LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061819\
Data File : VU032822.D
Acq On : 18 Jun 2019 14:23
Operator : JC/SP
Sample : K3363-04
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JT8

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\SOMULM061719WMA.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	1.180	24	28	34	rVB2	6135	5508	0.49%	0.055%
2	1.396	88	95	110	rVB	127339	128190	11.33%	1.283%
3	1.470	113	118	126	rVB	8316	8781	0.78%	0.088%
4	1.676	174	182	199	rVB	97140	120325	10.63%	1.204%
5	2.267	355	366	376	rBV	204183	310424	27.43%	3.107%
6	2.412	407	411	415	rBV4	556	430	0.04%	0.004%
7	2.566	456	459	465	rVB4	325	249	0.02%	0.002%
8	2.618	470	475	482	rVV3	1448	1986	0.18%	0.020%
9	2.695	490	499	508	rBV3	4573	7280	0.64%	0.073%
10	2.978	579	587	597	rBV4	2387	4211	0.37%	0.042%
11	3.020	597	600	605	rVB2	446	444	0.04%	0.004%
12	3.177	643	649	652	rBV4	1132	1502	0.13%	0.015%
13	3.254	668	673	678	rVB3	459	560	0.05%	0.006%
14	3.344	699	701	708	rVB2	377	337	0.03%	0.003%
15	3.409	716	721	722	rBV3	540	404	0.04%	0.004%
16	3.521	753	756	760	rBV3	420	382	0.03%	0.004%
17	3.698	807	811	814	rVB3	332	272	0.02%	0.003%
18	3.923	877	881	886	rVB3	405	294	0.03%	0.003%
19	3.955	886	891	897	rBV2	279	318	0.03%	0.003%
20	4.061	919	924	926	rBV3	297	283	0.03%	0.003%
21	4.113	935	940	944	rBV2	462	524	0.05%	0.005%
22	4.171	944	958	996	rBV	88214	262032	23.16%	2.622%
23	4.640	1087	1104	1124	rBV	156732	365306	32.28%	3.656%
24	4.833	1160	1164	1167	rBV2	315	371	0.03%	0.004%
25	4.884	1172	1180	1184	rBV4	519	775	0.07%	0.008%
26	5.129	1251	1256	1258	rBV2	296	270	0.02%	0.003%
27	5.331	1295	1319	1348	rBV2	314278	921832	81.46%	9.225%
28	5.441	1350	1353	1359	rVB3	485	458	0.04%	0.005%
29	5.547	1376	1386	1403	rBV3	5534	12692	1.12%	0.127%
30	5.611	1404	1406	1412	rVB3	826	580	0.05%	0.006%
31	5.643	1412	1416	1418	rBV2	361	253	0.02%	0.003%
32	5.672	1422	1425	1430	rVB3	289	240	0.02%	0.002%
33	5.714	1433	1438	1442	rBV2	358	269	0.02%	0.003%
34	5.807	1463	1467	1473	rVB2	417	399	0.04%	0.004%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061819\
Data File : VU032822.D
Acq On : 18 Jun 2019 14:23
Operator : JC/SP
Sample : K3363-04
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JT8

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\SOMULM061719WMA.M
Title : VOC Analysis

35	5.878	1473	1489	1517	rBV	274117	537200	47.47%	5.376%
36	6.000	1517	1527	1531	rBV5	1551	2825	0.25%	0.028%
37	6.180	1574	1583	1598	rVB7	6554	12935	1.14%	0.129%
38	6.248	1602	1604	1609	rVB4	335	255	0.02%	0.003%
39	6.277	1609	1613	1614	rBV	388	294	0.03%	0.003%
40	6.325	1614	1628	1649	rBV	209850	419991	37.12%	4.203%
41	6.425	1650	1659	1678	rVB2	6366	14223	1.26%	0.142%
42	6.531	1685	1692	1699	rBV2	2849	4795	0.42%	0.048%
43	6.576	1700	1706	1713	rBV	3600	5306	0.47%	0.053%
44	6.698	1731	1744	1765	rBV	638343	1131570	100.00%	11.324%
45	7.097	1865	1868	1870	rBV3	565	409	0.04%	0.004%
46	7.222	1895	1907	1922	rBV2	111148	195080	17.24%	1.952%
47	7.370	1950	1953	1955	rBV3	646	428	0.04%	0.004%
48	7.415	1955	1967	1991	rVV	131234	228631	20.20%	2.288%
49	7.560	1999	2012	2030	rBV	439665	760602	67.22%	7.612%
50	7.698	2051	2055	2063	rVB4	1493	1854	0.16%	0.019%
51	7.842	2088	2100	2124	rBV2	91845	161398	14.26%	1.615%
52	8.058	2163	2167	2170	rBV3	328	297	0.03%	0.003%
53	8.148	2183	2195	2211	rBV	76454	126336	11.16%	1.264%
54	8.257	2214	2229	2234	rVV5	20748	41049	3.63%	0.411%
55	8.306	2234	2244	2266	rVV	298139	517553	45.74%	5.179%
56	8.408	2266	2276	2302	rVV	344349	563959	49.84%	5.644%
57	8.521	2303	2311	2332	rVV	22224	40495	3.58%	0.405%
58	8.598	2332	2335	2337	rVV2	624	447	0.04%	0.004%
59	8.611	2337	2339	2342	rVV2	430	242	0.02%	0.002%
60	8.653	2348	2352	2356	rVV3	336	312	0.03%	0.003%
61	8.897	2416	2428	2450	rBV	302195	479379	42.36%	4.797%
62	9.084	2468	2486	2523	rBV	418880	697284	61.62%	6.978%
63	9.209	2523	2525	2529	rVB2	503	254	0.02%	0.003%
64	9.251	2535	2538	2541	rVB2	371	263	0.02%	0.003%
65	9.289	2547	2550	2556	rVB3	404	383	0.03%	0.004%
66	9.412	2583	2588	2590	rBV2	409	329	0.03%	0.003%
67	9.463	2601	2604	2610	rBV2	358	324	0.03%	0.003%
68	9.601	2640	2647	2655	rBV5	2777	4551	0.40%	0.046%
69	9.762	2689	2697	2712	rBV2	8256	12579	1.11%	0.126%
70	9.878	2730	2733	2737	rBV3	430	429	0.04%	0.004%
71	9.903	2737	2741	2747	rVB	320	364	0.03%	0.004%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061819\
Data File : VU032822.D
Acq On : 18 Jun 2019 14:23
Operator : JC/SP
Sample : K3363-04
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JT8

