LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU071618\
Data File : VU025424.D
Acq On : 16 Jul 2018 15:08
Operator : MD/SY
Sample : VLEB#01
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : VLEB01

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\SOMULM071618WMA.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	0.667	17	24	25	rBV4	553	467	0.04%	0.004%
2	0.680	25	28	32	rVB3	756	574	0.05%	0.005%
3	0.777	53	58	66	rVB4	1121	1380	0.12%	0.012%
4	0.970	116	118	121	rVB3	934	503	0.04%	0.004%
5	1.089	141	155	174	rBV	590075	716576	60.98%	6.314%
6	1.400	245	252	263	rBV	121665	132582	11.28%	1.168%
7	1.677	331	338	357	rVB	92813	131149	11.16%	1.156%
8	2.272	513	523	533	rBV	228297	344990	29.36%	3.040%
9	2.619	623	631	646	rVB2	6821	12289	1.05%	0.108%
10	2.703	646	657	675	rBV2	37155	70741	6.02%	0.623%
11	2.815	684	692	694	rBV6	1052	1424	0.12%	0.013%
12	3.076	770	773	778	rVB5	876	596	0.05%	0.005%
13	3.236	816	823	827	rBV7	658	887	0.08%	0.008%
14	3.355	855	860	865	rBV4	1104	1313	0.11%	0.012%
15	3.410	865	877	891	rVV3	8665	20366	1.73%	0.179%
16	3.571	924	927	930	rVB4	1009	650	0.06%	0.006%
17	3.590	930	933	939	rVB3	646	539	0.05%	0.005%
18	3.622	939	943	947	rBV4	1059	992	0.08%	0.009%
19	3.661	952	955	957	rVB3	942	483	0.04%	0.004%
20	3.757	981	985	987	rBV4	684	575	0.05%	0.005%
21	3.802	995	999	1003	rBV5	640	551	0.05%	0.005%
22	3.895	1024	1028	1032	rBV4	676	625	0.05%	0.006%
23	3.947	1041	1044	1046	rBV3	651	498	0.04%	0.004%
24	4.082	1082	1086	1089	rBV4	701	695	0.06%	0.006%
25	4.178	1099	1116	1138	rBV	112643	300287	25.56%	2.646%
26	4.651	1245	1263	1285	rBV	203150	472727	40.23%	4.166%
27	5.079	1389	1396	1401	rBV5	1099	1100	0.09%	0.010%
28	5.217	1436	1439	1443	rBV4	630	485	0.04%	0.004%
29	5.346	1451	1479	1496	rBV2	388112	1175012	100.00%	10.354%
30	5.551	1529	1543	1561	rBV	87781	180155	15.33%	1.587%
31	5.728	1595	1598	1603	rBV5	991	771	0.07%	0.007%
32	5.889	1625	1648	1668	rBV	446443	1090644	92.82%	9.611%
33	6.336	1773	1787	1806	rBV	264588	536011	45.62%	4.723%
34	6.583	1857	1864	1870	rBV2	4371	6858	0.58%	0.060%

LSC Area Percent Report

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Acq On : 16 Jul 2018 15:08
Operator : MD/SY
Sample : VLEB#01
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : VLEB01

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\SOMULM071618WMA.M
Title : VOC Analysis

