LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU102619\
Data File : VU035521.D
Acq On : 26 Oct 2019 16:21
Operator : JC/SP
Sample : K5536-01
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BEK31

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\SOMULM102619WMA.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	1.373	4	10	26	rBV	44062	57573	1.57%	0.198%
2	1.610	77	84	100	rVB	346771	386265	10.52%	1.326%
3	1.932	176	184	204	rVB	274669	358070	9.75%	1.230%
4	2.594	377	390	407	rBV	498735	810166	22.06%	2.782%
5	2.697	413	422	455	rVB2	26854	86341	2.35%	0.296%
6	3.083	532	542	563	rVB	48659	95805	2.61%	0.329%
7	3.228	579	587	588	rBV7	5177	5097	0.14%	0.018%
8	3.324	614	617	620	rBV2	775	541	0.01%	0.002%
9	3.385	631	636	638	rBV4	1268	1110	0.03%	0.004%
10	3.553	683	688	691	rBV3	341	304	0.01%	0.001%
11	3.704	731	735	738	rVB4	397	254	0.01%	0.001%
12	3.726	738	742	744	rBV3	555	360	0.01%	0.001%
13	3.813	764	769	772	rVB2	370	340	0.01%	0.001%
14	3.864	783	785	789	rVV2	700	495	0.01%	0.002%
15	3.958	811	814	816	rBV2	407	317	0.01%	0.001%
16	4.041	836	840	843	rVB	477	274	0.01%	0.001%
17	4.141	868	871	872	rBV	481	265	0.01%	0.001%
18	4.199	884	889	891	rBV2	449	437	0.01%	0.002%
19	4.231	891	899	902	rBV4	1355	1576	0.04%	0.005%
20	4.408	951	954	961	rVB4	771	864	0.02%	0.003%
21	4.462	967	971	975	rBV2	844	642	0.02%	0.002%
22	4.524	985	990	992	rVB	426	310	0.01%	0.001%
23	4.559	997	1001	1002	rBV	603	398	0.01%	0.001%
24	4.578	1002	1007	1008	rBV2	673	587	0.02%	0.002%
25	4.614	1016	1018	1024	rVB2	537	411	0.01%	0.001%
26	4.710	1031	1048	1097	rBV	186928	670034	18.25%	2.301%
27	4.983	1131	1133	1138	rVB3	604	368	0.01%	0.001%
28	5.115	1156	1174	1193	rBV	424835	933695	25.43%	3.206%
29	5.331	1234	1241	1242	rBV4	1822	1596	0.04%	0.005%
30	5.388	1254	1259	1261	rBV2	384	314	0.01%	0.001%
31	5.430	1261	1272	1282	rVB8	3399	7146	0.19%	0.025%
32	5.498	1290	1293	1296	rVB2	666	466	0.01%	0.002%
33	5.565	1310	1314	1315	rBV2	439	261	0.01%	0.001%
34	5.594	1319	1323	1327	rBV4	424	322	0.01%	0.001%

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Sample : K5536-01
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BEK31

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\SOMULM102619WMA.M
Title : VOC Analysis

35	5.646	1334	1339	1343	rBV2	625	636	0.02%	0.002%
36	5.771	1356	1378	1407	rBV2	957864	2461080	67.03%	8.451%
37	5.974	1428	1441	1462	rBV2	107153	223434	6.09%	0.767%
38	6.179	1470	1505	1508	rBV3	101575	486023	13.24%	1.669%
39	6.292	1531	1540	1604	rVB	977109	2506283	68.26%	8.606%
40	6.736	1663	1678	1696	rBV	566189	1115813	30.39%	3.832%
41	6.993	1748	1758	1775	rVB2	44415	100529	2.74%	0.345%
42	7.093	1775	1789	1823	rBV	1947068	3671808	100.00%	12.609%
43	7.604	1935	1948	1974	rBV	312098	569063	15.50%	1.954%
44	7.784	1993	2004	2016	rBV	269923	459437	12.51%	1.578%
45	7.935	2037	2051	2066	rBV	1130664	1972119	53.71%	6.772%
46	8.215	2124	2138	2164	rBV2	253893	489343	13.33%	1.680%
47	8.507	2216	2229	2247	rBV	414594	700894	19.09%	2.407%
48	8.613	2248	2262	2271	rVV3	58711	134000	3.65%	0.460%
49	8.681	2271	2283	2300	rVV2	777453	1551009	42.24%	5.326%
50	8.768	2301	2310	2332	rVB	710984	1195531	32.56%	4.105%
51	9.147	2425	2428	2434	rBV5	661	598	0.02%	0.002%
52	9.250	2447	2460	2496	rBV	861348	1403743	38.23%	4.820%
53	9.449	2501	2522	2558	rVV	1128317	2011223	54.77%	6.906%
54	9.601	2561	2569	2580	rVB2	11690	17845	0.49%	0.061%
55	9.723	2598	2607	2619	rVB	35735	58897	1.60%	0.202%
56	9.877	2651	2655	2660	rBV5	994	1205	0.03%	0.004%
57	9.954	2669	2679	2701	rBV	23491	42783	1.17%	0.147%
58	10.109	2715	2727	2746	rBV2	75598	158838	4.33%	0.545%
59	10.195	2752	2754	2759	rVB3	603	374	0.01%	0.001%
60	10.227	2761	2764	2768	rBV4	757	777	0.02%	0.003%
61	10.276	2771	2779	2791	rBV3	5286	9154	0.25%	0.031%
62	10.417	2820	2823	2826	rBV3	454	409	0.01%	0.001%
63	10.446	2829	2832	2835	rVB	617	316	0.01%	0.001%
64	10.462	2835	2837	2840	rBV3	558	364	0.01%	0.001%
65	10.510	2848	2852	2858	rVB5	1830	2065	0.06%	0.007%
66	10.572	2868	2871	2877	rVB4	963	992	0.03%	0.003%
67	10.607	2878	2882	2885	rBV3	881	747	0.02%	0.003%
68	10.726	2917	2919	2924	rBV4	479	359	0.01%	0.001%
69	10.787	2924	2938	2958	rBV	721570	1202551	32.75%	4.129%
70	11.022	3004	3011	3012	rBV5	1668	1566	0.04%	0.005%
71	11.115	3032	3040	3052	rVV4	4283	6582	0.18%	0.023%

LSC Area Percent Report

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ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BEK31

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\SOMULM102619WMA.M
Title : VOC Analysis