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\SOMULM061719WMA.M
Title : VOC Analysis

72	9.932	2747	2750	2753	rBV3	351	338	0.03%	0.003%
73	10.026	2776	2779	2783	rVB2	440	313	0.03%	0.003%
74	10.376	2881	2888	2890	rBV2	245	263	0.02%	0.003%
75	10.424	2892	2903	2923	rVV	302972	486693	43.01%	4.871%
76	10.585	2948	2953	2956	rVV3	251	286	0.03%	0.003%
77	10.604	2956	2959	2964	rVV3	403	340	0.03%	0.003%
78	10.653	2970	2974	2980	rVB3	449	420	0.04%	0.004%
79	10.768	3007	3010	3012	rBV	430	285	0.03%	0.003%
80	10.868	3036	3041	3044	rBV3	233	288	0.03%	0.003%
81	10.993	3077	3080	3084	rBV3	367	348	0.03%	0.003%
82	11.106	3110	3115	3118	rBV3	432	393	0.03%	0.004%
83	11.193	3139	3142	3146	rVB	380	272	0.02%	0.003%
84	11.219	3146	3150	3153	rBV2	341	261	0.02%	0.003%
85	11.280	3167	3169	3173	rVB	339	239	0.02%	0.002%
86	11.421	3209	3213	3218	rBV2	333	336	0.03%	0.003%
87	11.476	3218	3230	3250	rBV	418856	672865	59.46%	6.734%
88	11.575	3259	3261	3265	rVB2	869	529	0.05%	0.005%
89	11.752	3314	3316	3322	rBV2	237	249	0.02%	0.002%
90	11.855	3335	3348	3367	rBV	422431	701047	61.95%	7.016%
91	12.064	3409	3413	3423	rVB6	621	884	0.08%	0.009%
92	12.614	3582	3584	3589	rVV2	386	271	0.02%	0.003%
93	12.772	3631	3633	3637	rVB	408	240	0.02%	0.002%
94	12.794	3637	3640	3643	rBV2	402	299	0.03%	0.003%
95	13.344	3808	3811	3814	rBV	392	329	0.03%	0.003%
96	13.444	3838	3842	3844	rBV2	447	345	0.03%	0.003%
97	13.669	3908	3912	3917	rBV4	538	585	0.05%	0.006%
98	13.723	3926	3929	3932	rBV2	356	292	0.03%	0.003%
99	14.215	4079	4082	4084	rBV3	500	336	0.03%	0.003%
100	14.495	4167	4169	4174	rVB3	701	408	0.04%	0.004%