35	6.709	1892	1903	1922	rBV	139694	255188	21.72%	2.249%
36	6.905	1961	1964	1968	rBV4	806	646	0.05%	0.006%
37	7.230	2054	2065	2086	rBV	155600	279505	23.79%	2.463%
38	7.426	2119	2126	2134	rBV3	4981	7070	0.60%	0.062%
39	7.571	2156	2171	2207	rBV	541337	989009	84.17%	8.715%
40	7.850	2247	2258	2274	rBV	109378	187934	15.99%	1.656%
41	8.156	2347	2353	2361	rBV5	3202	5262	0.45%	0.046%
42	8.236	2368	2378	2380	rBV8	4702	6614	0.56%	0.058%
43	8.265	2381	2387	2392	rVV3	15693	22923	1.95%	0.202%
44	8.313	2392	2402	2425	rVV	393462	696271	59.26%	6.135%
45	8.419	2427	2435	2447	rVB	69032	111263	9.47%	0.980%
46	8.526	2461	2468	2478	rVB	21706	32795	2.79%	0.289%
47	8.773	2541	2545	2551	rBV6	1392	1618	0.14%	0.014%
48	8.908	2576	2587	2604	rVB2	71137	112811	9.60%	0.994%
49	9.095	2632	2645	2675	rVB	561039	953469	81.15%	8.402%
50	9.365	2727	2729	2731	rBV3	775	479	0.04%	0.004%
51	9.381	2731	2734	2738	rVV4	1561	1394	0.12%	0.012%
52	9.397	2738	2739	2743	rVB2	796	514	0.04%	0.005%
53	9.432	2747	2750	2755	rBV4	708	615	0.05%	0.005%
54	9.632	2809	2812	2815	rBV3	645	472	0.04%	0.004%
55	9.651	2816	2818	2824	rVB5	744	652	0.06%	0.006%
56	9.689	2824	2830	2831	rBV4	801	646	0.05%	0.006%
57	9.770	2847	2855	2859	rBV6	2375	3521	0.30%	0.031%
58	9.821	2869	2871	2875	rVB4	1062	667	0.06%	0.006%
59	9.905	2894	2897	2899	rBV3	878	568	0.05%	0.005%
60	9.995	2920	2925	2928	rBV3	479	538	0.05%	0.005%
61	10.197	2985	2988	2993	rBV5	666	618	0.05%	0.005%
62	10.313	3020	3024	3028	rBV6	1158	1078	0.09%	0.009%
63	10.435	3047	3062	3079	rBV	389636	633343	53.90%	5.581%
64	10.558	3096	3100	3102	rBV4	828	708	0.06%	0.006%
65	10.715	3144	3149	3152	rBV4	793	567	0.05%	0.005%
66	10.776	3166	3168	3177	rVB7	1881	1929	0.16%	0.017%
67	10.818	3179	3181	3188	rVV6	586	640	0.05%	0.006%
68	10.882	3197	3201	3206	rVB3	666	492	0.04%	0.004%
69	10.992	3232	3235	3240	rBV4	783	571	0.05%	0.005%
70	11.082	3260	3263	3266	rBV3	737	674	0.06%	0.006%
71	11.146	3279	3283	3285	rBV3	1003	820	0.07%	0.007%

LSC Area Percent Report

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Acq On : 16 Jul 2018 15:08
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Sample : VLEB#01
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : VLEB01

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\SOMULM071618WMA.M
Title : VOC Analysis