72	11.269	3082	3088	3093	rBV5	1422	2077	0.06%	0.007%
73	11.494	3149	3158	3165	rBV2	8409	12030	0.33%	0.041%
74	11.552	3174	3176	3179	rBV2	575	290	0.01%	0.001%
75	11.649	3203	3206	3210	rVB	850	511	0.01%	0.002%
76	11.671	3210	3213	3215	rBV	361	249	0.01%	0.001%
77	11.716	3223	3227	3230	rBV3	656	497	0.01%	0.002%
78	11.777	3234	3246	3252	rBV9	3239	5866	0.16%	0.020%
79	11.838	3252	3265	3281	rVB	941991	1561301	42.52%	5.361%
80	11.919	3286	3290	3297	rVB5	2180	2489	0.07%	0.009%
81	12.073	3336	3338	3339	rBV	552	284	0.01%	0.001%
82	12.218	3368	3383	3400	rBV	908940	1513838	41.23%	5.198%
83	12.420	3443	3446	3448	rBV4	484	260	0.01%	0.001%
84	12.481	3463	3465	3469	rVV2	719	424	0.01%	0.001%
85	12.510	3469	3474	3480	rVB5	1078	1175	0.03%	0.004%
86	12.549	3484	3486	3487	rBV2	705	295	0.01%	0.001%
87	12.903	3591	3596	3599	rBV4	917	1119	0.03%	0.004%
88	13.038	3634	3638	3640	rBV3	1133	1000	0.03%	0.003%
89	13.186	3682	3684	3690	rVB4	813	601	0.02%	0.002%
90	13.240	3695	3701	3712	rVB5	4193	6467	0.18%	0.022%
91	13.288	3712	3716	3718	rBV3	428	322	0.01%	0.001%
92	13.366	3734	3740	3744	rBV3	602	843	0.02%	0.003%
93	13.588	3805	3809	3810	rBV	641	477	0.01%	0.002%
94	13.616	3815	3818	3821	rBV3	671	502	0.01%	0.002%
95	13.716	3845	3849	3851	rBV4	837	752	0.02%	0.003%
96	13.806	3875	3877	3883	rVB4	805	604	0.02%	0.002%
97	13.867	3888	3896	3903	rBV5	3371	5243	0.14%	0.018%
98	14.108	3964	3971	3981	rVB2	8345	12749	0.35%	0.044%
99	14.353	4041	4047	4054	rVB8	3148	4319	0.12%	0.015%
100	14.716	4151	4160	4164	rBV9	1701	3052	0.08%	0.010%

Sum of corrected areas: 29121030

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU102619\
Data File : VU035521.D
Acq On : 26 Oct 2019 16:21
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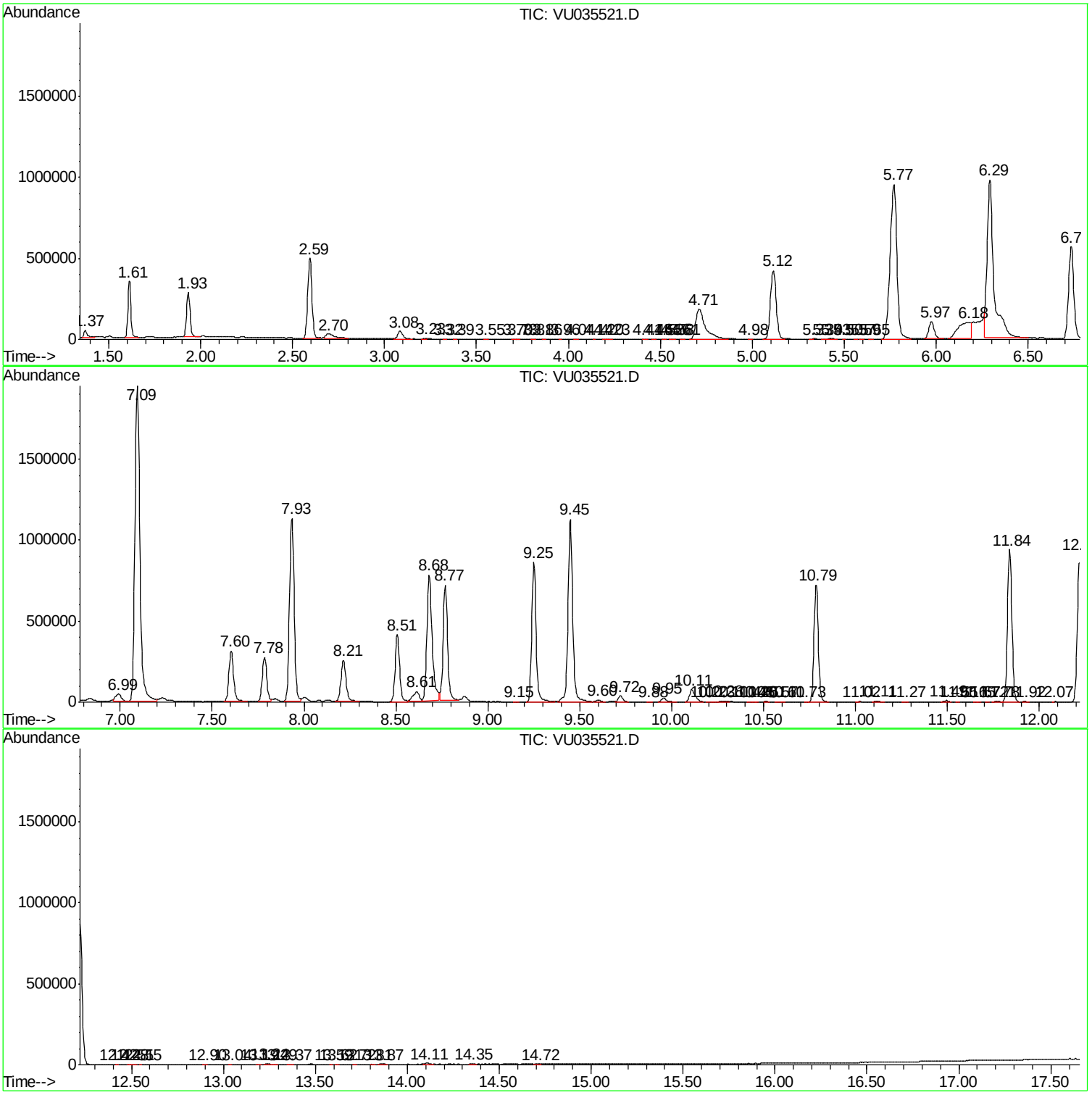
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BEK31

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102619WMA.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\VU102619\
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Quant Title : VOC Analysis

