LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061319\
Data File : VU032688.D
Acq On : 13 Jun 2019 12:50
Operator : JC/SP
Sample : K3286-11
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JP4

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\SOMULM060619WMA.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	35	rVB2	4990	4589	0.48%	0.066%
2	1.395	88	95	108	rBV	64453	67406	7.04%	0.967%
3	1.675	175	182	198	rVB	56564	69466	7.25%	0.997%
4	2.267	356	366	376	rBV	114405	172023	17.95%	2.469%
5	2.318	377	382	398	rVB	9850	15578	1.63%	0.224%
6	2.447	416	422	426	rBV3	692	872	0.09%	0.013%
7	2.514	439	443	449	rBV2	210	217	0.02%	0.003%
8	2.604	468	471	473	rBV	284	198	0.02%	0.003%
9	2.698	491	500	512	rVB2	7013	11425	1.19%	0.164%
10	3.096	621	624	630	rBV2	173	176	0.02%	0.003%
11	3.157	637	643	647	rBV2	230	242	0.03%	0.003%
12	3.254	670	673	677	rBV	222	168	0.02%	0.002%
13	3.418	720	724	730	rBV2	229	299	0.03%	0.004%
14	3.469	736	740	743	rBV2	150	160	0.02%	0.002%
15	3.563	764	769	773	rVB2	168	171	0.02%	0.002%
16	3.749	824	827	832	rBV2	182	164	0.02%	0.002%
17	4.003	902	906	913	rBV	331	402	0.04%	0.006%
18	4.093	928	934	937	rVB2	253	267	0.03%	0.004%
19	4.170	946	958	989	rBV	59516	158442	16.54%	2.274%
20	4.370	1017	1020	1026	rVB3	472	444	0.05%	0.006%
21	4.643	1088	1105	1129	rBV	95315	224247	23.40%	3.218%
22	4.804	1153	1155	1160	rVB2	419	242	0.03%	0.003%
23	4.894	1179	1183	1188	rVB3	301	306	0.03%	0.004%
24	4.971	1203	1207	1211	rBV2	224	180	0.02%	0.003%
25	4.993	1211	1214	1218	rBV2	251	234	0.02%	0.003%
26	5.048	1223	1231	1234	rBV2	228	299	0.03%	0.004%
27	5.138	1255	1259	1268	rBB2	197	277	0.03%	0.004%
28	5.228	1282	1287	1290	rBV2	215	184	0.02%	0.003%
29	5.334	1297	1320	1350	rBV2	183078	551150	57.52%	7.910%
30	5.553	1378	1388	1401	rBV3	3125	6861	0.72%	0.098%
31	5.681	1426	1428	1433	rVB2	300	239	0.02%	0.003%
32	5.797	1458	1464	1467	rBV2	338	410	0.04%	0.006%
33	5.881	1467	1490	1513	rBV	214589	453905	47.37%	6.515%
34	6.183	1574	1584	1602	rVB2	25740	52264	5.45%	0.750%

LSC Area Percent Report

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Acq On : 13 Jun 2019 12:50
Operator : JC/SP
Sample : K3286-11
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JP4

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\SOMULM060619WMA.M
Title : VOC Analysis

35	6.324	1615	1628	1650	rBV	126289	253923	26.50%	3.644%
36	6.424	1653	1659	1680	rVB2	5085	10223	1.07%	0.147%
37	6.530	1688	1692	1700	rBV4	1567	2391	0.25%	0.034%
38	6.579	1701	1707	1714	rBV	3282	5377	0.56%	0.077%
39	6.701	1733	1745	1777	rBV	527530	958147	100.00%	13.752%
40	7.006	1838	1840	1845	rVB4	497	243	0.03%	0.003%
41	7.048	1849	1853	1854	rBV3	251	185	0.02%	0.003%
42	7.225	1896	1908	1927	rBV	71909	130178	13.59%	1.868%
43	7.347	1943	1946	1949	rBV3	401	313	0.03%	0.004%
44	7.415	1955	1967	1994	rBV	95853	168743	17.61%	2.422%
45	7.559	2000	2012	2031	rBV	244958	427437	44.61%	6.135%
46	7.791	2082	2084	2086	rBV2	474	319	0.03%	0.005%
47	7.845	2090	2101	2124	rVV2	54985	98520	10.28%	1.414%
48	8.006	2148	2151	2154	rBV3	208	179	0.02%	0.003%
49	8.151	2185	2196	2211	rBV	48484	81062	8.46%	1.163%
50	8.228	2211	2220	2224	rBV5	13069	20582	2.15%	0.295%
51	8.305	2235	2244	2266	rVV	199735	341224	35.61%	4.897%
52	8.411	2267	2277	2305	rVV	321558	520246	54.30%	7.467%
53	8.524	2305	2312	2329	rVB	16866	29143	3.04%	0.418%
54	8.813	2398	2402	2405	rVB2	366	258	0.03%	0.004%
55	8.829	2405	2407	2411	rBV2	278	225	0.02%	0.003%
56	8.900	2414	2429	2452	rBV	207803	334821	34.94%	4.805%
57	9.083	2471	2486	2514	rBV	310149	519180	54.19%	7.451%
58	9.263	2539	2542	2545	rBV3	255	171	0.02%	0.002%
59	9.324	2557	2561	2563	rBV2	295	165	0.02%	0.002%
60	9.373	2569	2576	2578	rBV2	396	343	0.04%	0.005%
61	9.411	2584	2588	2591	rBV	203	195	0.02%	0.003%
62	9.498	2612	2615	2620	rBV2	269	276	0.03%	0.004%
63	9.527	2621	2624	2628	rVB	286	231	0.02%	0.003%
64	9.553	2628	2632	2635	rBV	311	230	0.02%	0.003%
65	9.614	2643	2651	2663	rVV4	1891	3448	0.36%	0.049%
66	9.768	2691	2699	2709	rBV2	6144	10926	1.14%	0.157%
67	9.848	2721	2724	2727	rBV	235	160	0.02%	0.002%
68	10.276	2855	2857	2861	rVB3	275	193	0.02%	0.003%
69	10.315	2861	2869	2871	rBV	223	231	0.02%	0.003%
70	10.427	2892	2904	2928	rBV	196188	319067	33.30%	4.579%
71	10.511	2928	2930	2933	rVB2	324	186	0.02%	0.003%