72	11.185	3290	3295	3299	rBV4	812	763	0.06%	0.007%
73	11.233	3305	3310	3313	rVB5	501	531	0.05%	0.005%
74	11.255	3313	3317	3321	rBV4	689	502	0.04%	0.004%
75	11.371	3349	3353	3358	rBV4	473	486	0.04%	0.004%
76	11.487	3376	3389	3408	rBV	560603	887309	75.51%	7.819%
77	11.699	3451	3455	3457	rVB4	634	479	0.04%	0.004%
78	11.757	3462	3473	3477	rBV5	1679	2610	0.22%	0.023%
79	11.863	3493	3506	3522	rBV	557571	895780	76.24%	7.893%
80	12.136	3587	3591	3596	rVB6	1032	841	0.07%	0.007%
81	12.242	3621	3624	3630	rVB5	683	543	0.05%	0.005%
82	12.271	3630	3633	3638	rBV4	655	658	0.06%	0.006%
83	12.352	3653	3658	3665	rVB4	734	874	0.07%	0.008%
84	12.390	3667	3670	3675	rBV5	748	887	0.08%	0.008%
85	12.480	3695	3698	3699	rBV2	995	516	0.04%	0.005%
86	12.570	3715	3726	3738	rBV2	15442	23963	2.04%	0.211%
87	12.641	3744	3748	3752	rVB6	1443	1179	0.10%	0.010%
88	12.821	3802	3804	3810	rVB4	756	580	0.05%	0.005%
89	12.943	3838	3842	3843	rBV4	949	685	0.06%	0.006%
90	13.037	3866	3871	3874	rBV4	756	911	0.08%	0.008%
91	13.303	3952	3954	3959	rVB4	896	601	0.05%	0.005%
92	13.336	3959	3964	3966	rBV5	1148	1169	0.10%	0.010%
93	13.480	4007	4009	4014	rVB4	1326	888	0.08%	0.008%
94	13.506	4014	4017	4023	rVV6	1406	1737	0.15%	0.015%
95	13.538	4023	4027	4030	rVB3	1310	1065	0.09%	0.009%
96	13.648	4059	4061	4065	rVB3	884	539	0.05%	0.005%
97	13.689	4071	4074	4075	rBV3	890	497	0.04%	0.004%
98	13.799	4104	4108	4112	rBV4	867	787	0.07%	0.007%
99	13.821	4112	4115	4117	rBV2	1077	689	0.06%	0.006%
100	14.104	4200	4203	4208	rVB5	1195	960	0.08%	0.008%

Sum of corrected areas: 11348408

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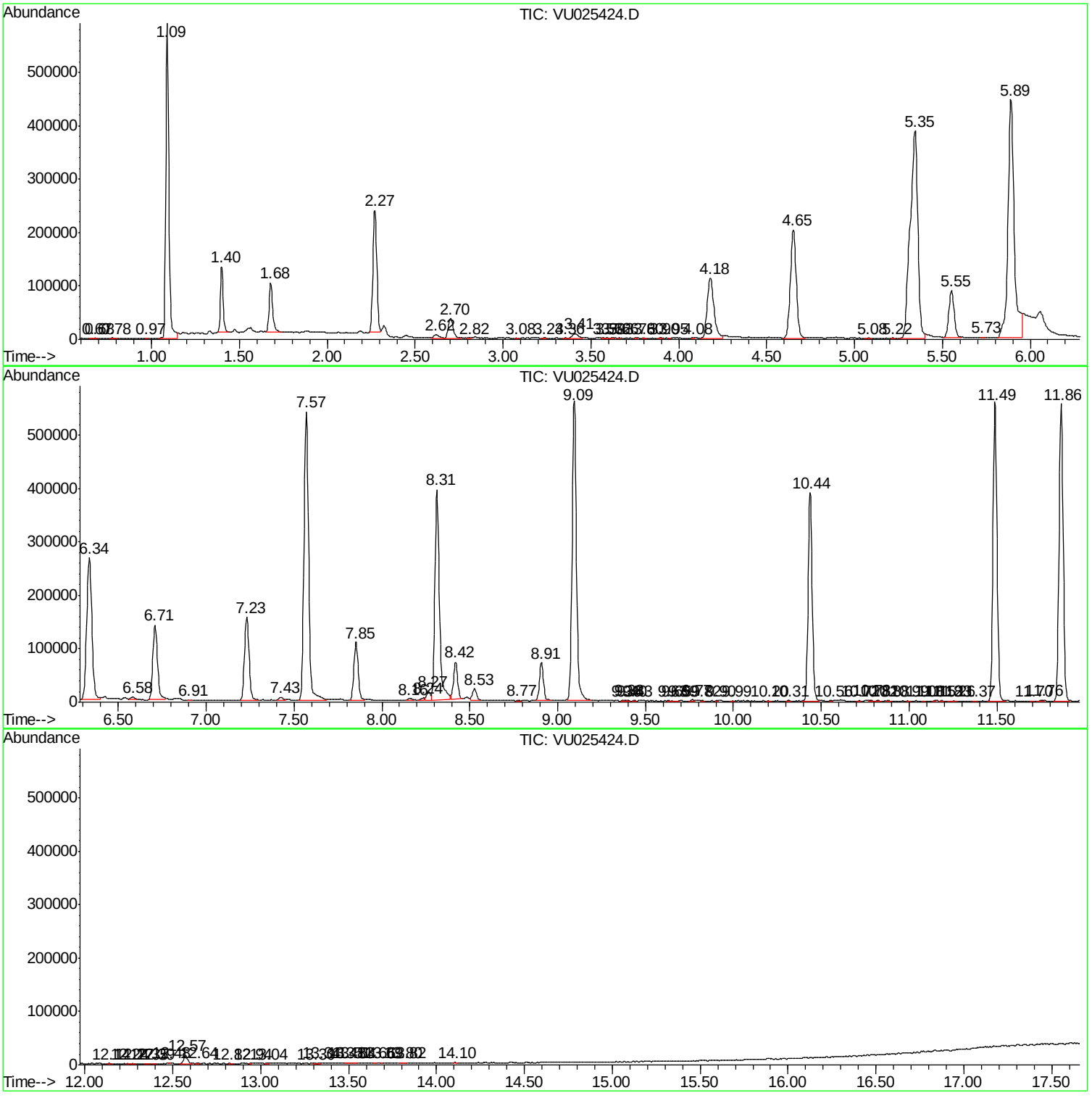
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : VLEB01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM071618WMA.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\VU071618\
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Quant Title : VOC Analysis

