LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU110519\
Data File : VU035619.D
Acq On : 05 Nov 2019 10:48
Operator : JC/SP
Sample : PB124534TB
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 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\SOMULM103119WMA.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	1.375	6	11	31	rBV3	15148	27480	0.87%	0.109%
2	1.485	40	45	58	rBV2	13415	23270	0.74%	0.092%
3	1.617	78	86	101	rVB	320245	352806	11.23%	1.401%
4	1.935	176	185	203	rBV	263038	352329	11.21%	1.399%
5	2.597	378	391	405	rBV	465054	780238	24.83%	3.098%
6	2.996	508	515	523	rBV4	2746	4838	0.15%	0.019%
7	3.086	532	543	561	rVB2	18439	37584	1.20%	0.149%
8	3.150	561	563	566	rVB3	552	289	0.01%	0.001%
9	3.205	577	580	581	rBV2	1191	695	0.02%	0.003%
10	3.333	617	620	626	rBV4	615	538	0.02%	0.002%
11	3.382	632	635	639	rBV4	643	588	0.02%	0.002%
12	3.440	651	653	659	rVB	330	269	0.01%	0.001%
13	3.469	659	662	665	rBV	445	299	0.01%	0.001%
14	3.588	694	699	703	rVB	464	322	0.01%	0.001%
15	3.639	712	715	721	rVB2	633	568	0.02%	0.002%
16	3.739	741	746	748	rBV2	306	250	0.01%	0.001%
17	3.851	771	781	788	rBV3	886	1608	0.05%	0.006%
18	3.983	818	822	831	rVB2	504	618	0.02%	0.002%
19	4.041	836	840	842	rVV2	293	226	0.01%	0.001%
20	4.099	855	858	861	rBV	338	288	0.01%	0.001%
21	4.147	867	873	883	rVB4	828	1702	0.05%	0.007%
22	4.205	883	891	893	rBV2	380	306	0.01%	0.001%
23	4.256	904	907	912	rVB2	375	275	0.01%	0.001%
24	4.285	912	916	922	rBV2	442	299	0.01%	0.001%
25	4.391	946	949	952	rVB2	398	244	0.01%	0.001%
26	4.420	952	958	963	rBV2	402	532	0.02%	0.002%
27	4.494	977	981	984	rBV2	556	431	0.01%	0.002%
28	4.690	1026	1042	1090	rBV	198451	524243	16.68%	2.081%
29	5.112	1156	1173	1204	rBV	409727	919436	29.26%	3.650%
30	5.417	1264	1268	1274	rBV2	988	899	0.03%	0.004%
31	5.575	1312	1317	1318	rBV2	384	324	0.01%	0.001%
32	5.597	1320	1324	1326	rBV2	340	243	0.01%	0.001%
33	5.623	1330	1332	1338	rVB2	628	378	0.01%	0.002%
34	5.658	1338	1343	1345	rBV2	478	439	0.01%	0.002%

LSC Area Percent Report

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Sample : PB124534TB
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 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\SOMULM103119WMA.M
Title : VOC Analysis