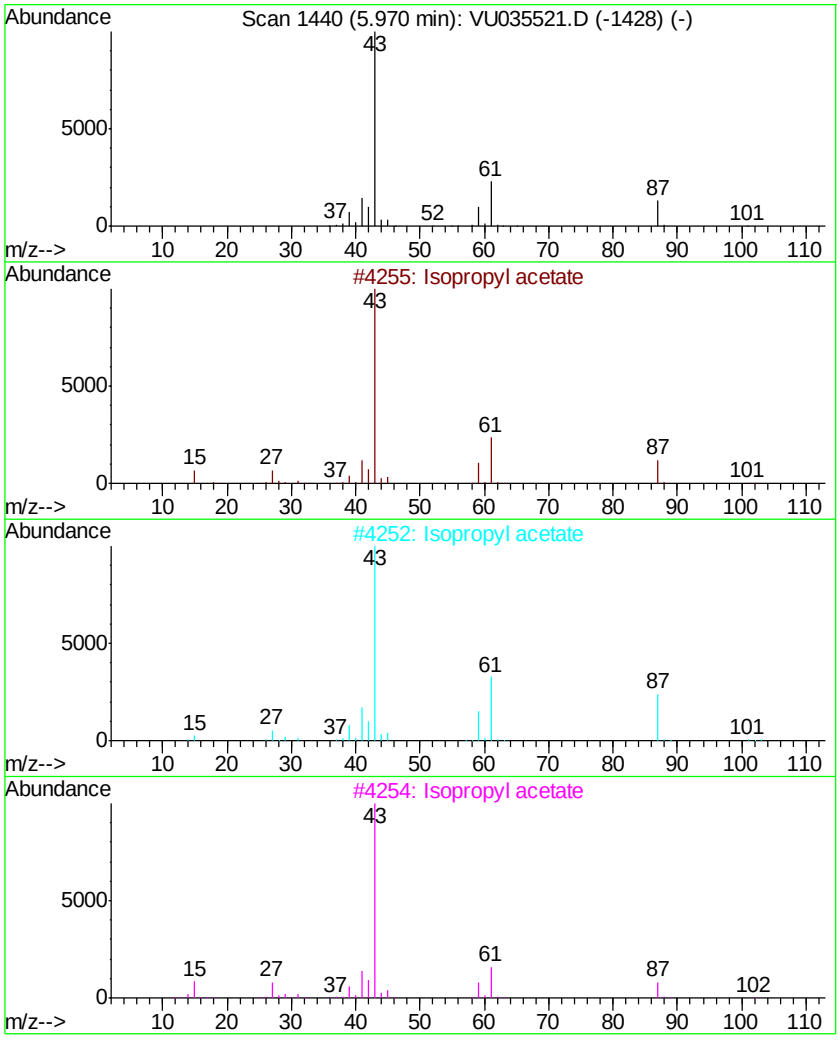
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

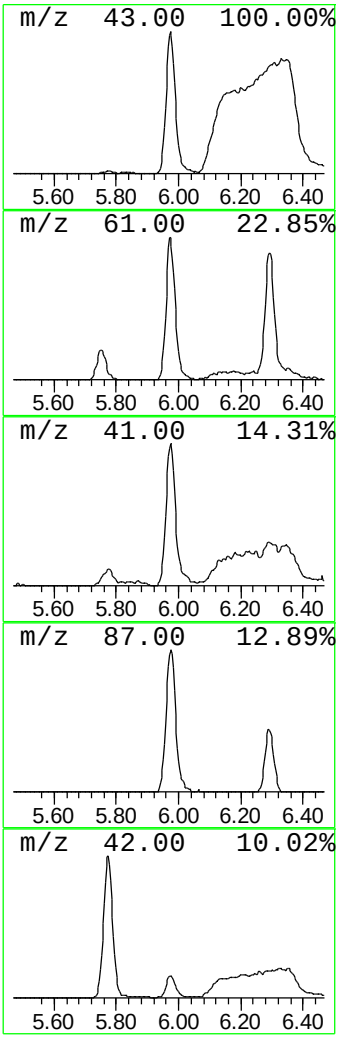
****

Peak Number 1 Isopropyl acetate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.97	4.46 ug/L	223434	1,4-Difluorobenzene	6.29

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	64
3	Isopropyl acetate	102	C5H10O2	000108-21-4	50
4	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	25
5	Acetaldehyde, O-ethyloxime-	87	C4H9NO	1000288-34-6	16





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU102619\
Data File : VU035521.D
Acq On : 26 Oct 2019 16:21
Operator : JC/SP
Sample : K5536-01
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BEK31

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102619WMA.M
Quant Title : VOC Analysis

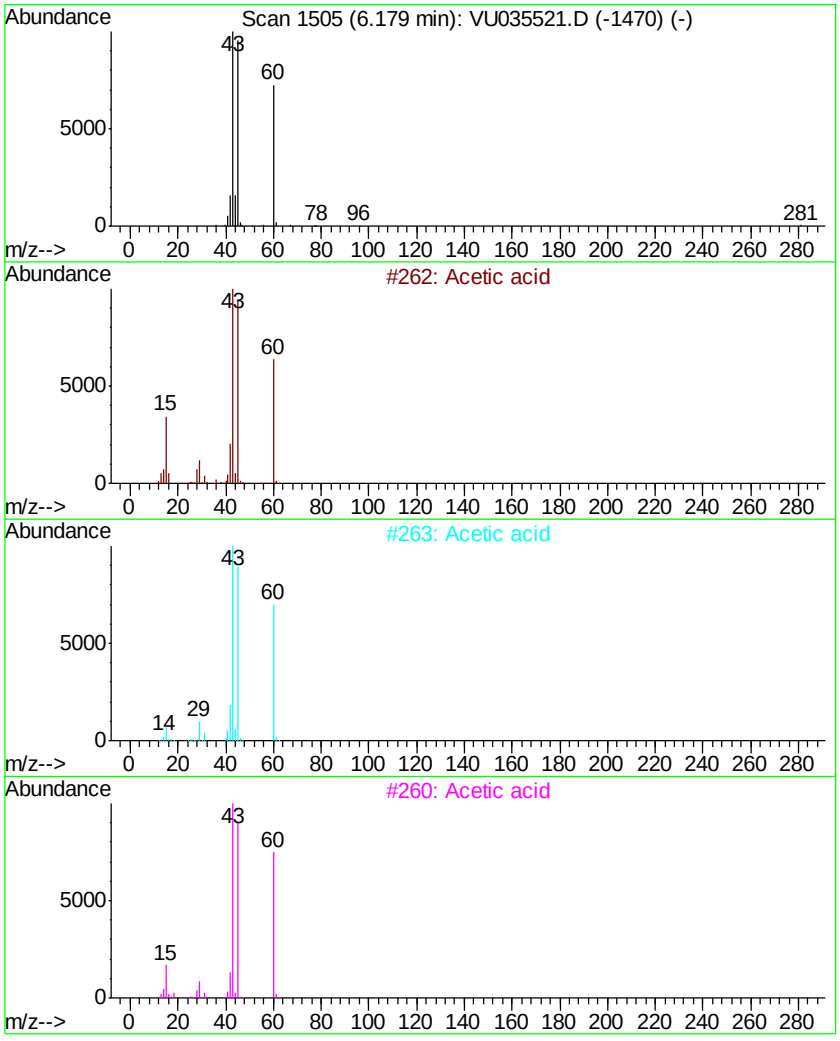
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

