LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU072318\
Data File : VU025599.D
Acq On : 23 Jul 2018 14:01
Operator : MD/SY
Sample : VLEB#03
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : VLEB#03

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	0.613	3	7	10	rVB3	239	224	0.02%	0.002%
2	0.992	121	125	129	rVB2	218	216	0.02%	0.002%
3	1.024	129	135	136	rBV2	296	249	0.02%	0.003%
4	1.092	142	156	168	rBV	173369	198404	18.66%	1.992%
5	1.403	246	253	265	rBV	109359	112058	10.54%	1.125%
6	1.683	332	340	358	rVB	93682	119050	11.19%	1.195%
7	2.275	514	524	534	rBV	202455	302181	28.42%	3.034%
8	2.442	570	576	587	rBV3	3615	5397	0.51%	0.054%
9	2.619	624	631	640	rVB	3869	5385	0.51%	0.054%
10	2.709	648	659	669	rVB2	9034	16237	1.53%	0.163%
11	2.786	679	683	685	rVB	408	247	0.02%	0.002%
12	2.805	685	689	691	rBV2	511	339	0.03%	0.003%
13	2.821	691	694	695	rBV	561	256	0.02%	0.003%
14	2.844	696	701	703	rBV4	605	575	0.05%	0.006%
15	2.889	713	715	718	rBV2	365	223	0.02%	0.002%
16	2.960	732	737	741	rVB3	762	677	0.06%	0.007%
17	3.011	748	753	756	rBV2	313	287	0.03%	0.003%
18	3.075	770	773	776	rBV	318	256	0.02%	0.003%
19	3.172	800	803	805	rBV2	376	228	0.02%	0.002%
20	3.394	868	872	873	rBV	740	499	0.05%	0.005%
21	3.403	873	875	877	rBV3	736	422	0.04%	0.004%
22	3.464	891	894	897	rBV3	335	232	0.02%	0.002%
23	3.558	919	923	926	rBV2	626	445	0.04%	0.004%
24	3.847	1008	1013	1016	rBV3	318	382	0.04%	0.004%
25	3.911	1029	1033	1038	rBV2	410	386	0.04%	0.004%
26	3.937	1038	1041	1046	rBV3	262	283	0.03%	0.003%
27	4.095	1086	1090	1092	rVB3	271	213	0.02%	0.002%
28	4.178	1100	1116	1134	rBV	99172	258026	24.26%	2.591%
29	4.371	1173	1176	1180	rBV3	497	484	0.05%	0.005%
30	4.419	1187	1191	1192	rBV3	386	279	0.03%	0.003%
31	4.580	1238	1241	1244	rVV2	423	314	0.03%	0.003%
32	4.654	1245	1264	1288	rVV	197692	471976	44.38%	4.739%
33	4.812	1307	1313	1317	rBV4	387	412	0.04%	0.004%
34	4.889	1328	1337	1351	rVB4	1178	3062	0.29%	0.031%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU072318\
Data File : VU025599.D
Acq On : 23 Jul 2018 14:01
Operator : MD/SY
Sample : VLEB#03
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : VLEB#03