LSC Area Percent Report

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Acq On : 13 Jun 2019 12:50
Operator : JC/SP
Sample : K3286-11
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JP4

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\SOMULM060619WMA.M
Title : VOC Analysis

72	10.623	2960	2965	2970	rBV2	187	207	0.02%	0.003%
73	10.813	3018	3024	3028	rBV2	175	182	0.02%	0.003%
74	10.958	3060	3069	3071	rBV2	233	325	0.03%	0.005%
75	11.048	3093	3097	3101	rBV3	307	288	0.03%	0.004%
76	11.141	3120	3126	3129	rBV2	257	265	0.03%	0.004%
77	11.209	3145	3147	3153	rVB2	296	212	0.02%	0.003%
78	11.244	3153	3158	3159	rBV	191	169	0.02%	0.002%
79	11.479	3219	3231	3258	rBV	305934	495951	51.76%	7.118%
80	11.688	3292	3296	3299	rVB3	274	191	0.02%	0.003%
81	11.736	3307	3311	3313	rBV	336	216	0.02%	0.003%
82	11.797	3328	3330	3334	rBV2	194	181	0.02%	0.003%
83	11.855	3336	3348	3378	rVV	260004	432735	45.16%	6.211%
84	12.376	3507	3510	3515	rVB2	164	157	0.02%	0.002%
85	12.504	3546	3550	3563	rVB2	412	515	0.05%	0.007%
86	12.700	3608	3611	3615	rBV	203	163	0.02%	0.002%
87	12.749	3624	3626	3630	rBV	210	164	0.02%	0.002%
88	12.829	3646	3651	3656	rBV2	166	231	0.02%	0.003%
89	12.874	3662	3665	3671	rVB2	386	324	0.03%	0.005%
90	12.964	3690	3693	3697	rVB3	217	184	0.02%	0.003%
91	13.106	3734	3737	3741	rBV	296	182	0.02%	0.003%
92	13.643	3900	3904	3908	rVB	295	311	0.03%	0.004%
93	13.874	3974	3976	3982	rVB	286	233	0.02%	0.003%
94	13.906	3983	3986	3988	rBV	232	164	0.02%	0.002%
95	13.951	3996	4000	4002	rBV2	301	245	0.03%	0.004%
96	13.993	4011	4013	4016	rBV	234	171	0.02%	0.002%
97	14.250	4088	4093	4095	rBV	286	275	0.03%	0.004%
98	14.318	4110	4114	4118	rBV2	325	306	0.03%	0.004%
99	14.491	4163	4168	4175	rBV3	362	580	0.06%	0.008%
100	14.761	4250	4252	4255	rBV	254	183	0.02%	0.003%