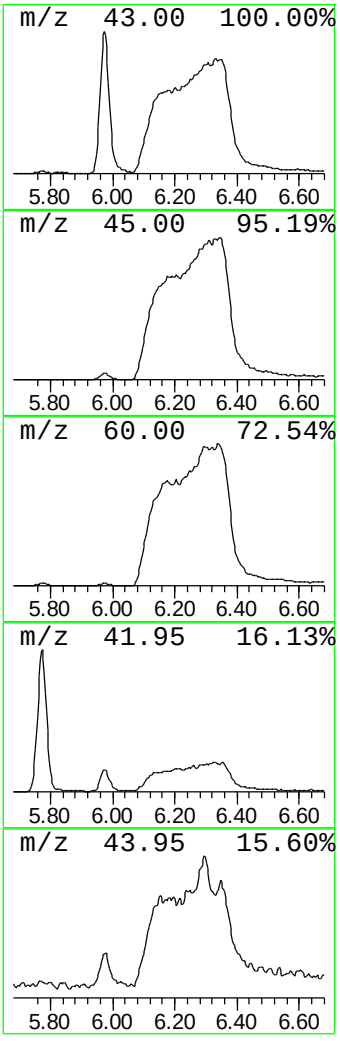
****

Peak Number 2 Acetic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.18	9.70 ug/L	486023	1,4-Difluorobenzene	6.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid	60	C2H4O2	000064-19-7	90
2	Acetic acid	60	C2H4O2	000064-19-7	90
3	Acetic acid	60	C2H4O2	000064-19-7	86
4	Acetic acid	60	C2H4O2	000064-19-7	86
5	Acetic acid	60	C2H4O2	000064-19-7	78





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ClientSampleId : BEK31

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102619WMA.M
Quant Title : VOC Analysis

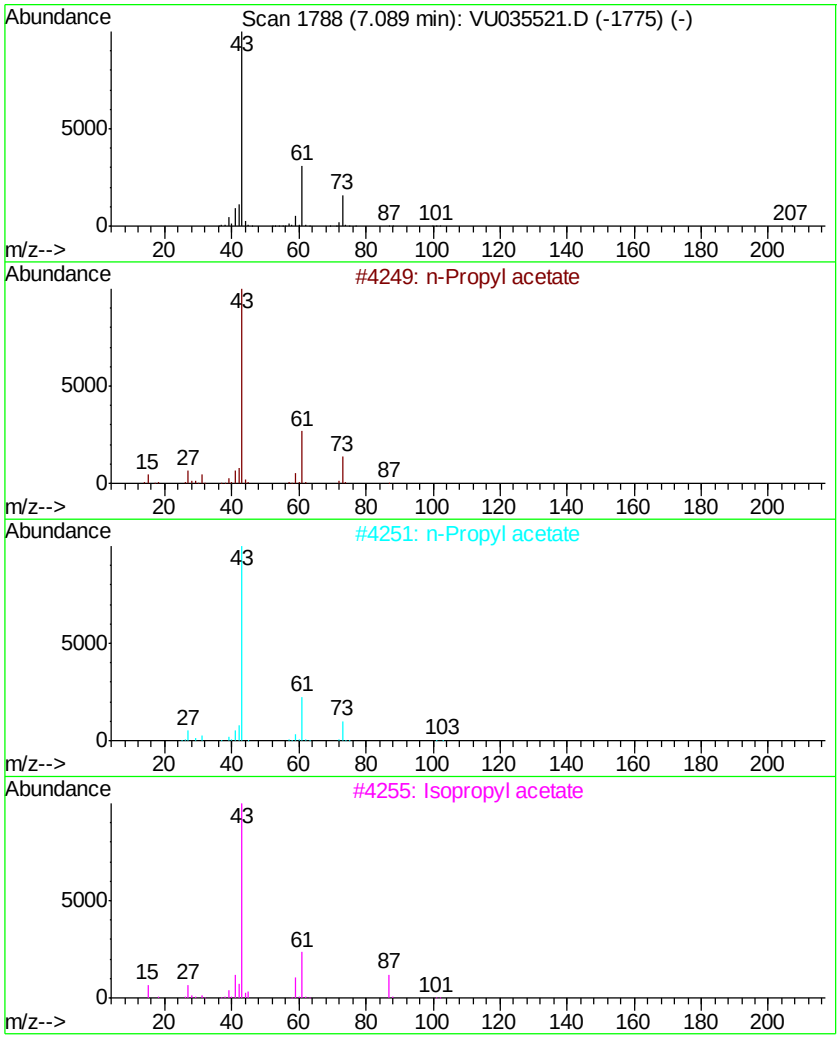
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

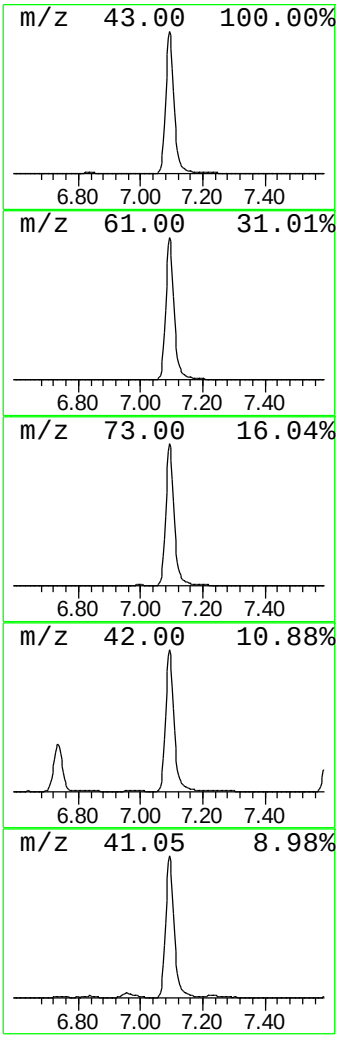
****

Peak Number 3 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.09	73.25 ug/L	3671810	1,4-Difluorobenzene	6.29

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	83
3	Isopropyl acetate	102	C5H10O2	000108-21-4	36
4	n-Propyl acetate	102	C5H10O2	000109-60-4	9
5	1-Butanamine	73	C4H11N	000109-73-9	7





Library Search Compound Report

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ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BEK31