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

35	4.989	1362	1368	1371	rBV4	717	939	0.09%	0.009%
36	5.124	1407	1410	1413	rBV	358	207	0.02%	0.002%
37	5.220	1438	1440	1446	rVB2	256	227	0.02%	0.002%
38	5.246	1446	1448	1451	rBV2	354	229	0.02%	0.002%
39	5.345	1454	1479	1505	rBV2	354079	1063442	100.00%	10.678%
40	5.464	1513	1516	1518	rBV2	445	268	0.03%	0.003%
41	5.551	1528	1543	1568	rVV	97299	199567	18.77%	2.004%
42	5.638	1568	1570	1575	rVB3	717	524	0.05%	0.005%
43	5.677	1575	1582	1586	rBV4	860	860	0.08%	0.009%
44	5.744	1600	1603	1610	rBV3	439	340	0.03%	0.003%
45	5.892	1630	1649	1669	rBV	401017	845471	79.50%	8.489%
46	6.336	1773	1787	1805	rVB	248428	489649	46.04%	4.916%
47	6.580	1858	1863	1872	rVB2	4693	6846	0.64%	0.069%
48	6.709	1891	1903	1927	rBV	145244	262217	24.66%	2.633%
49	6.831	1938	1941	1942	rBV2	815	532	0.05%	0.005%
50	7.230	2051	2065	2086	rBV	150950	267265	25.13%	2.684%
51	7.423	2118	2125	2134	rBV2	5776	9121	0.86%	0.092%
52	7.570	2155	2171	2202	rBV	503548	882158	82.95%	8.857%
53	7.702	2208	2212	2217	rBV4	614	788	0.07%	0.008%
54	7.853	2246	2259	2279	rBV	109937	188519	17.73%	1.893%
55	7.979	2296	2298	2299	rBV	481	218	0.02%	0.002%
56	8.185	2344	2362	2369	rBV5	9878	27520	2.59%	0.276%
57	8.313	2392	2402	2424	rVB	337163	577997	54.35%	5.803%
58	8.419	2426	2435	2448	rVB	75304	118152	11.11%	1.186%
59	8.525	2460	2468	2482	rVB	22210	36058	3.39%	0.362%
60	8.651	2504	2507	2508	rBV2	403	243	0.02%	0.002%
61	8.754	2537	2539	2544	rVB3	512	321	0.03%	0.003%
62	8.786	2547	2549	2554	rVB2	406	294	0.03%	0.003%
63	8.821	2554	2560	2563	rBV2	486	466	0.04%	0.005%
64	8.908	2571	2587	2600	rBV	84796	134956	12.69%	1.355%
65	9.014	2618	2620	2624	rBV	269	252	0.02%	0.003%
66	9.094	2628	2645	2663	rBV	560731	931992	87.64%	9.358%
67	9.246	2689	2692	2697	rBV4	567	628	0.06%	0.006%
68	9.519	2773	2777	2778	rBV2	471	310	0.03%	0.003%
69	9.680	2825	2827	2830	rVB2	548	255	0.02%	0.003%
70	9.718	2837	2839	2843	rBV	325	285	0.03%	0.003%
71	9.770	2848	2855	2861	rBV5	2537	3758	0.35%	0.038%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU072318\
Data File : VU025599.D
Acq On : 23 Jul 2018 14:01
Operator : MD/SY
Sample : VLEB#03
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : VLEB#03

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

72	9.918	2899	2901	2904	rVB2	412	206	0.02%	0.002%
73	10.027	2932	2935	2942	rBV3	478	581	0.05%	0.006%
74	10.059	2942	2945	2952	rVV3	366	393	0.04%	0.004%
75	10.181	2981	2983	2988	rVB3	454	316	0.03%	0.003%
76	10.233	2990	2999	3010	rVV4	4069	6310	0.59%	0.063%
77	10.339	3031	3032	3037	rVB3	347	209	0.02%	0.002%
78	10.435	3050	3062	3076	rBV	360360	572492	53.83%	5.748%
79	10.619	3111	3119	3133	rVB5	3833	7265	0.68%	0.073%
80	10.731	3150	3154	3158	rBV2	631	558	0.05%	0.006%
81	10.776	3162	3168	3178	rVB3	3032	4097	0.39%	0.041%
82	10.837	3182	3187	3189	rBV	468	446	0.04%	0.004%
83	10.927	3212	3215	3220	rBV3	432	367	0.03%	0.004%
84	10.992	3231	3235	3238	rBV2	371	313	0.03%	0.003%
85	11.223	3303	3307	3309	rBV2	366	252	0.02%	0.003%
86	11.274	3320	3323	3328	rBV3	385	285	0.03%	0.003%
87	11.307	3329	3333	3337	rBV2	457	423	0.04%	0.004%
88	11.371	3350	3353	3357	rVB	575	437	0.04%	0.004%
89	11.487	3376	3389	3404	rBV	600700	936640	88.08%	9.404%
90	11.750	3467	3471	3474	rBV3	585	470	0.04%	0.005%
91	11.802	3482	3487	3490	rBV2	427	490	0.05%	0.005%
92	11.863	3494	3506	3525	rVV	544677	869199	81.73%	8.727%
93	12.406	3672	3675	3678	rBV2	436	305	0.03%	0.003%
94	12.532	3711	3714	3719	rBV2	490	443	0.04%	0.004%
95	12.580	3723	3729	3731	rBV4	750	813	0.08%	0.008%
96	12.638	3744	3747	3752	rBV4	978	873	0.08%	0.009%
97	12.741	3777	3779	3782	rVB	427	233	0.02%	0.002%
98	12.853	3810	3814	3818	rBV2	623	565	0.05%	0.006%
99	13.165	3908	3911	3913	rBV2	430	308	0.03%	0.003%
100	13.995	4161	4169	4173	rBV4	960	1468	0.14%	0.015%