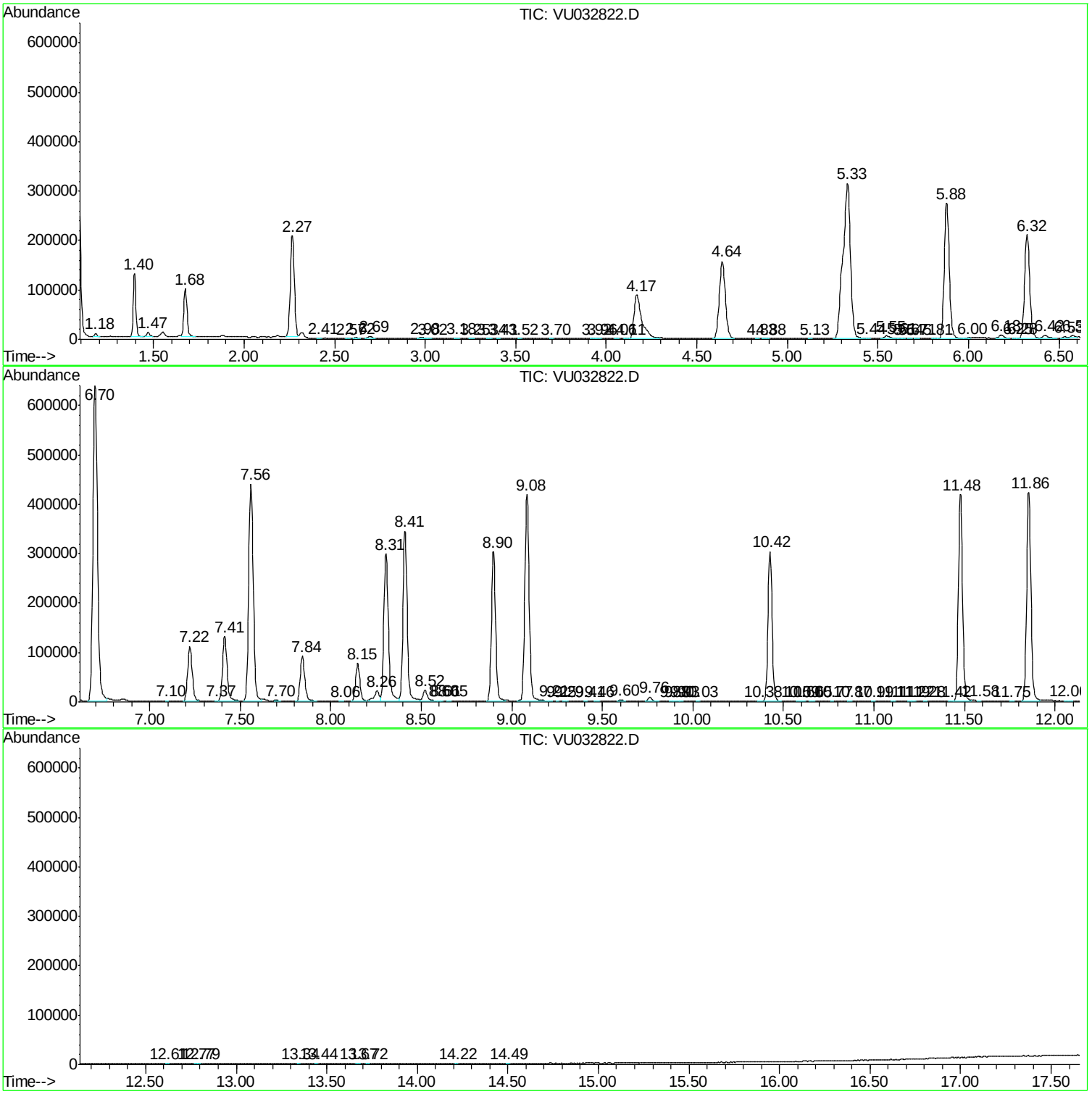
Sum of corrected areas: 9992560

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061819\
Data File : VU032822.D
Acq On : 18 Jun 2019 14:23
Operator : JC/SP
Sample : K3363-04
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JT8

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.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\VU061819\
Data File : VU032822.D
Acq On : 18 Jun 2019 14:23
Operator : JC/SP
Sample : K3363-04
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JT8

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

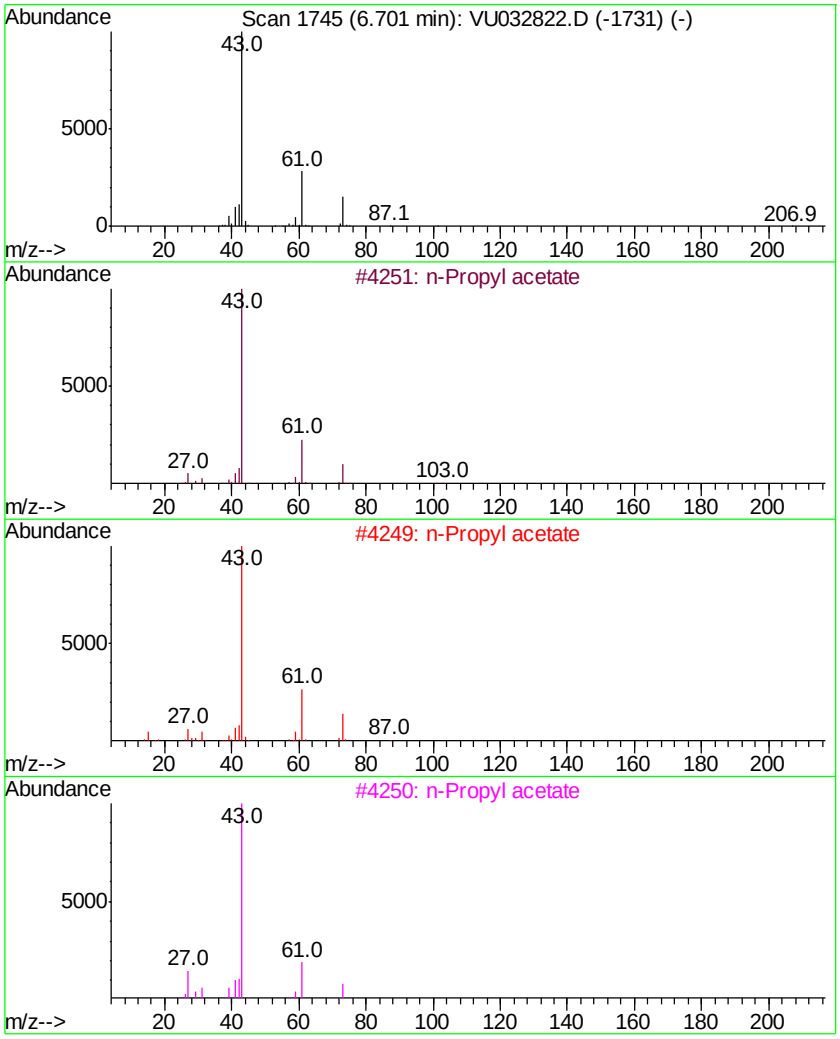
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