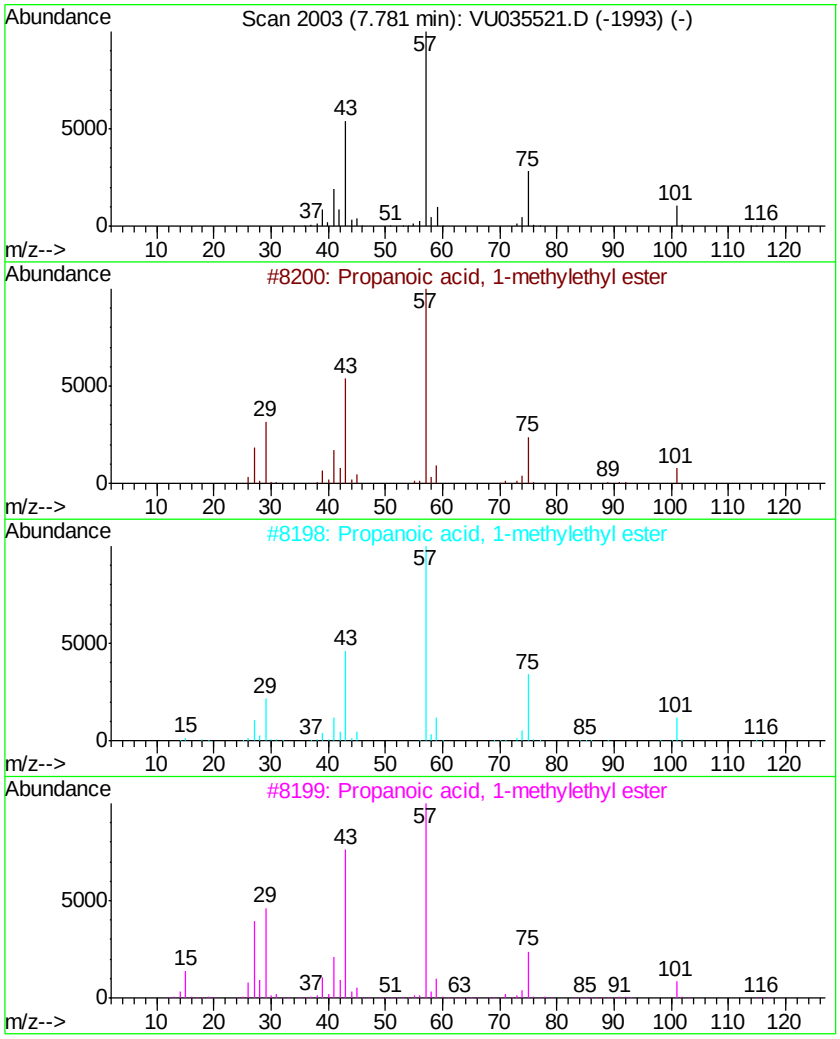
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102619WMA.M
Quant Title : VOC Analysis

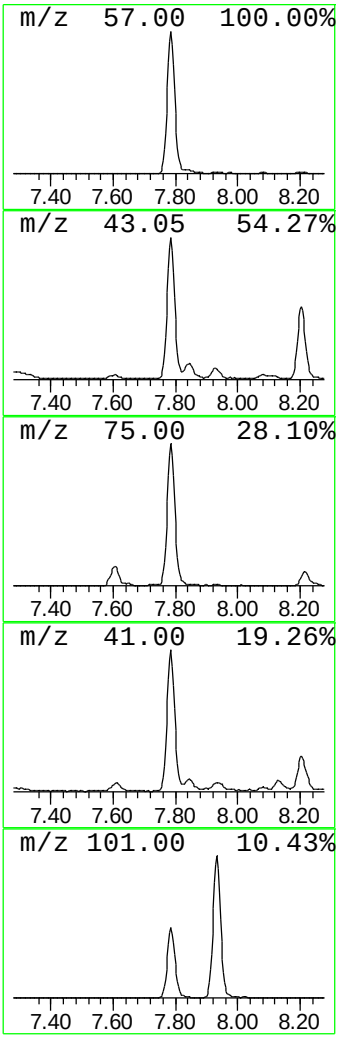
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Propanoic acid, 1-methyleth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.78	9.17 ug/L	459437	1,4-Difluorobenzene	6.29

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	83
3	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	74
4	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	42
5	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	42





Library Search Compound Report

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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BEK31

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102619WMA.M
Quant Title : VOC Analysis

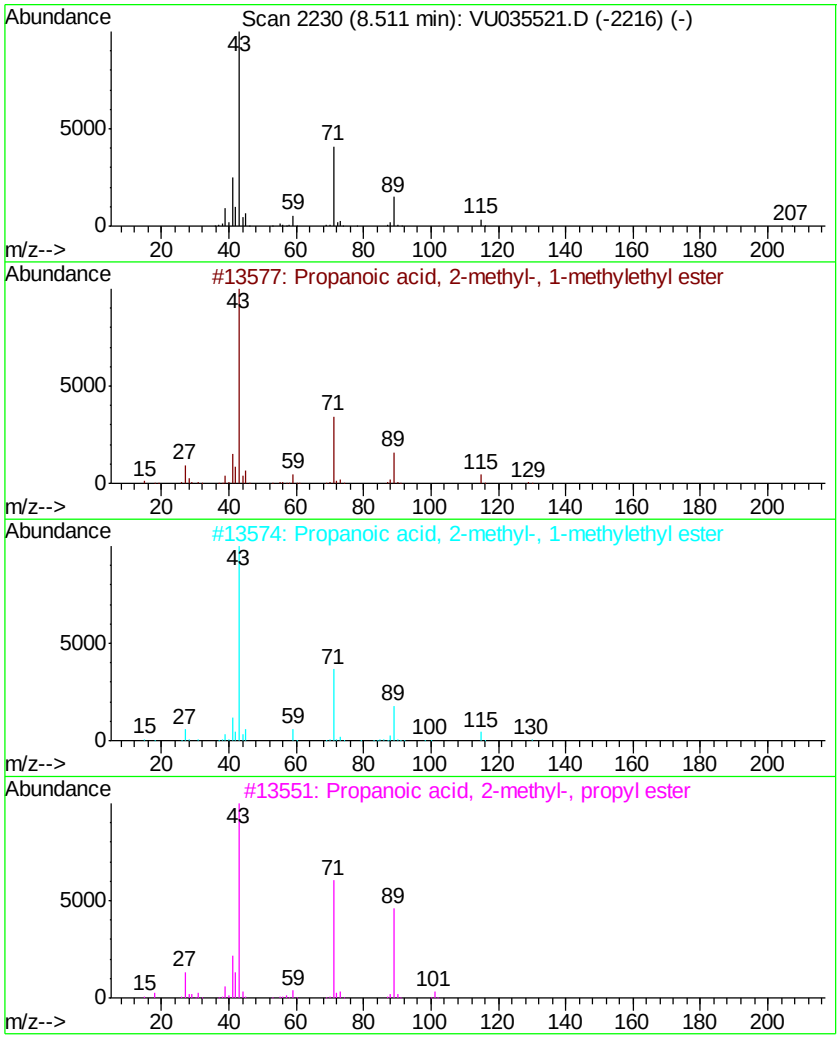
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