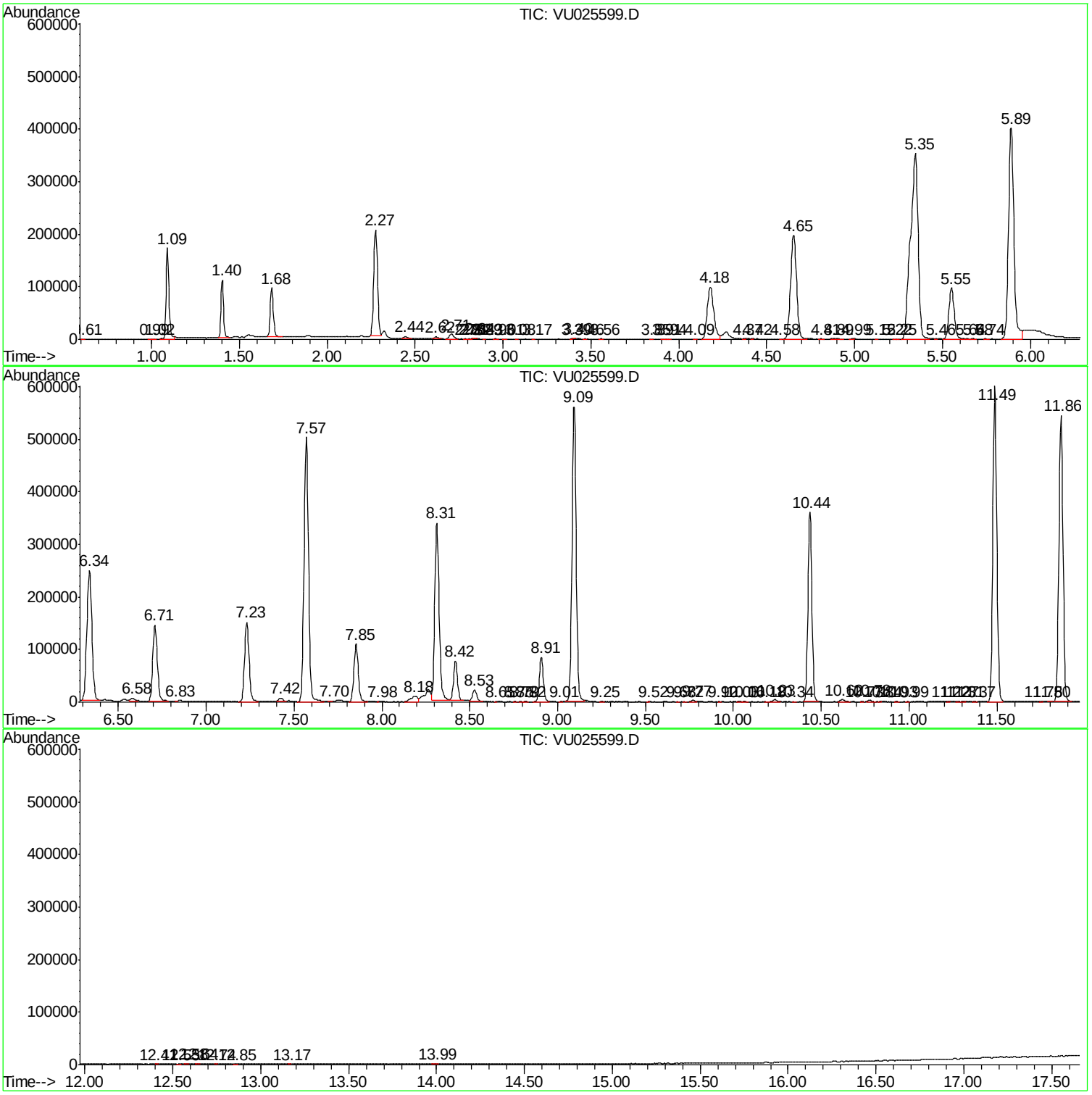
Sum of corrected areas: 9959535

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU072318\
Data File : VU025599.D
Acq On : 23 Jul 2018 14:01
Operator : MD/SY
Sample : VLEB#03
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB#03

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