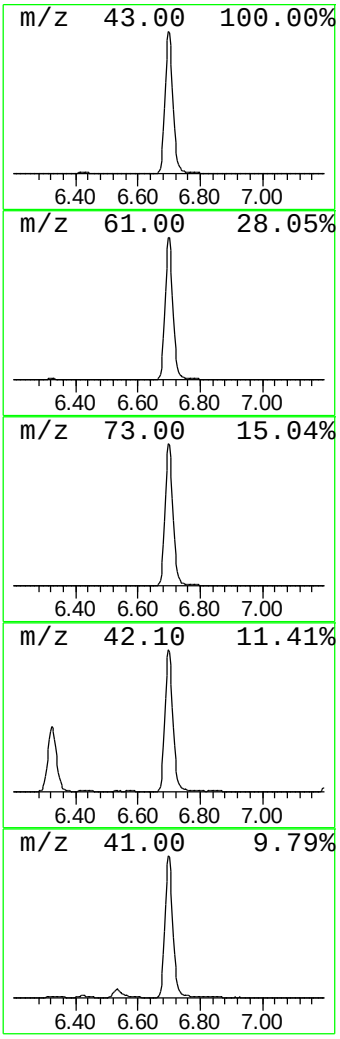
****

Peak Number 1 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	105.32 ug/L	1131570	1,4-Difluorobenzene	5.88

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





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061819\
Data File : VU032822.D
Acq On : 18 Jun 2019 14:23
Operator : JC/SP
Sample : K3363-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JT8

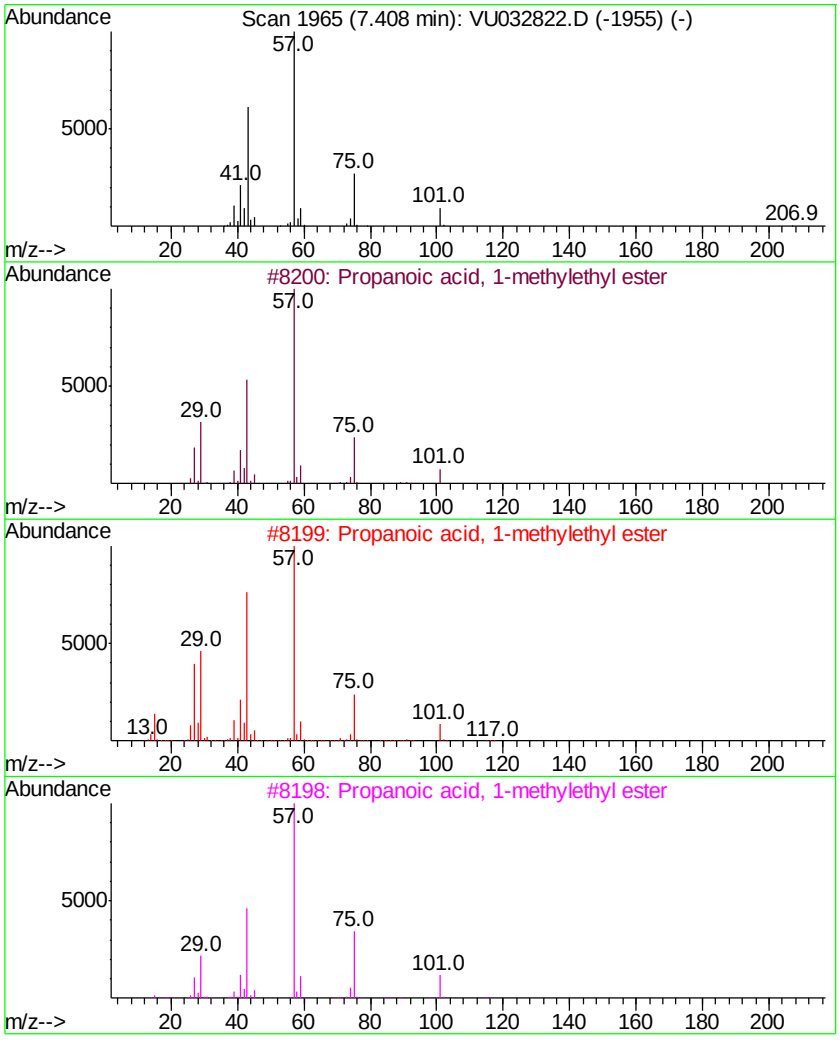
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

