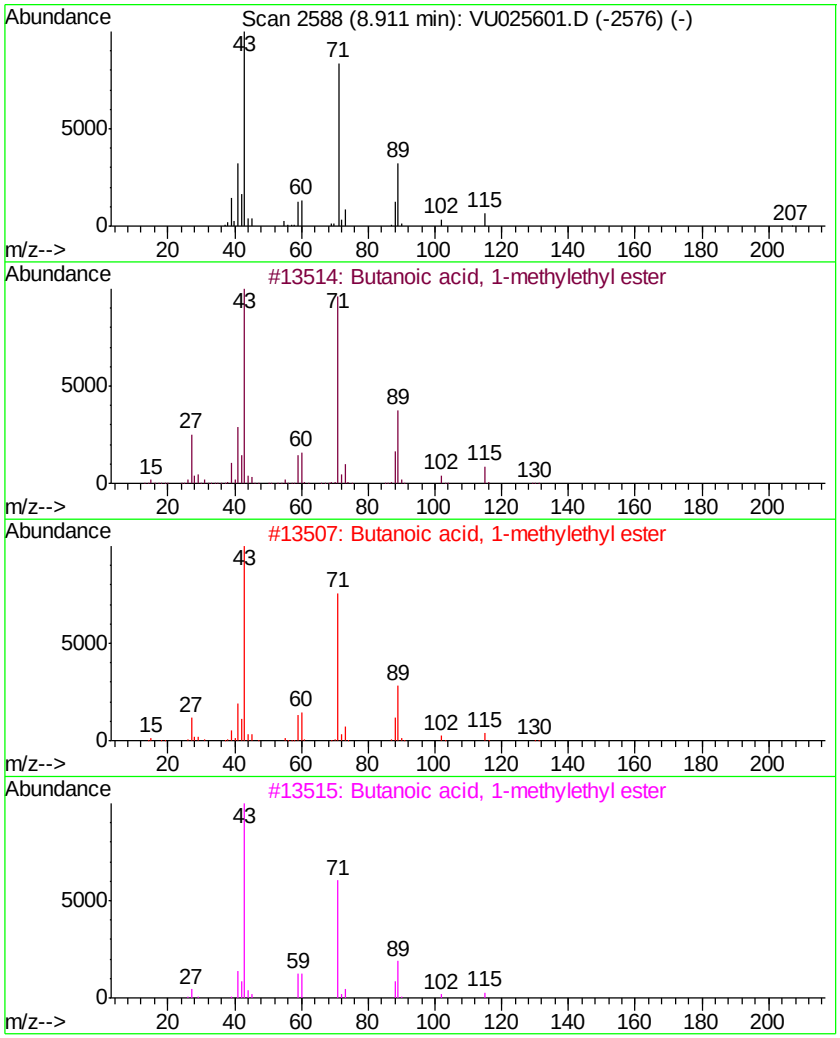
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

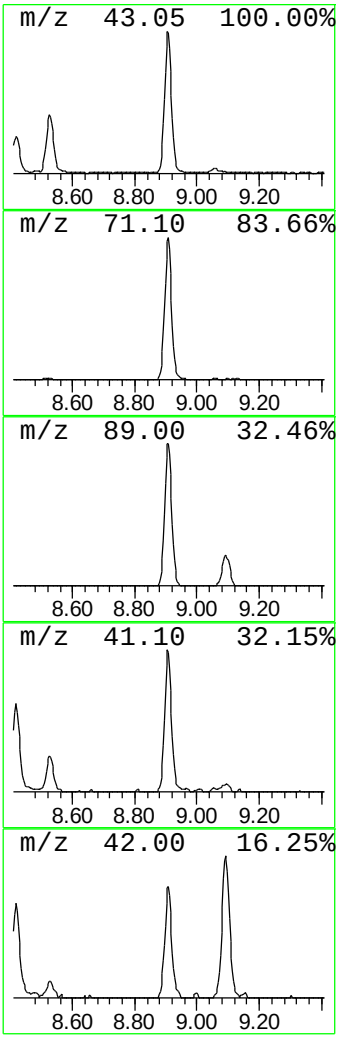
****

Peak Number 6 Butanoic acid, 1-methylethy... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.91	7.37 ug/L	131410	Chlorobenzene-d5	9.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	91
2	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	90
3	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	83
4	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
5	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64





Tentatively Identified Compound (LSC) summary

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ClientSampleId : PB111343ZHE#07

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM072018WMA.M
Quant Title : VOC Analysis

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Isopropyl acetate	5.55	11.9	ug/L	201669	1	5.89	843965	50.0
n-Propyl acetate	6.71	15.6	ug/L	262763	1	5.89	843965	50.0
Propanoic acid, p...	8.42	6.6	ug/L	117154	2	9.09	890948	50.0
Butanoic acid, 1-...	8.91	7.4	ug/L	131410	2	9.09	890948	50.0