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU072318\
Data File : VU025599.D
Acq On : 23 Jul 2018 14:01
Operator : MD/SY
Sample : VLEB#03
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : VLEB#03

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

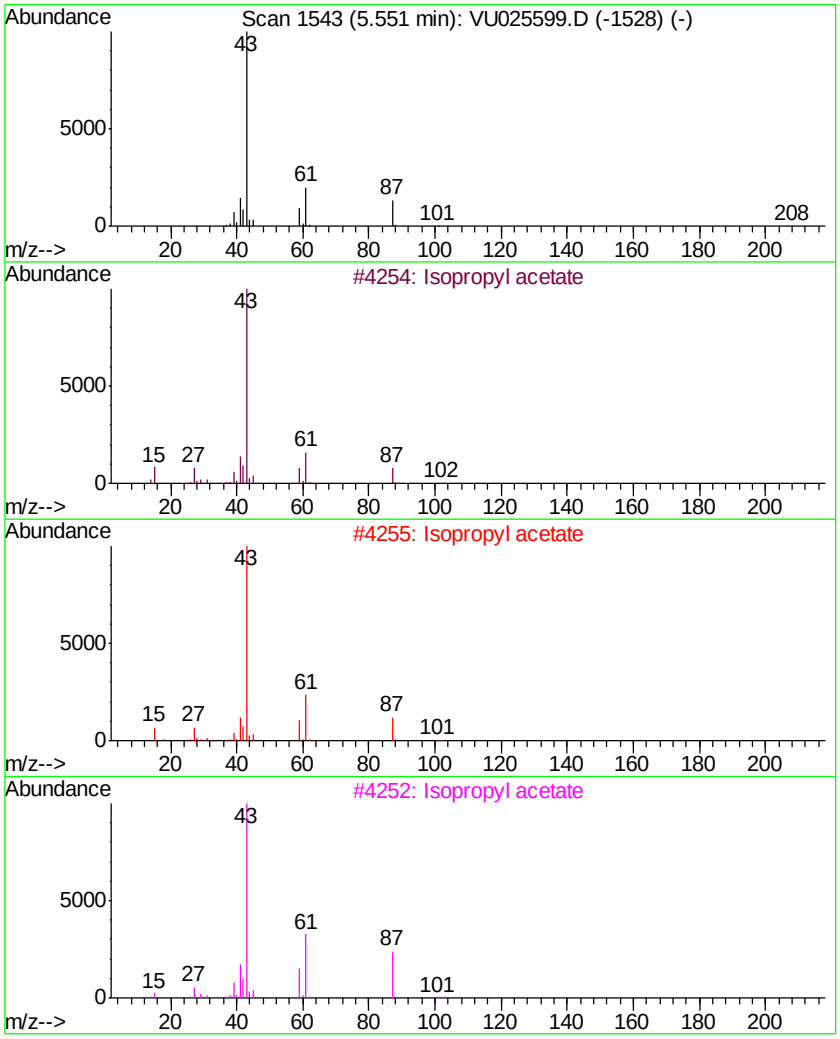
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