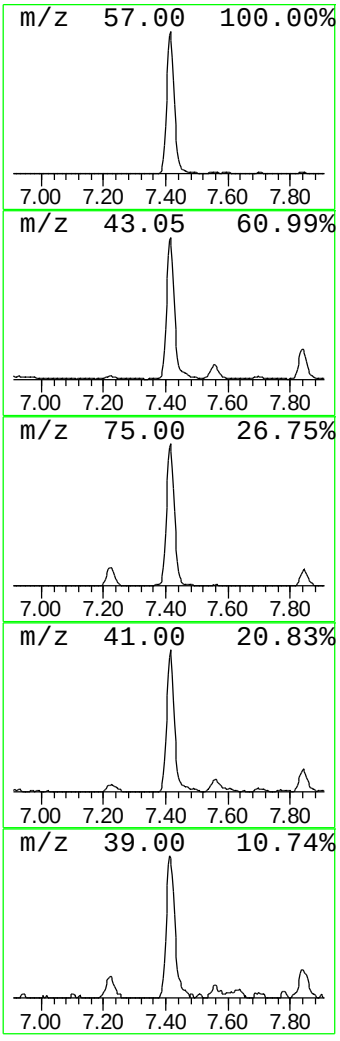
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.41	21.28 ug/L	228631	1,4-Difluorobenzene	5.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	83
2	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	83
3	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	78
4	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	45
5	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	40





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061819\
Data File : VU032822.D
Acq On : 18 Jun 2019 14:23
Operator : JC/SP
Sample : K3363-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JT8

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

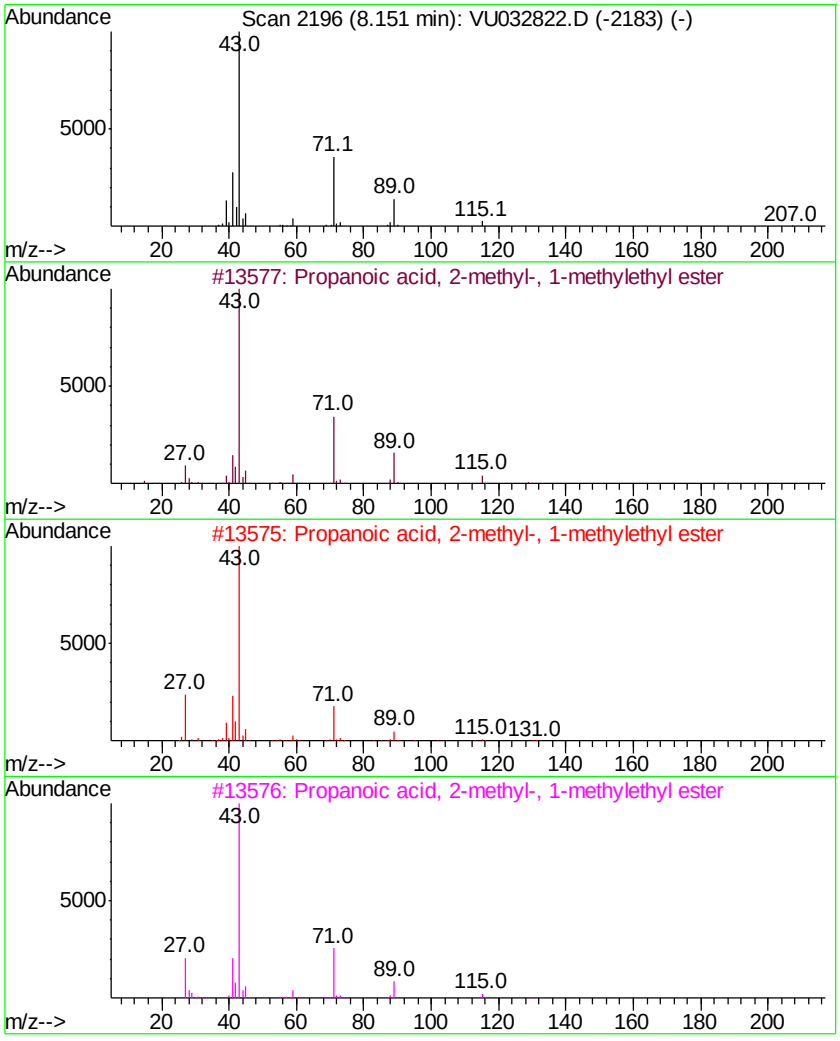
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