Sum of corrected areas: 6967558

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061319\
Data File : VU032688.D
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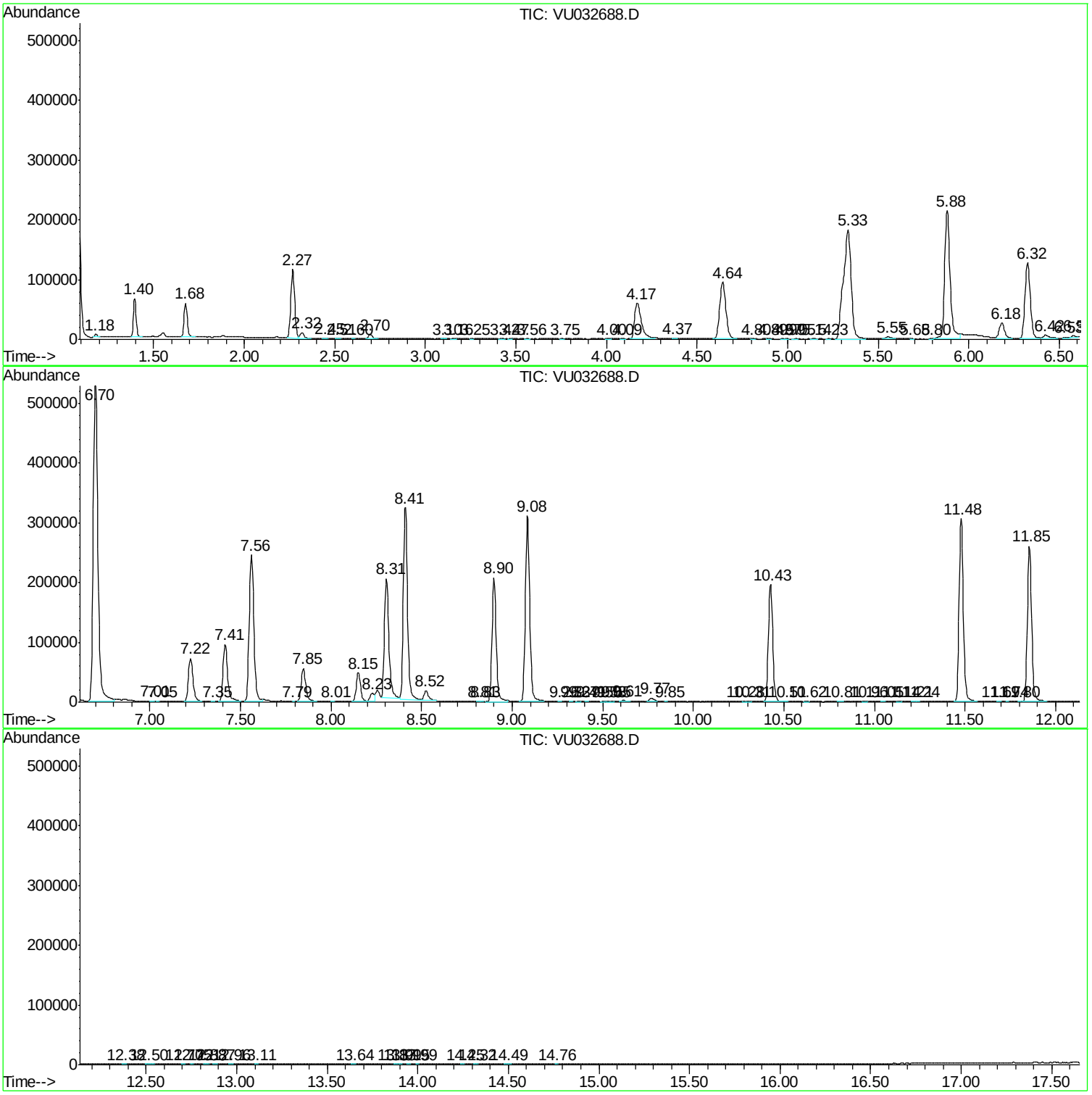
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JP4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.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\VU061319\
Data File : VU032688.D
Acq On : 13 Jun 2019 12:50
Operator : JC/SP
Sample : K3286-11
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JP4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

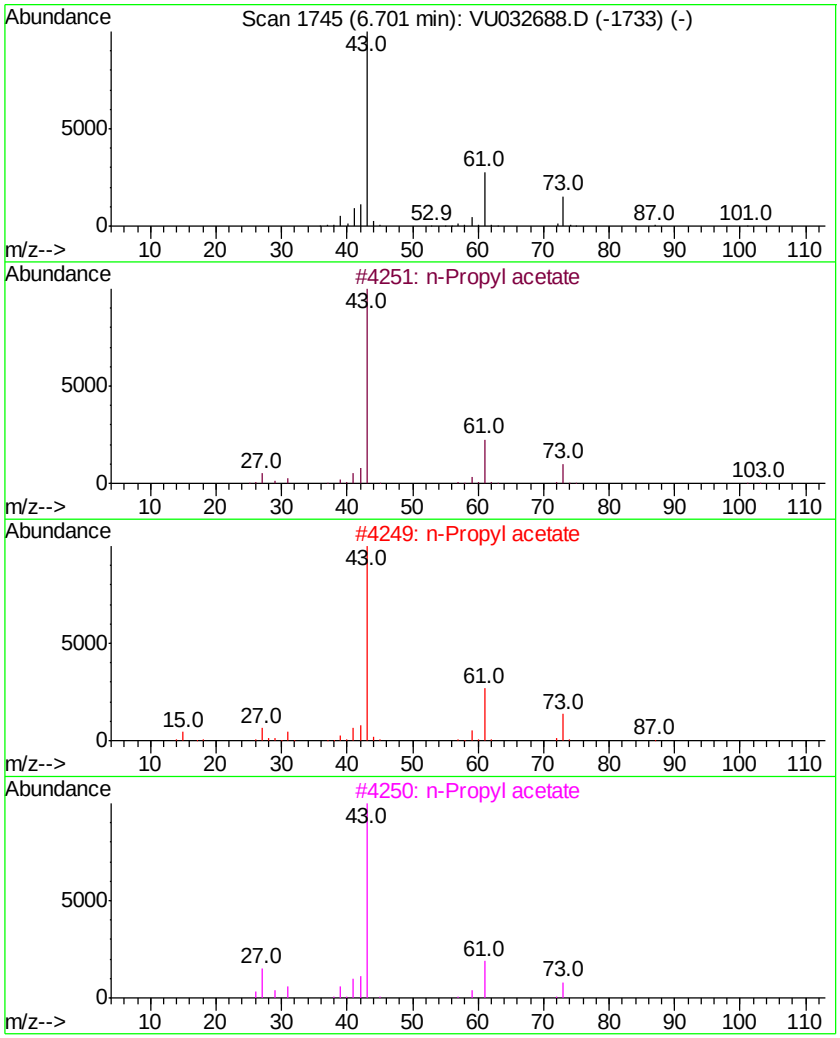
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