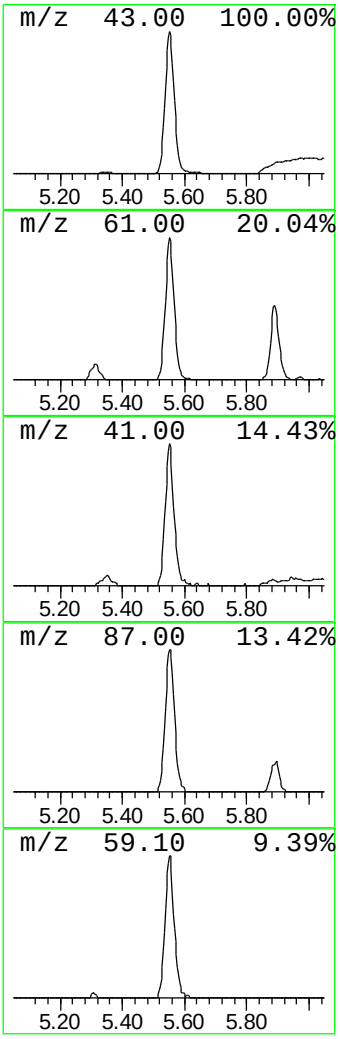
****

Peak Number 2 Isopropyl acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.55	11.80 ug/L	199567	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	83
3	Isopropyl acetate	102	C5H10O2	000108-21-4	64
4	Acetaldehyde, O-ethyloxime-	87	C4H9NO	1000288-34-6	12
5	2-Pentanol, acetate	130	C7H14O2	000626-38-0	9





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU072318\
Data File : VU025599.D
Acq On : 23 Jul 2018 14:01
Operator : MD/SY
Sample : VLEB#03
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : VLEB#03

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

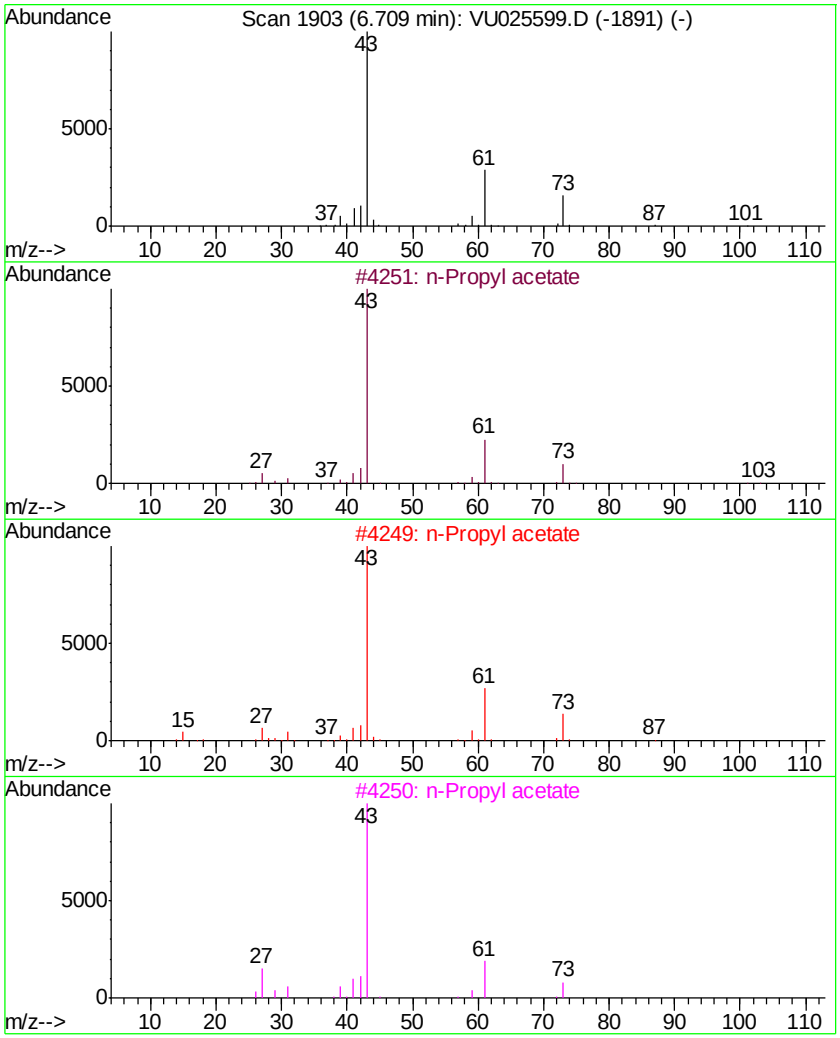
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