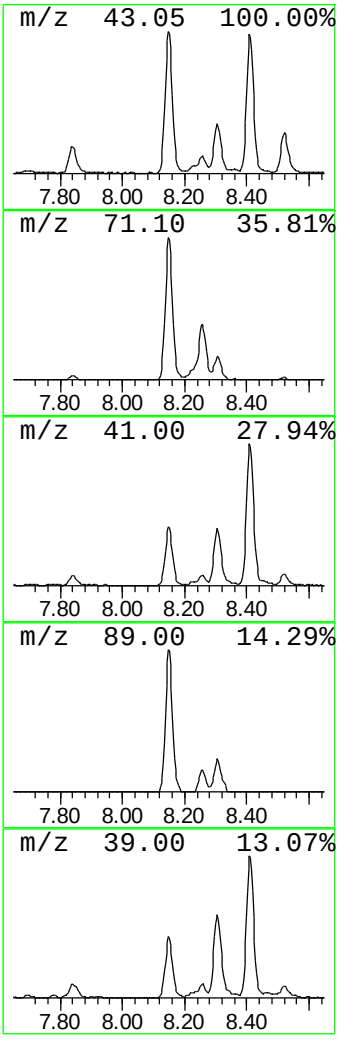
****

Peak Number 4 Propanoic acid, 2-methyl-, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.15	9.06 ug/L	126336	Chlorobenzene-d5	9.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
2	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
3	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
4	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64
5	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	56





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061819\
Data File : VU032822.D
Acq On : 18 Jun 2019 14:23
Operator : JC/SP
Sample : K3363-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JT8

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

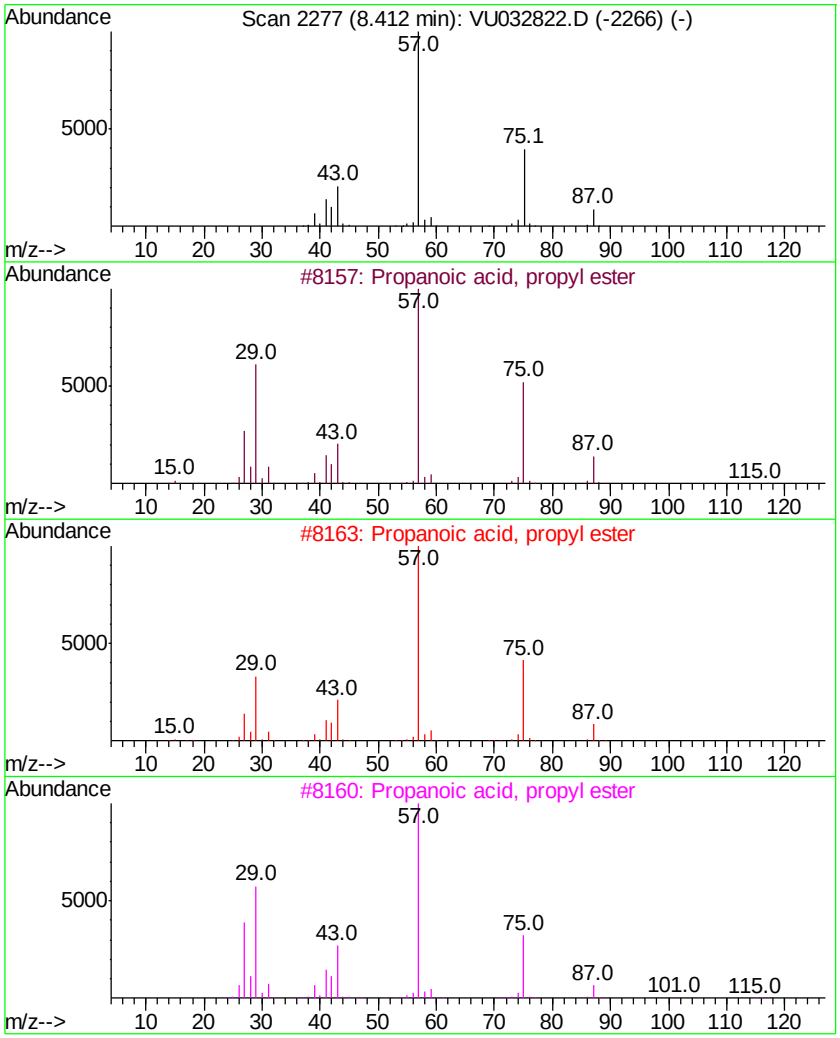
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

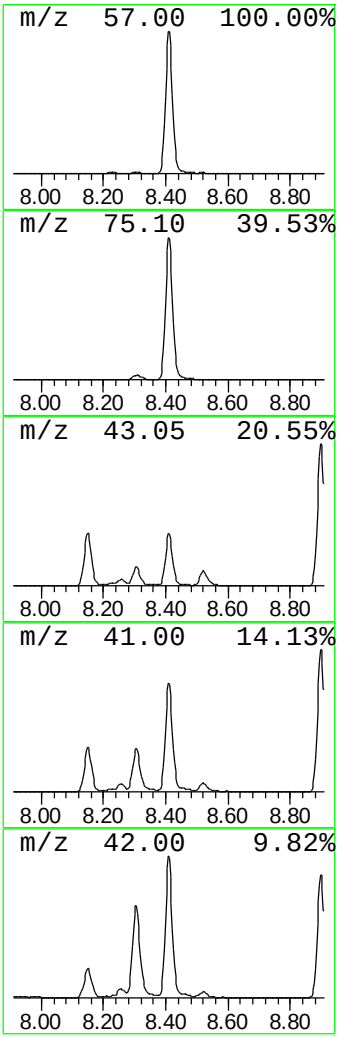
****

Peak Number 5 Propanoic acid, propyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.41	40.44 ug/L	563959	Chlorobenzene-d5	9.08