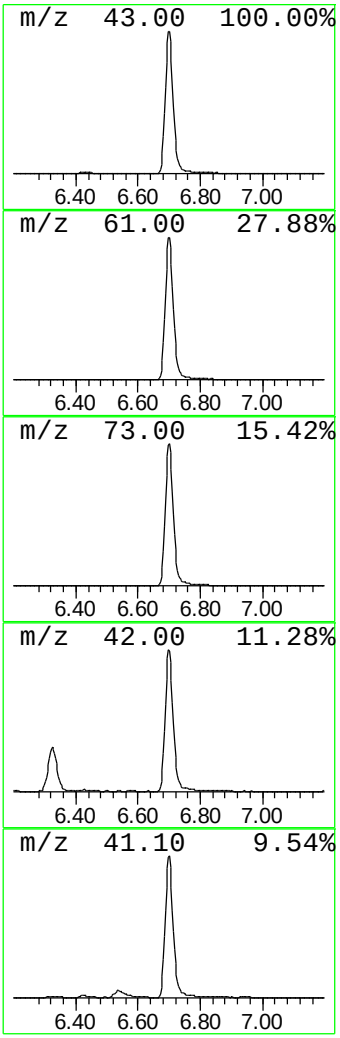
****

Peak Number 1 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	105.55 ug/L	958147	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	Isobutyl acetate	116	C6H12O2	000110-19-0	9





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061319\
Data File : VU032688.D
Acq On : 13 Jun 2019 12:50
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ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JP4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

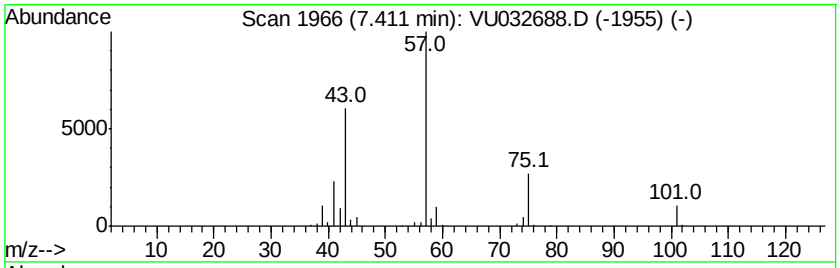
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

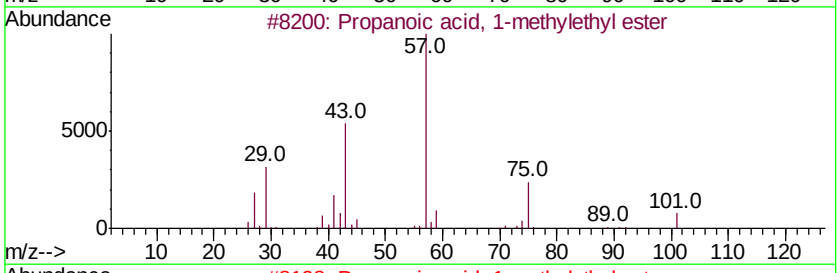
****

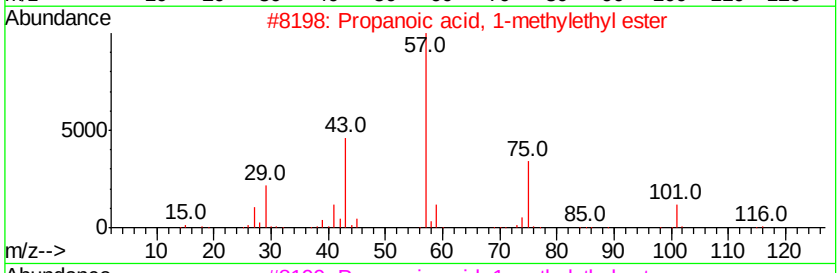
Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 4