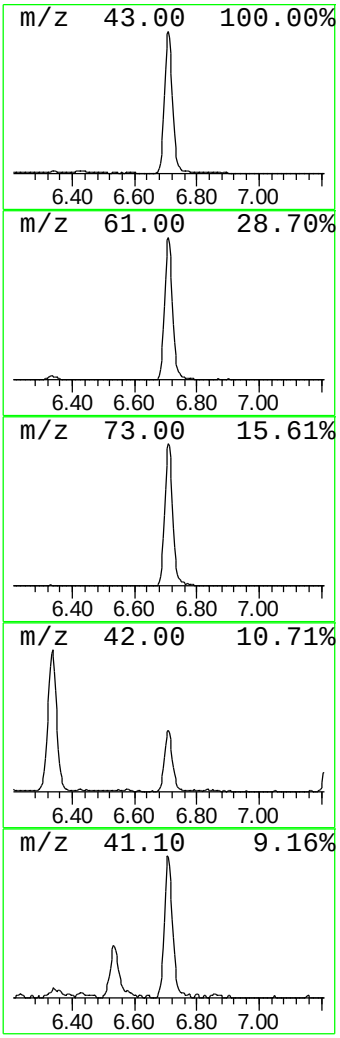
****

Peak Number 3 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.71	15.51 ug/L	262217	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	Isopropyl acetate	102	C5H10O2	000108-21-4	9





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU072318\
Data File : VU025599.D
Acq On : 23 Jul 2018 14:01
Operator : MD/SY
Sample : VLEB#03
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : VLEB#03