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





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061819\
Data File : VU032822.D
Acq On : 18 Jun 2019 14:23
Operator : JC/SP
Sample : K3363-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JT8

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

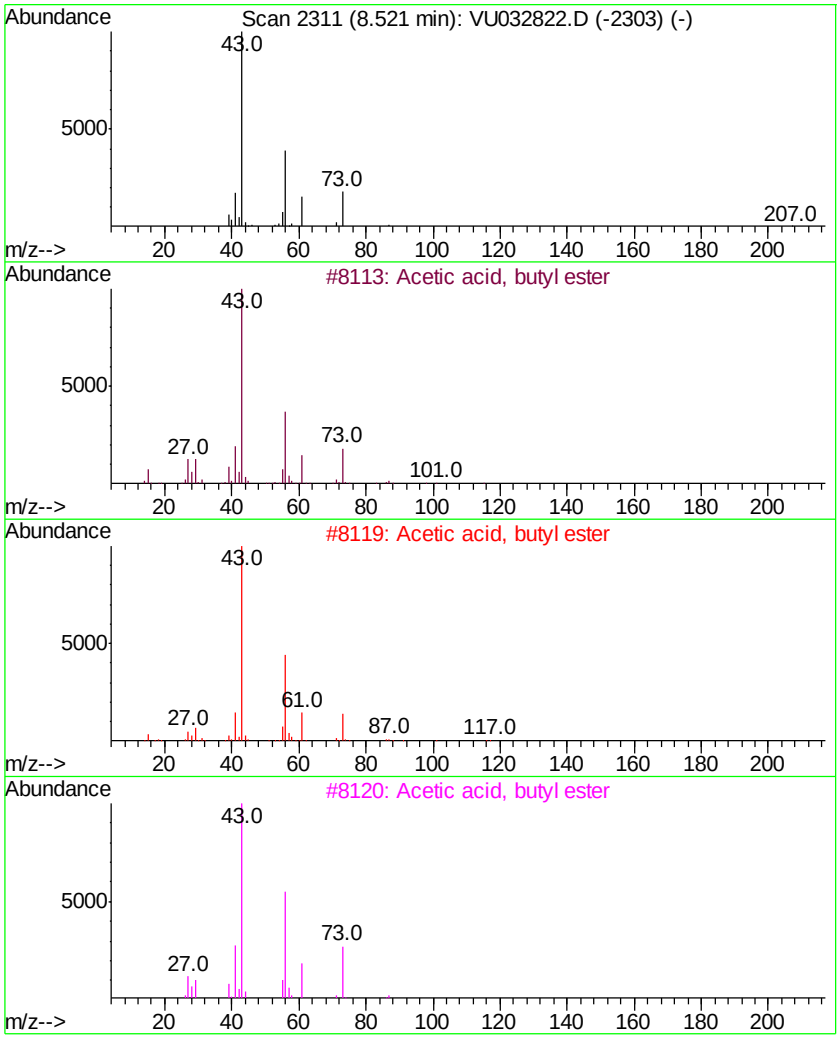
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

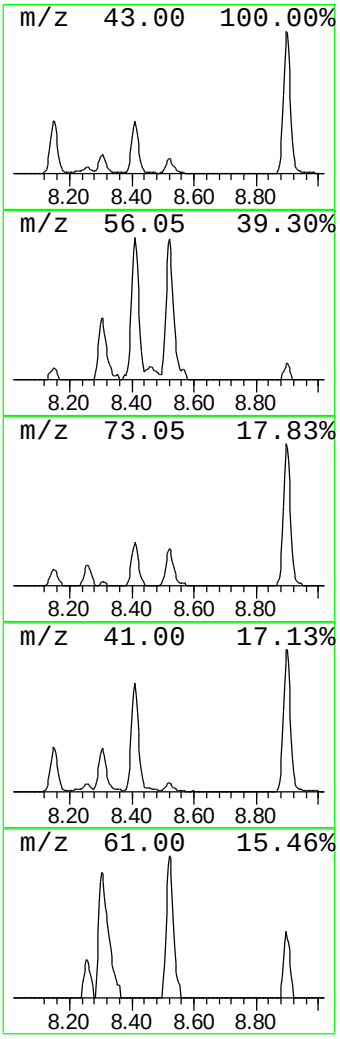
****

Peak Number 6 Acetic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.52	2.90 ug/L	40495	Chlorobenzene-d5	9.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78
2	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78
3	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	64
4	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	39
5	1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	17





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061819\
Data File : VU032822.D
Acq On : 18 Jun 2019 14:23
Operator : JC/SP
Sample : K3363-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JT8