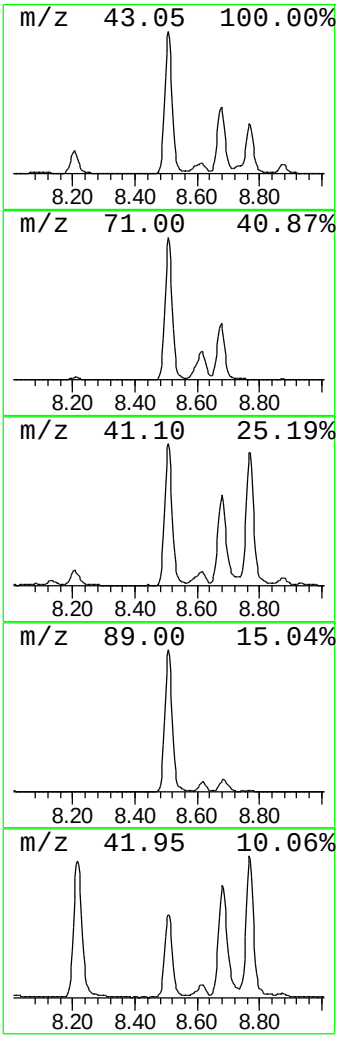
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.51	17.42 ug/L	700894	Chlorobenzene-d5	9.45

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	78
3	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
4	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU102619\
Data File : VU035521.D
Acq On : 26 Oct 2019 16:21
Operator : JC/SP
Sample : K5536-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BEK31

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102619WMA.M
Quant Title : VOC Analysis

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

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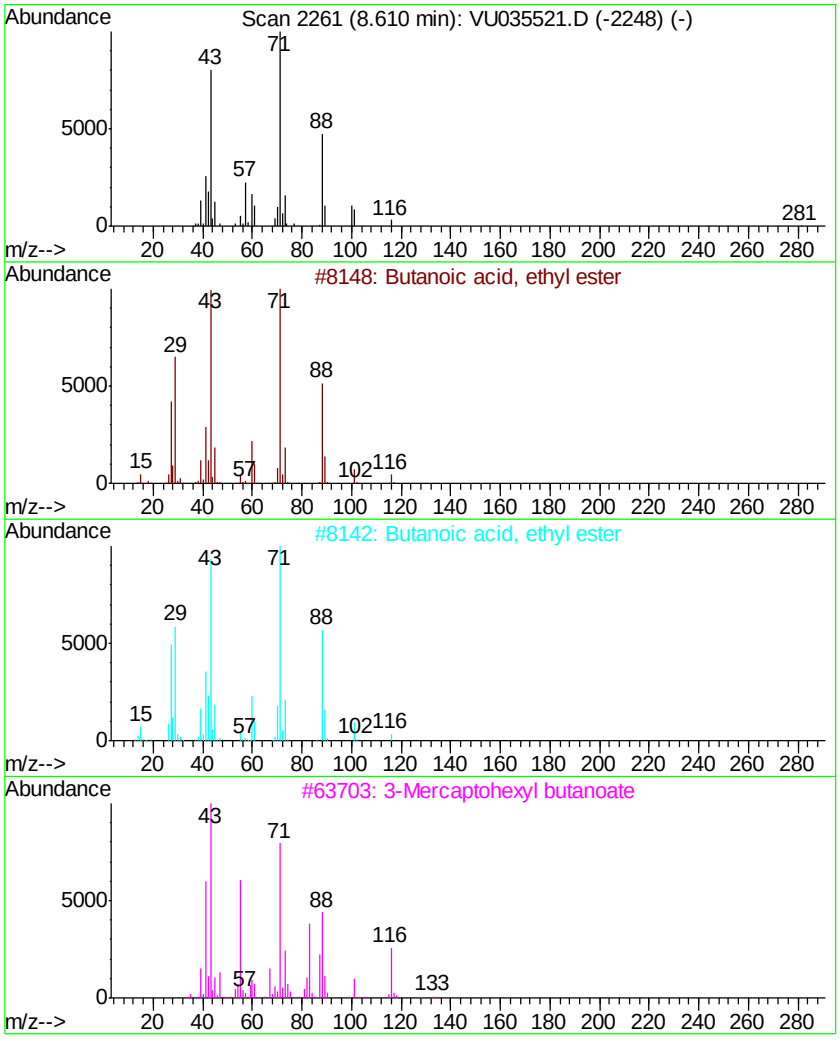
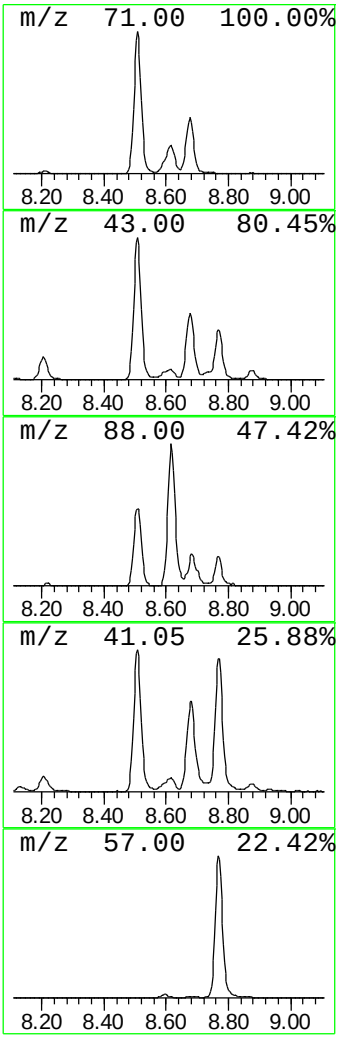
Peak Number 7 Butanoic acid, ethyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.61	3.33 ug/L	134000	Chlorobenzene-d5	9.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	96
2	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	60
3	3-Mercaptohexyl butanoate	204	C10H20O2S	136954-21-7	56
4	Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	53
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	53





Library Search Compound Report

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Data File : VU035521.D
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ALS Vial : 15 Sample Multiplier: 1

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ClientSampleId : BEK31

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102619WMA.M
Quant Title : VOC Analysis