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

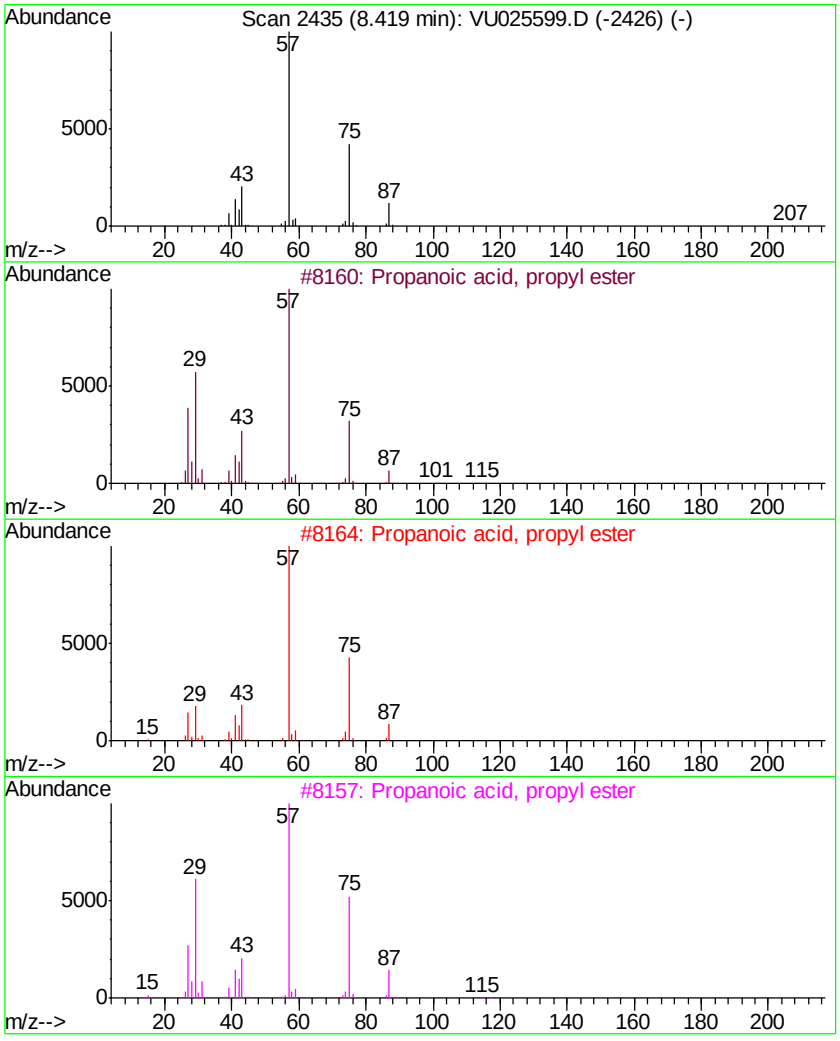
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

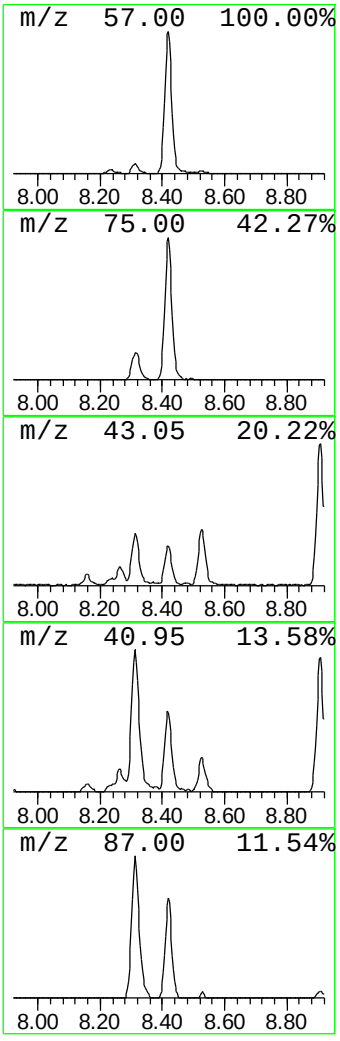
****

Peak Number 5 Propanoic acid, propyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.42	6.34 ug/L	118152	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	72
5	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	39





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU072318\
Data File : VU025599.D
Acq On : 23 Jul 2018 14:01
Operator : MD/SY
Sample : VLEB#03
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : VLEB#03