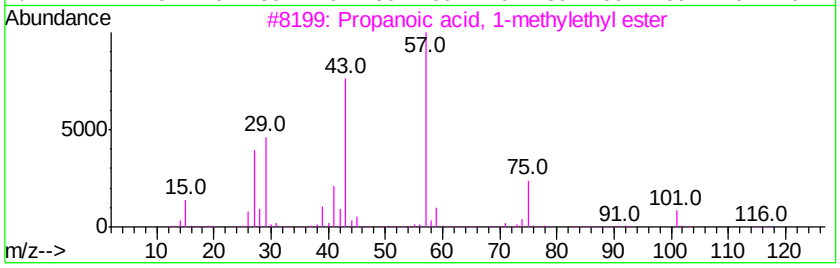
R.T.	EstConc	Area	Relative to ISTD	R.T.
7.41	18.59 ug/L	168743	1,4-Difluorobenzene	5.88

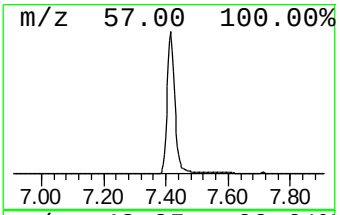
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	90
2	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	78
3	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	74
4	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	59
5	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	45

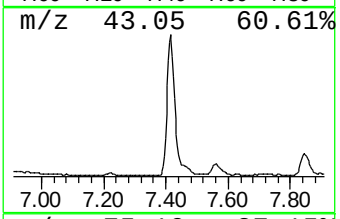


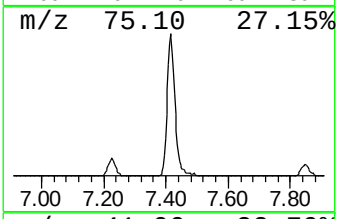


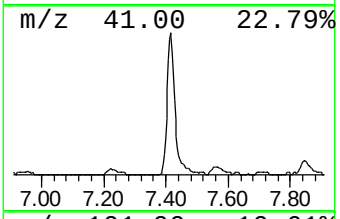


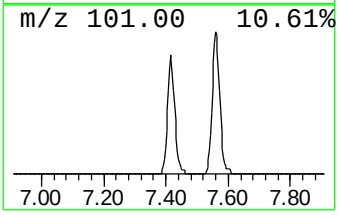












Library Search Compound Report

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Data File : VU032688.D
Acq On : 13 Jun 2019 12:50
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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JP4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

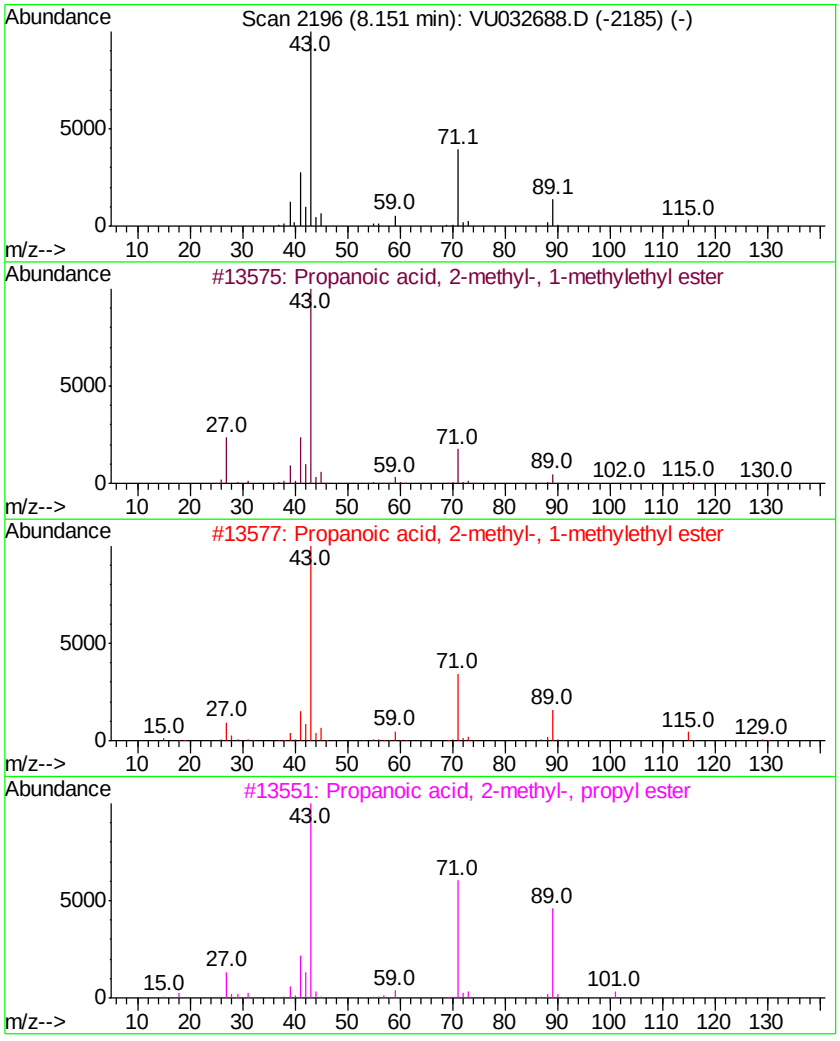
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