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

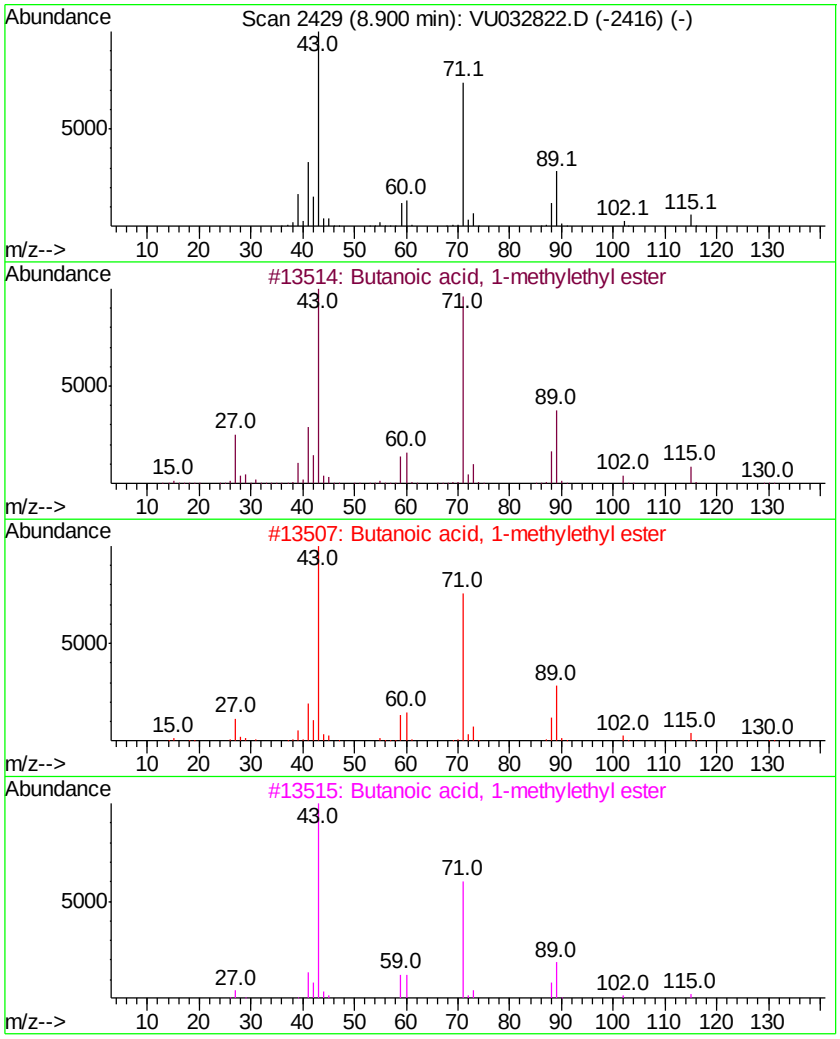
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

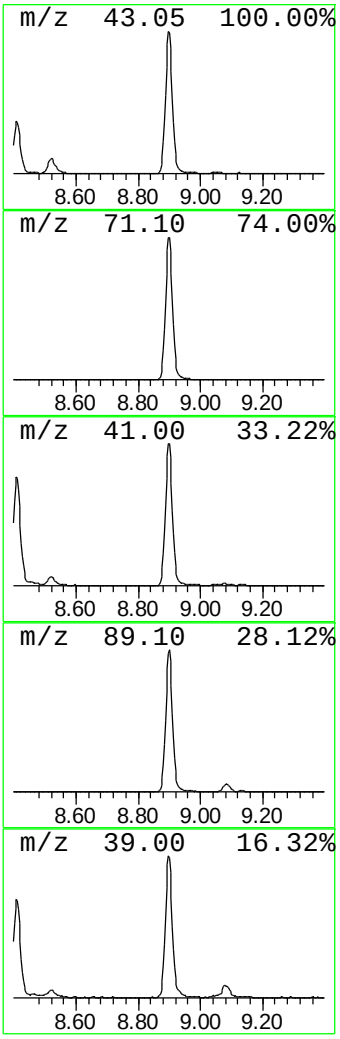
****

Peak Number 7 Butanoic acid, 1-methylethy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.90	34.37 ug/L	479379	Chlorobenzene-d5	9.08

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	83
4	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
5	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061819\
Data File : VU032822.D
Acq On : 18 Jun 2019 14:23
Operator : JC/SP
Sample : K3363-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JT8

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.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
n-Propyl acetate	6.70	105.3	ug/L	1131570	1	5.88	537200	50.0
Propanoic acid, 1...	7.41	21.3	ug/L	228631	1	5.88	537200	50.0
Propanoic acid, 2...	8.15	9.1	ug/L	126336	2	9.08	697284	50.0
Propanoic acid, p...	8.41	40.4	ug/L	563959	2	9.08	697284	50.0
Acetic acid, buty...	8.52	2.9	ug/L	40495	2	9.08	697284	50.0
Butanoic acid, 1-...	8.90	34.4	ug/L	479379	2	9.08	697284	50.0