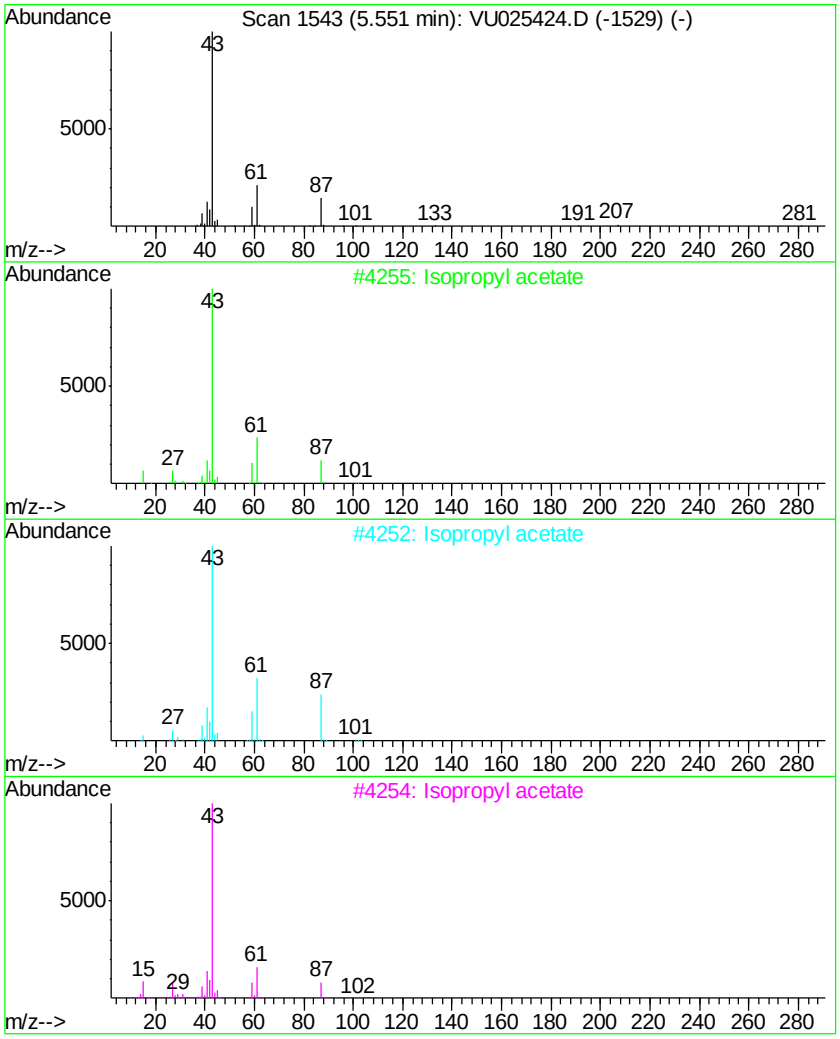
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