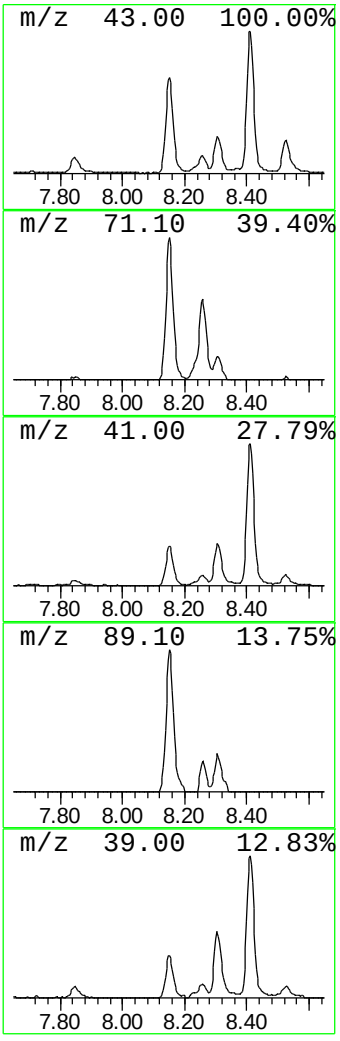
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.15	7.81 ug/L	81062	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-, propy...	130	C7H14O2	000644-49-5	78
4	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	64
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061319\
Data File : VU032688.D
Acq On : 13 Jun 2019 12:50
Operator : JC/SP
Sample : K3286-11
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JP4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

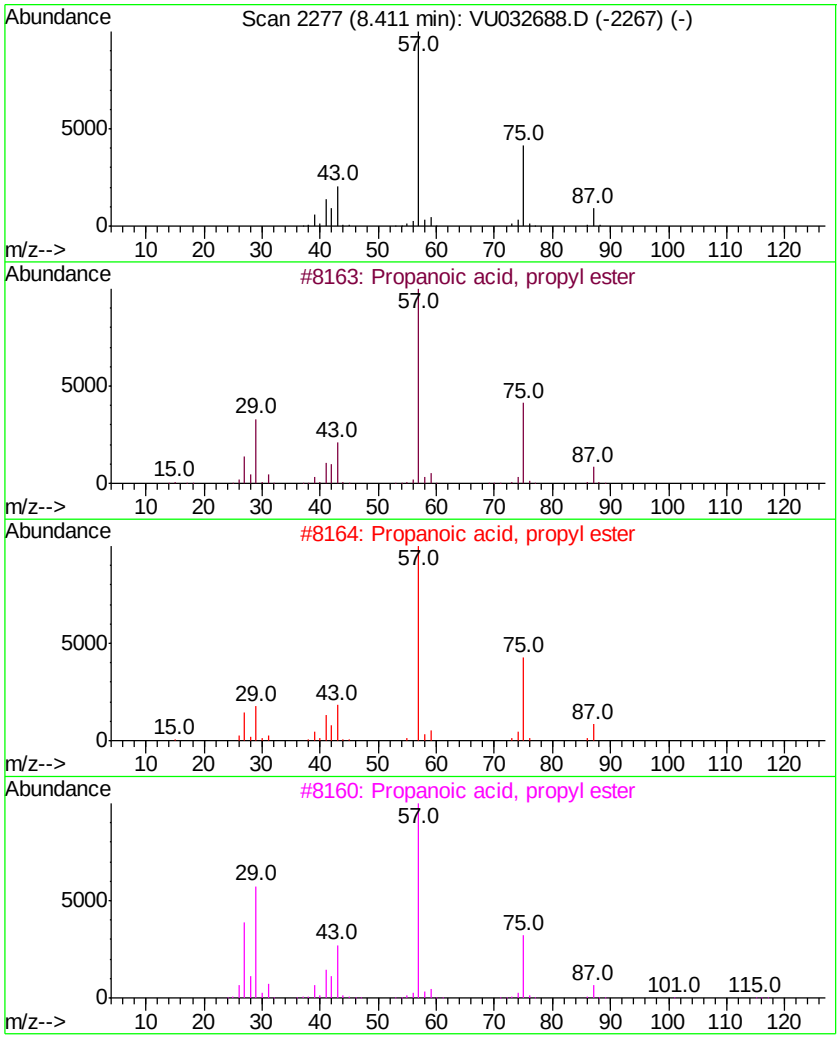
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

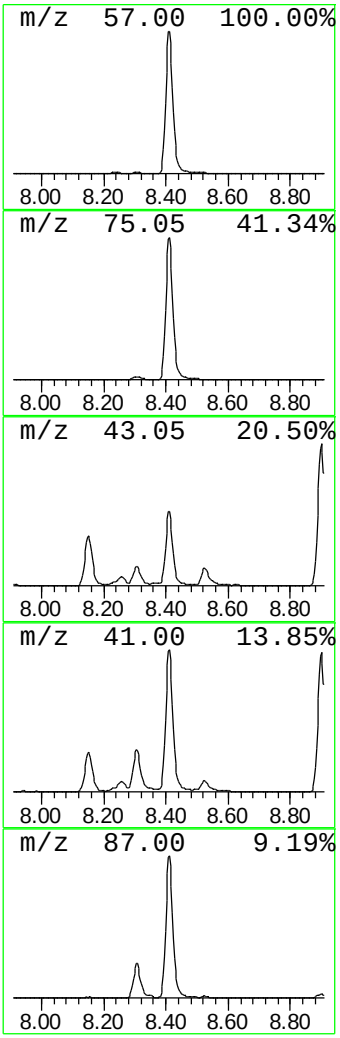
****

Peak Number 5 Propanoic acid, propyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.41	50.10 ug/L	520246	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	83
5	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	39