35	5.671	1345	1347	1350	rVB3	585	262	0.01%	0.001%
36	5.771	1353	1378	1406	rBV2	880098	2330519	74.15%	9.253%
37	5.970	1429	1440	1458	rVB	83680	165764	5.27%	0.658%
38	6.234	1485	1522	1524	rBV2	58991	261704	8.33%	1.039%
39	6.292	1530	1540	1592	rVB	875993	1971030	62.72%	7.826%
40	6.735	1663	1678	1697	rBV	526625	1053091	33.51%	4.181%
41	6.989	1746	1757	1770	rVB2	29288	67856	2.16%	0.269%
42	7.089	1774	1788	1823	rBV	1668641	3142799	100.00%	12.478%
43	7.504	1914	1917	1920	rBV2	586	372	0.01%	0.001%
44	7.603	1934	1948	1969	rBV	291951	540206	17.19%	2.145%
45	7.783	1992	2004	2016	rBV	204475	344595	10.96%	1.368%
46	7.935	2037	2051	2089	rBV	1062415	1985952	63.19%	7.885%
47	8.214	2125	2138	2170	rBV2	230570	480249	15.28%	1.907%
48	8.439	2206	2208	2210	rBV2	408	217	0.01%	0.001%
49	8.507	2216	2229	2247	rBV	325089	581347	18.50%	2.308%
50	8.677	2271	2282	2301	rBV2	445210	1115193	35.48%	4.428%
51	8.767	2302	2310	2336	rVB	595228	1111992	35.38%	4.415%
52	9.079	2403	2407	2410	rVB5	666	476	0.02%	0.002%
53	9.095	2410	2412	2416	rBV3	387	301	0.01%	0.001%
54	9.192	2440	2442	2446	rBV3	825	571	0.02%	0.002%
55	9.250	2446	2460	2494	rVV	609116	1216722	38.71%	4.831%
56	9.449	2500	2522	2561	rVB	1057329	1999887	63.63%	7.940%
57	9.590	2563	2566	2567	rBV2	691	440	0.01%	0.002%
58	9.677	2587	2593	2602	rBV6	2798	4867	0.15%	0.019%
59	9.877	2652	2655	2660	rVB2	610	468	0.01%	0.002%
60	9.912	2663	2666	2669	rBV2	947	686	0.02%	0.003%
61	9.960	2669	2681	2705	rBV3	9567	26518	0.84%	0.105%
62	10.057	2709	2711	2714	rVB	582	301	0.01%	0.001%
63	10.115	2716	2729	2750	rBV3	57870	141131	4.49%	0.560%
64	10.227	2761	2764	2766	rBV3	680	445	0.01%	0.002%
65	10.275	2775	2779	2781	rBV2	1367	1179	0.04%	0.005%
66	10.513	2847	2853	2856	rBV3	1390	1343	0.04%	0.005%
67	10.600	2877	2880	2882	rBV	418	324	0.01%	0.001%
68	10.635	2886	2891	2895	rVV5	720	582	0.02%	0.002%
69	10.658	2895	2898	2901	rBV2	646	617	0.02%	0.002%
70	10.690	2905	2908	2911	rBV2	354	215	0.01%	0.001%
71	10.735	2919	2922	2924	rVB	652	398	0.01%	0.002%

LSC Area Percent Report

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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 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\SOMULM103119WMA.M
Title : VOC Analysis

72	10.787	2924	2938	2960	rBV	667797	1169920	37.23%	4.645%
73	10.899	2969	2973	2974	rBV2	1144	802	0.03%	0.003%
74	11.041	3014	3017	3024	rVB3	792	648	0.02%	0.003%
75	11.115	3030	3040	3052	rVB4	3409	5716	0.18%	0.023%
76	11.195	3059	3065	3068	rBV3	743	840	0.03%	0.003%
77	11.356	3112	3115	3117	rBV2	480	281	0.01%	0.001%
78	11.372	3118	3120	3125	rVB2	444	266	0.01%	0.001%
79	11.439	3139	3141	3143	rVV3	726	288	0.01%	0.001%
80	11.497	3151	3159	3161	rBV4	1932	2135	0.07%	0.008%
81	11.581	3182	3185	3189	rBV2	584	379	0.01%	0.002%
82	11.738	3232	3234	3237	rBV2	425	254	0.01%	0.001%
83	11.777	3237	3246	3253	rVB7	1875	3389	0.11%	0.013%
84	11.844	3253	3267	3290	rBV	668028	1200745	38.21%	4.767%
85	11.928	3290	3293	3294	rBV2	574	258	0.01%	0.001%
86	12.034	3321	3326	3327	rBV	583	433	0.01%	0.002%
87	12.127	3352	3355	3359	rBV	591	535	0.02%	0.002%
88	12.224	3371	3385	3406	rBV	702668	1208228	38.44%	4.797%
89	12.317	3411	3414	3416	rBV2	593	400	0.01%	0.002%
90	12.359	3423	3427	3430	rBV2	446	383	0.01%	0.002%
91	12.507	3471	3473	3476	rBV3	441	250	0.01%	0.001%
92	12.542	3481	3484	3487	rBV4	459	331	0.01%	0.001%
93	12.587	3494	3498	3504	rBV5	781	866	0.03%	0.003%
94	12.877	3585	3588	3592	rBV2	553	481	0.02%	0.002%
95	13.008	3625	3629	3632	rVV2	627	572	0.02%	0.002%
96	13.024	3632	3634	3636	rVB2	604	269	0.01%	0.001%
97	13.127	3661	3666	3669	rBV2	604	614	0.02%	0.002%
98	13.420	3754	3757	3759	rBV3	620	386	0.01%	0.002%
99	13.761	3858	3863	3865	rBV3	983	865	0.03%	0.003%
100	14.076	3957	3961	3963	rBV5	775	682	0.02%	0.003%