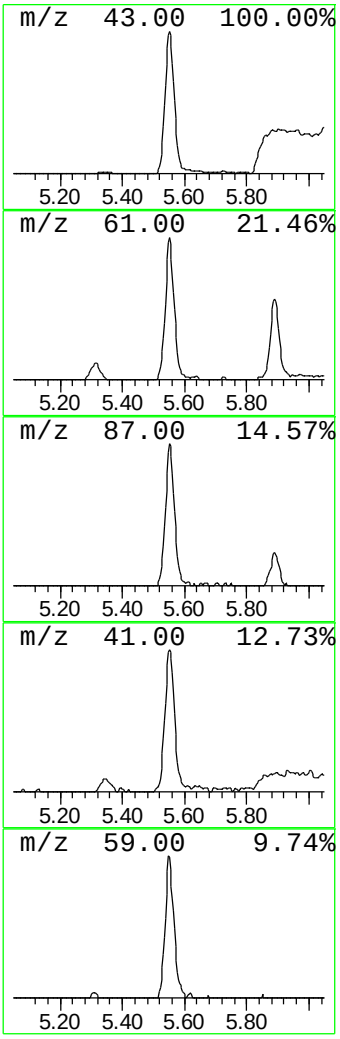
****

Peak Number 2 Isopropyl acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.55	8.26 ug/L	180155	1,4-Difluorobenzene	5.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl acetate	102	C5H10O2	000108-21-4	72
2	Isopropyl acetate	102	C5H10O2	000108-21-4	56
3	Isopropyl acetate	102	C5H10O2	000108-21-4	38
4	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	12
5	Acetaldehyde, O-ethyloxime-	87	C4H9NO	1000288-34-6	9





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU071618\
Data File : VU025424.D
Acq On : 16 Jul 2018 15:08
Operator : MD/SY
Sample : VLEB#01
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : VLEB01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM071618WMA.M
Quant Title : VOC Analysis

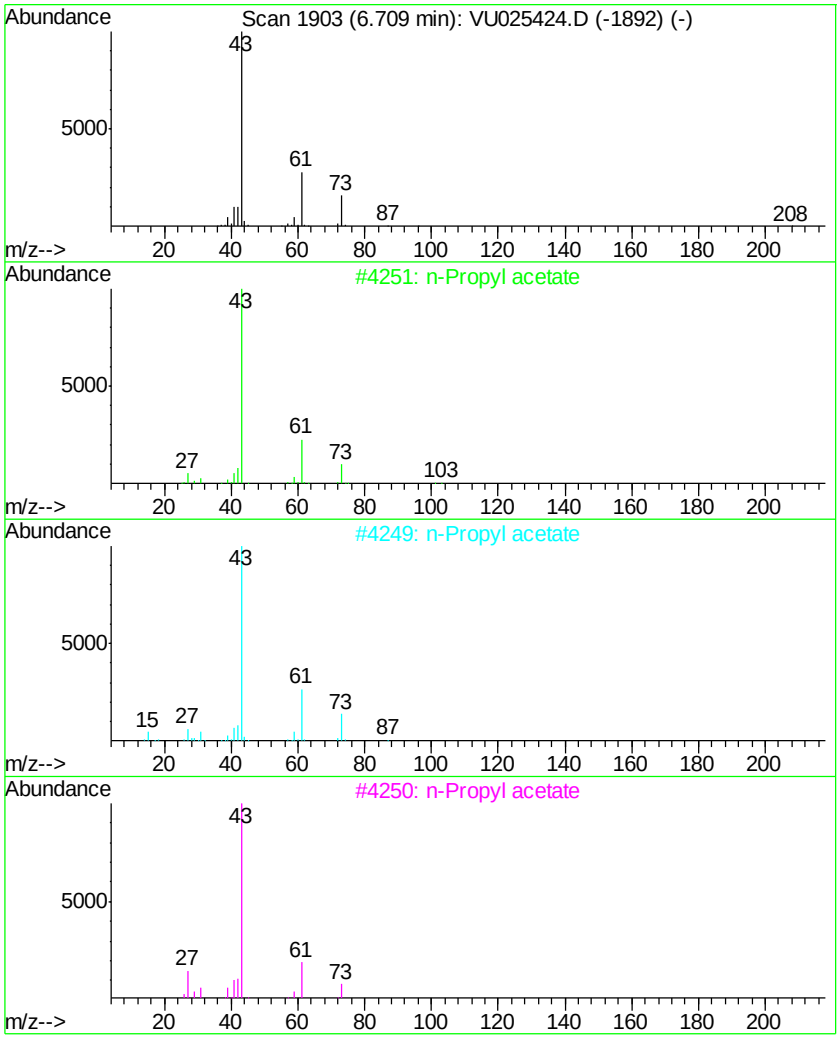
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