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

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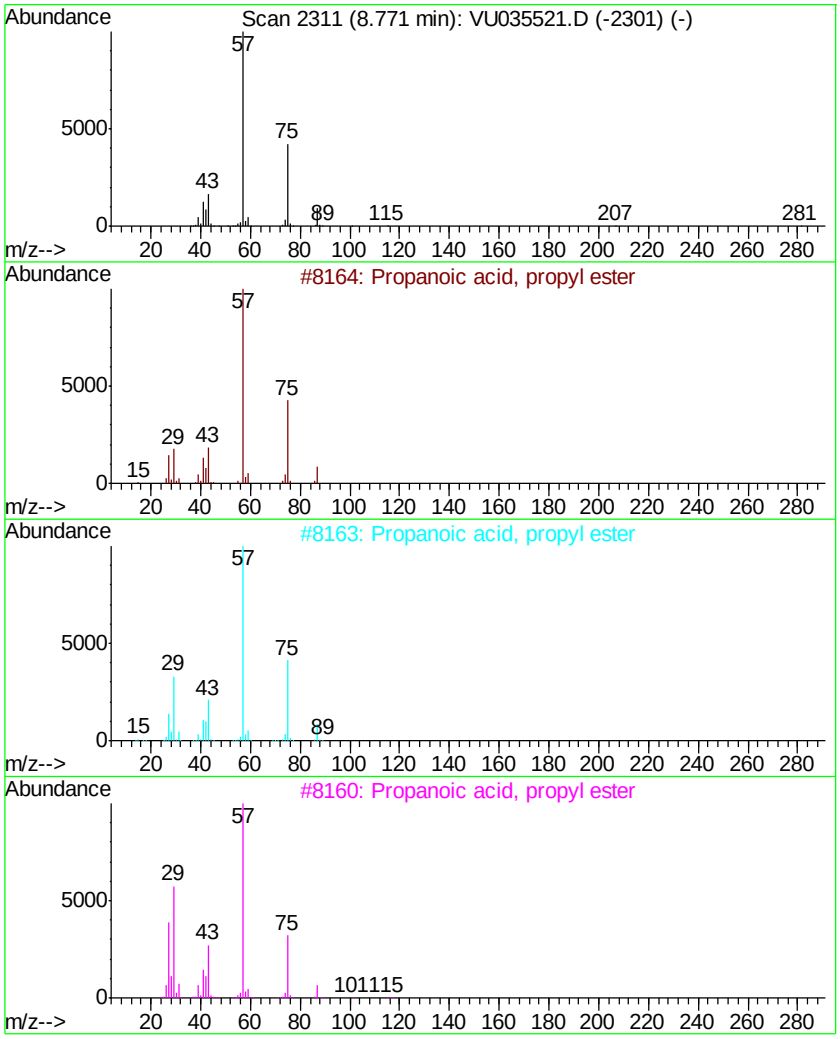
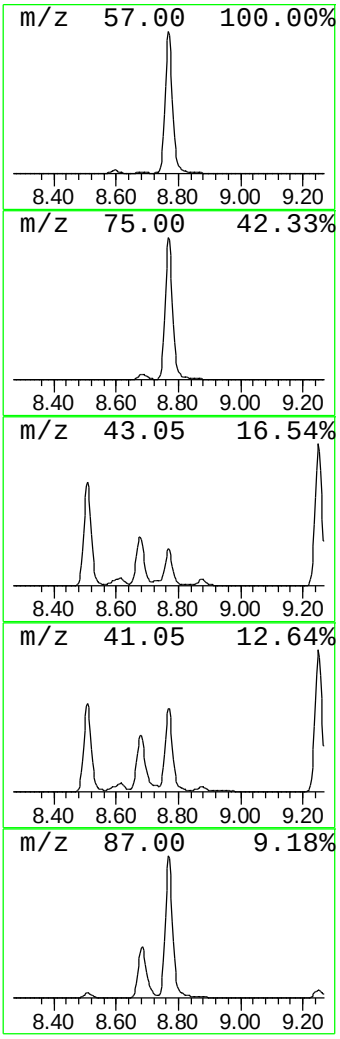
Peak Number 8 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.77	29.72 ug/L	1195530	Chlorobenzene-d5	9.45

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	28





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Data File : VU035521.D
Acq On : 26 Oct 2019 16:21
Operator : JC/SP
Sample : K5536-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BEK31

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102619WMA.M
Quant Title : VOC Analysis

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

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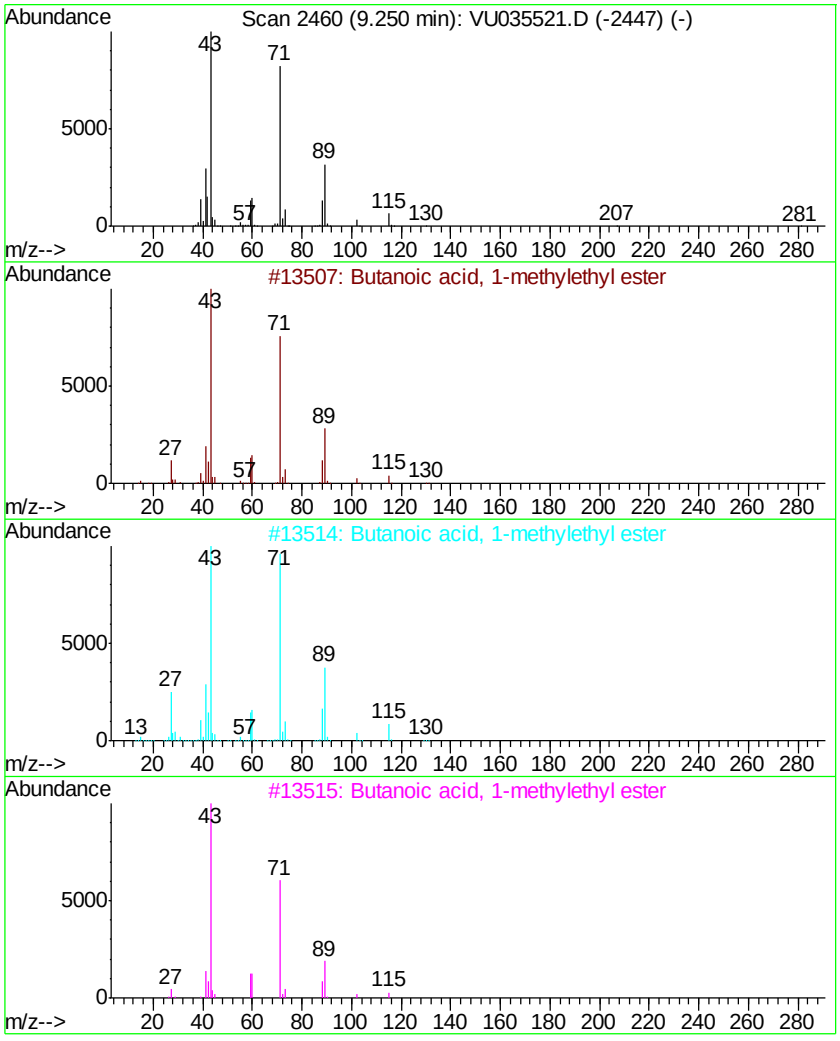
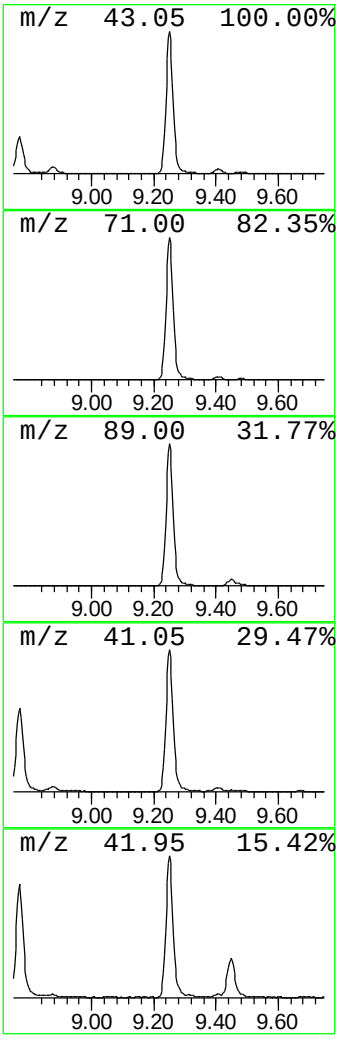
Peak Number 9 Butanoic acid, 1-methylethy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.25	34.90 ug/L	1403740	Chlorobenzene-d5	9.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	95
2	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	91
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	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72