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061319\
Data File : VU032688.D
Acq On : 13 Jun 2019 12:50
Operator : JC/SP
Sample : K3286-11
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JP4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

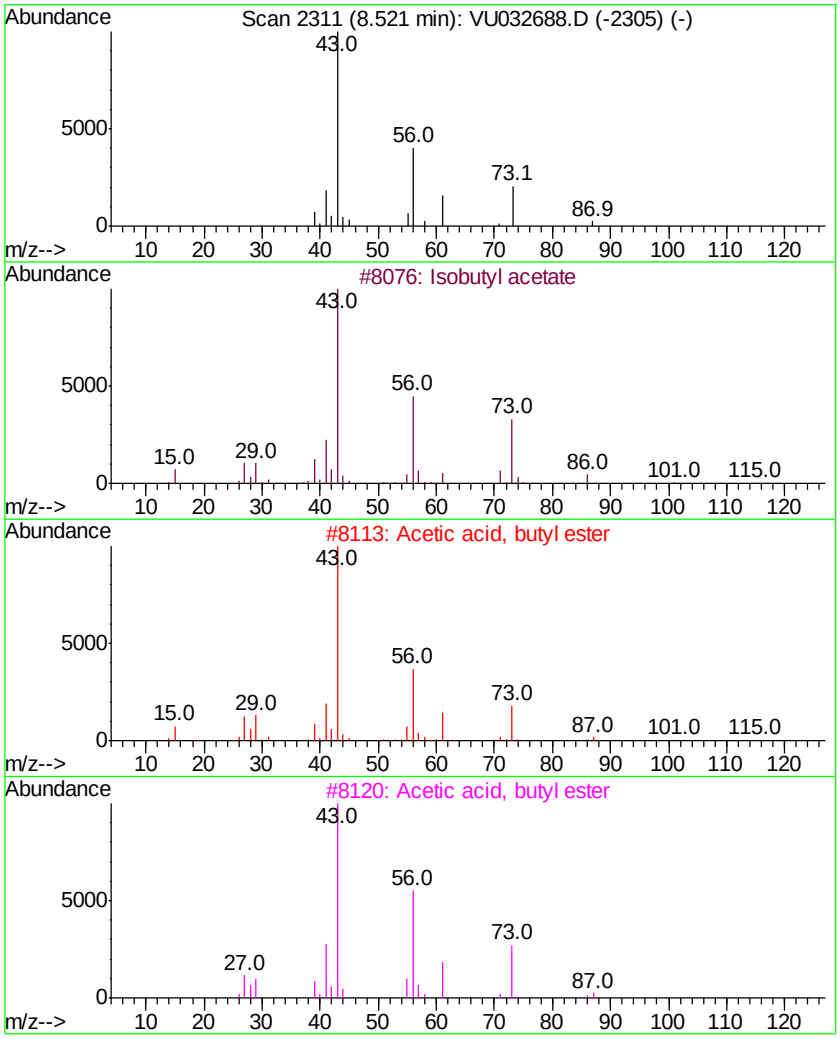
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

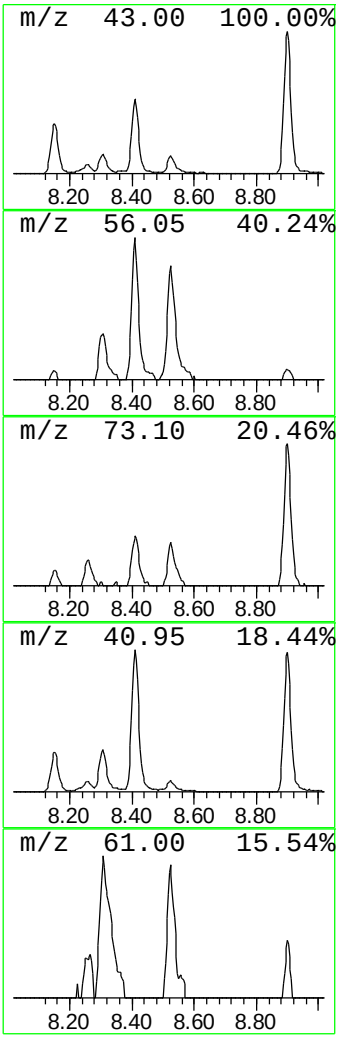
****

Peak Number 6 Isobutyl acetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.52	2.81 ug/L	29143	Chlorobenzene-d5	9.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutyl acetate	116	C6H12O2	000110-19-0	78
2	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78
3	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
4	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	40
5	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	39