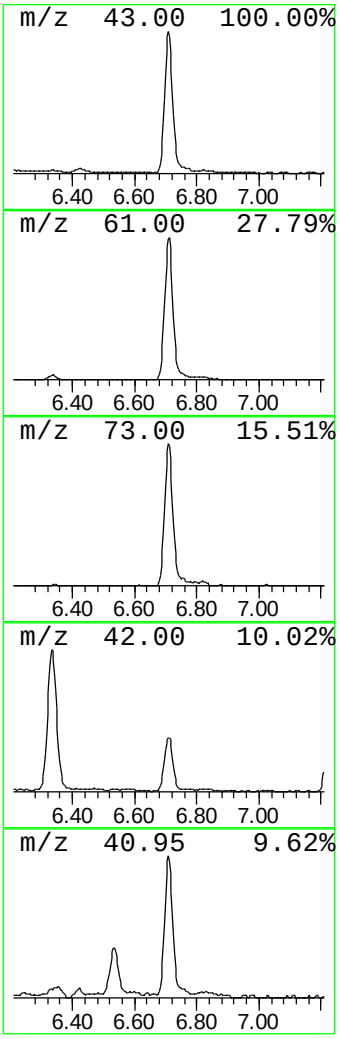
****

Peak Number 3 n-Propyl acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.71	11.70 ug/L	255188	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	Isobutyl acetate	116	C6H12O2	000110-19-0	9





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ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : VLEB01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM071618WMA.M
Quant Title : VOC Analysis