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

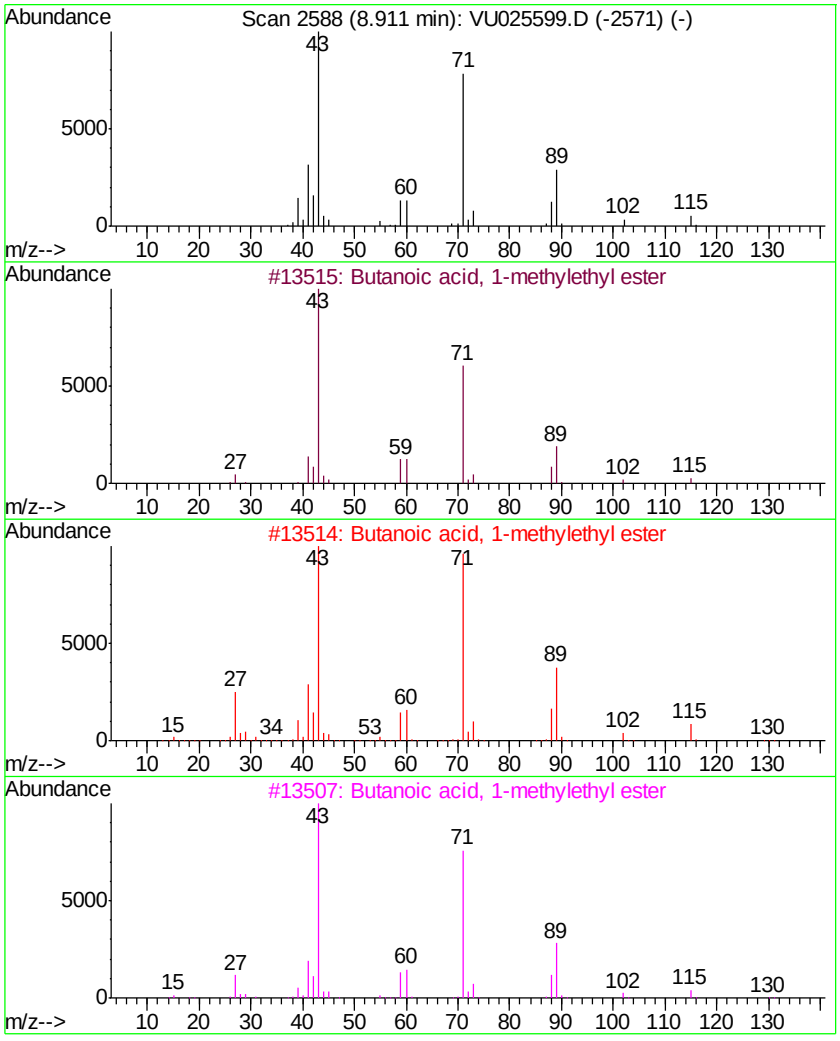
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

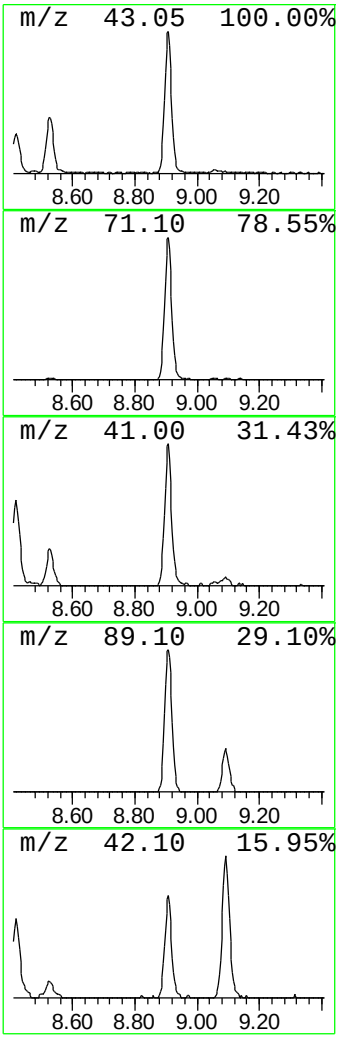
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.91	7.24 ug/L	134956	Chlorobenzene-d5	9.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	90
2	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	90
3	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	90
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

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU072318\
Data File : VU025599.D
Acq On : 23 Jul 2018 14:01
Operator : MD/SY
Sample : VLEB#03
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : VLEB#03

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	11.8	ug/L	199567	1	5.89	845471	50.0
n-Propyl acetate	6.71	15.5	ug/L	262217	1	5.89	845471	50.0
Propanoic acid, p...	8.42	6.3	ug/L	118152	2	9.09	931992	50.0
Butanoic acid, 1-...	8.91	7.2	ug/L	134956	2	9.09	931992	50.0