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ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BEK31

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102619WMA.M
Quant Title : VOC Analysis

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

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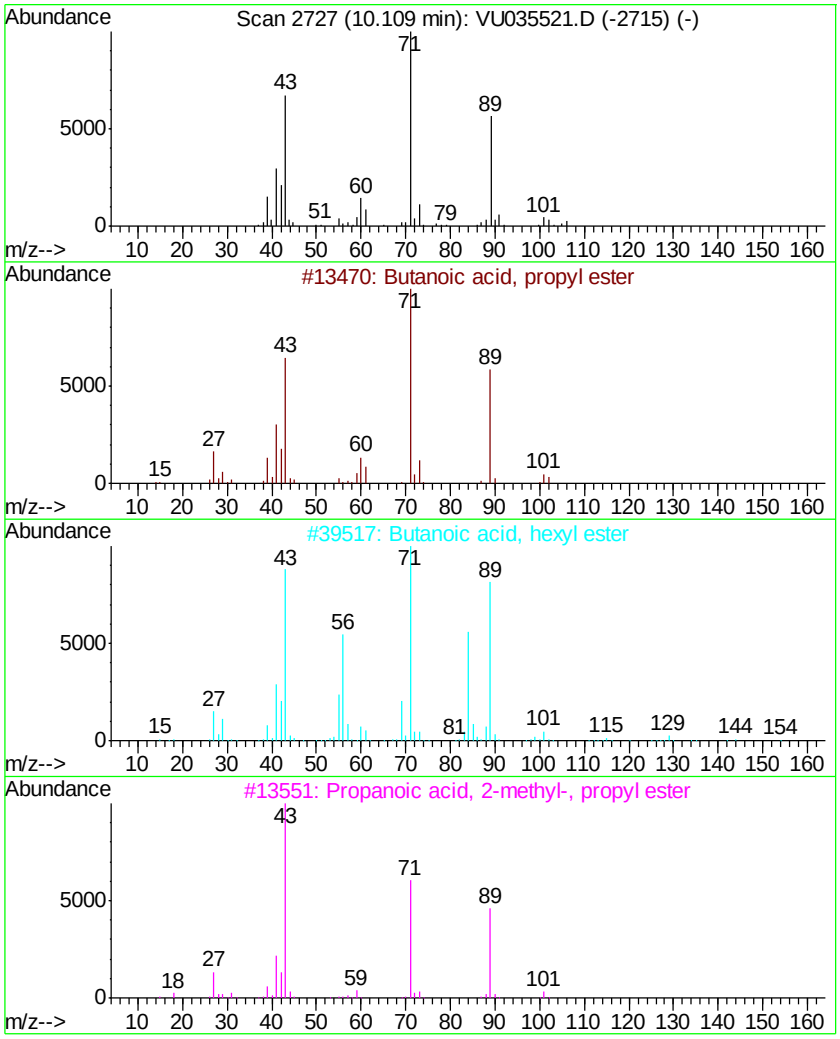
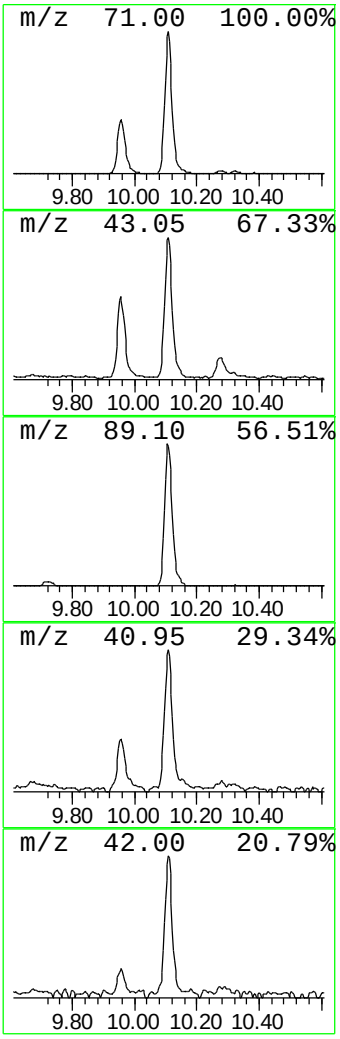
Peak Number 10 Butanoic acid, propyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.11	3.95 ug/L	158838	Chlorobenzene-d5	9.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	90
2	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	64
3	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	59
4	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	56
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	52





Tentatively Identified Compound (LSC) summary

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Data File : VU035521.D
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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	5.97	4.5	ug/L	223434	1	6.29	2506280	50.0
Acetic acid	6.18	9.7	ug/L	486023	1	6.29	2506280	50.0
n-Propyl acetate	7.09	73.3	ug/L	3671810	1	6.29	2506280	50.0
Propanoic acid, 1...	7.78	9.2	ug/L	459437	1	6.29	2506280	50.0
Propanoic acid, 2...	8.51	17.4	ug/L	700894	2	9.45	2011220	50.0
Butanoic acid, et...	8.61	3.3	ug/L	134000	2	9.45	2011220	50.0
Propanoic acid, p...	8.77	29.7	ug/L	1195530	2	9.45	2011220	50.0
Butanoic acid, 1-...	9.25	34.9	ug/L	1403740	2	9.45	2011220	50.0
Butanoic acid, pr...	10.11	4.0	ug/L	158838	2	9.45	2011220	50.0