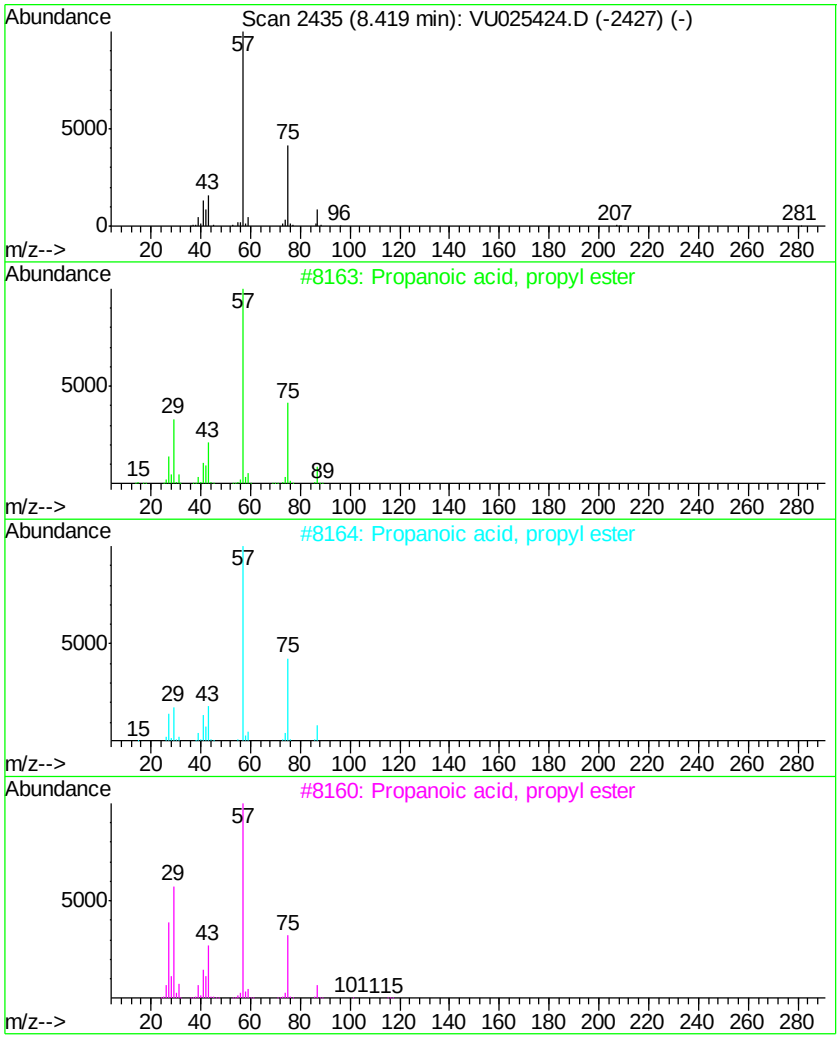
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

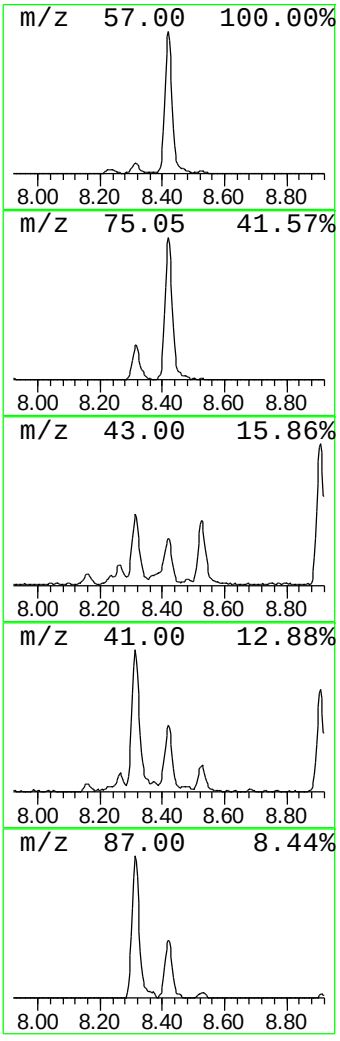
****

Peak Number 5 Propanoic acid, propyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.42	5.83 ug/L	111263	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	74
4	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	74
5	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	9





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Data File : VU025424.D
Acq On : 16 Jul 2018 15:08
Operator : MD/SY
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Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : VLEB01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM071618WMA.M
Quant Title : VOC Analysis