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061319\
Data File : VU032688.D
Acq On : 13 Jun 2019 12:50
Operator : JC/SP
Sample : K3286-11
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JP4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

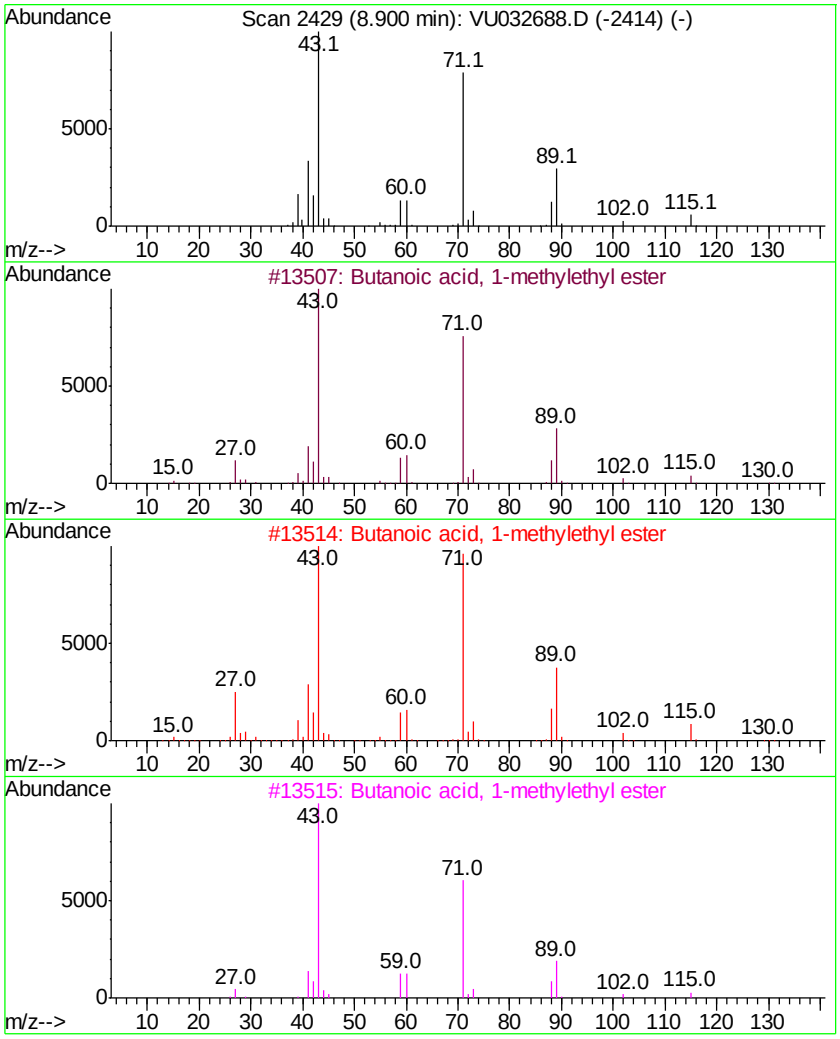
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

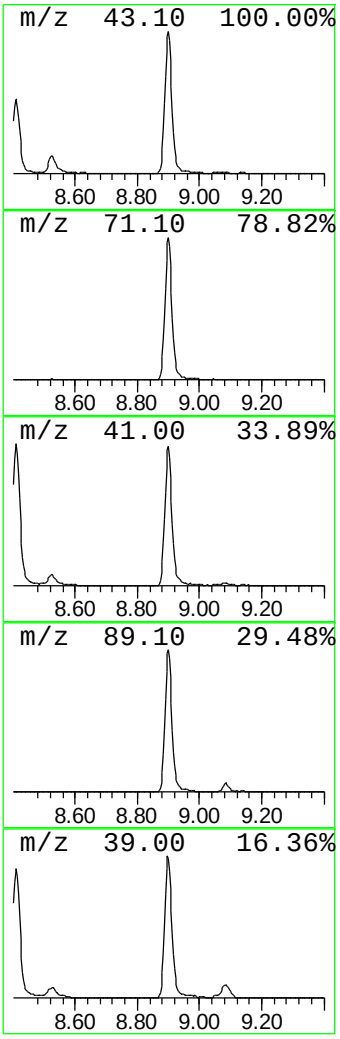
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.90	32.25 ug/L	334821	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-, propy...	130	C7H14O2	000644-49-5	72
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061319\
Data File : VU032688.D
Acq On : 13 Jun 2019 12:50
Operator : JC/SP
Sample : K3286-11
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JP4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.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	105.6	ug/L	958147	1	5.88	453905	50.0
Propanoic acid, 1...	7.41	18.6	ug/L	168743	1	5.88	453905	50.0
Propanoic acid, 2...	8.15	7.8	ug/L	81062	2	9.08	519180	50.0
Propanoic acid, p...	8.41	50.1	ug/L	520246	2	9.08	519180	50.0
Isobutyl acetate	8.52	2.8	ug/L	29143	2	9.08	519180	50.0
Butanoic acid, 1-...	8.90	32.3	ug/L	334821	2	9.08	519180	50.0