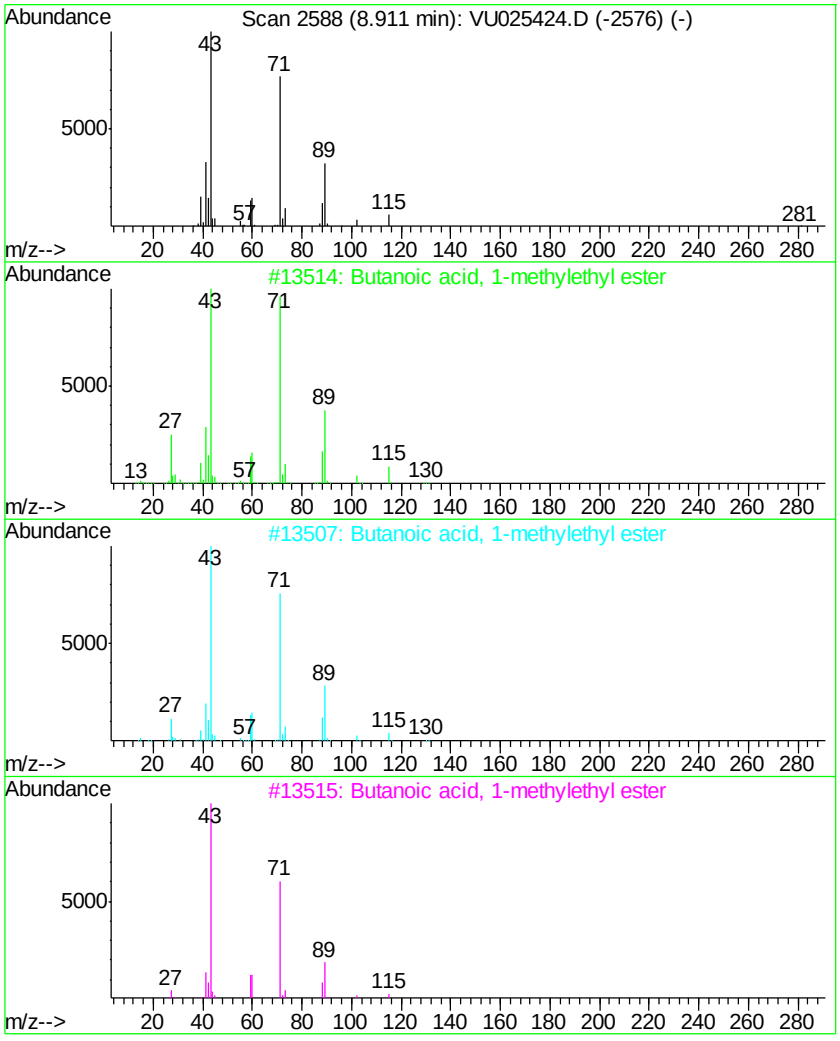
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

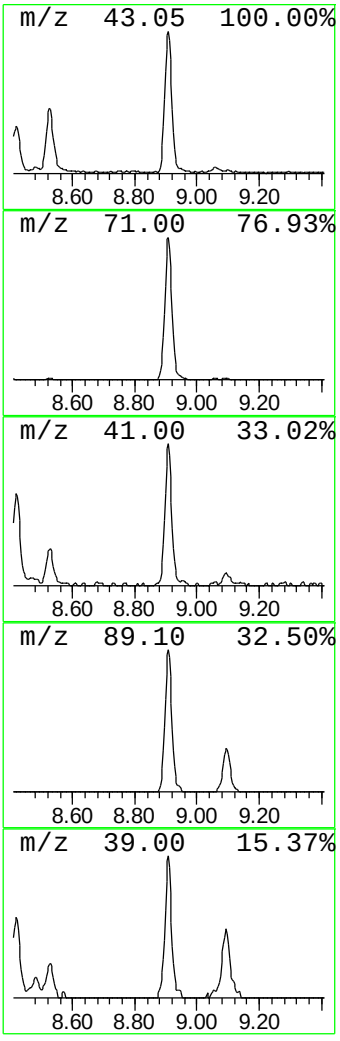
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.91	5.92 ug/L	112811	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	78
4	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	64
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU071618\
Data File : VU025424.D
Acq On : 16 Jul 2018 15:08
Operator : MD/SY
Sample : VLEB#01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : VLEB01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM071618WMA.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	8.3	ug/L	180155	1	5.89	1090640	50.0
n-Propyl acetate	6.71	11.7	ug/L	255188	1	5.89	1090640	50.0
Propanoic acid, p...	8.42	5.8	ug/L	111263	2	9.09	953469	50.0
Butanoic acid, 1-...	8.91	5.9	ug/L	112811	2	9.09	953469	50.0