Sum of corrected areas: 25186689

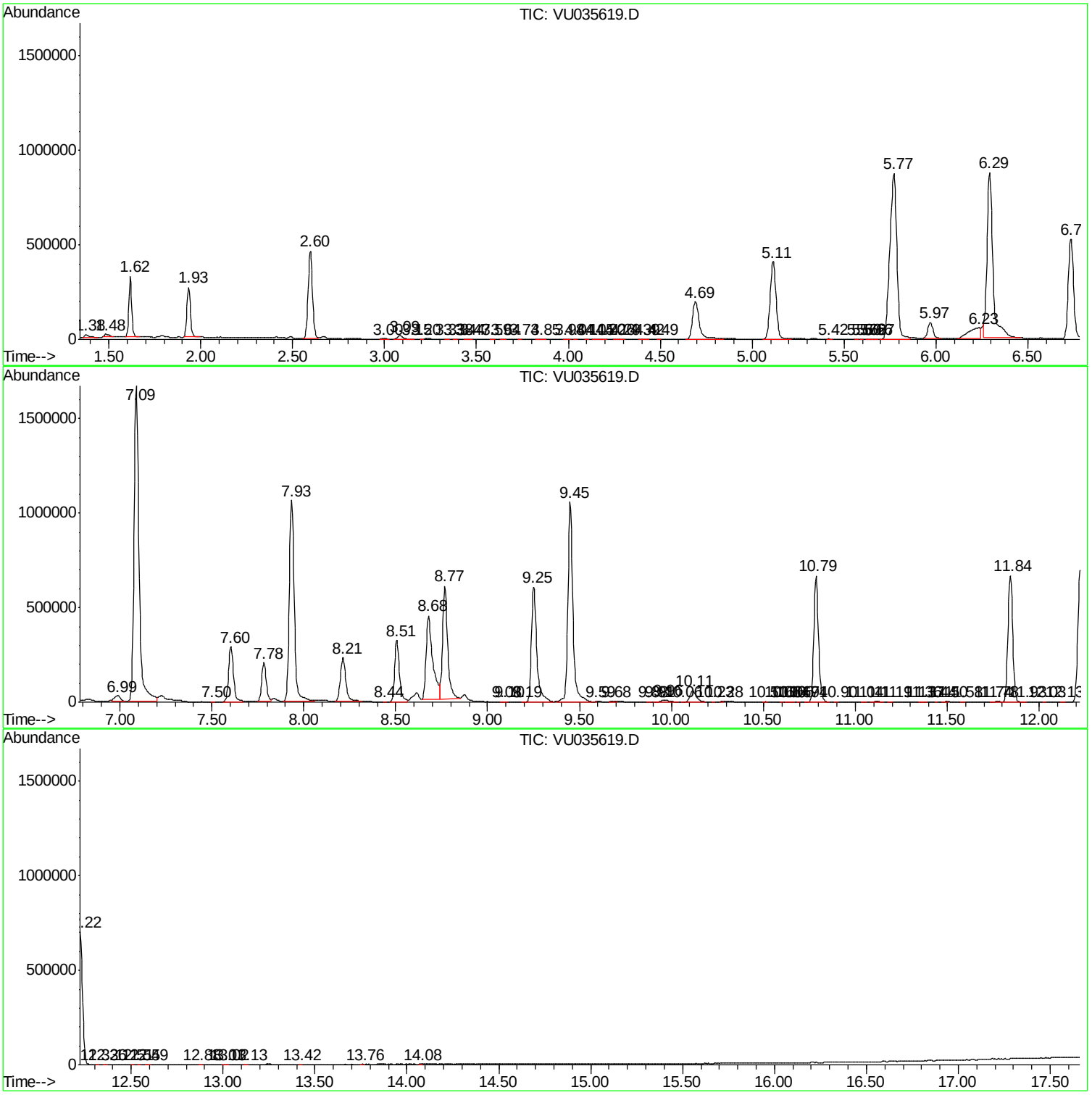
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU110519\
Data File : VU035619.D
Acq On : 05 Nov 2019 10:48
Operator : JC/SP
Sample : PB124534TB
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM103119WMA.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\VU110519\
Data File : VU035619.D
Acq On : 05 Nov 2019 10:48
Operator : JC/SP
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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : VLEB01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM103119WMA.M
Quant Title : VOC Analysis

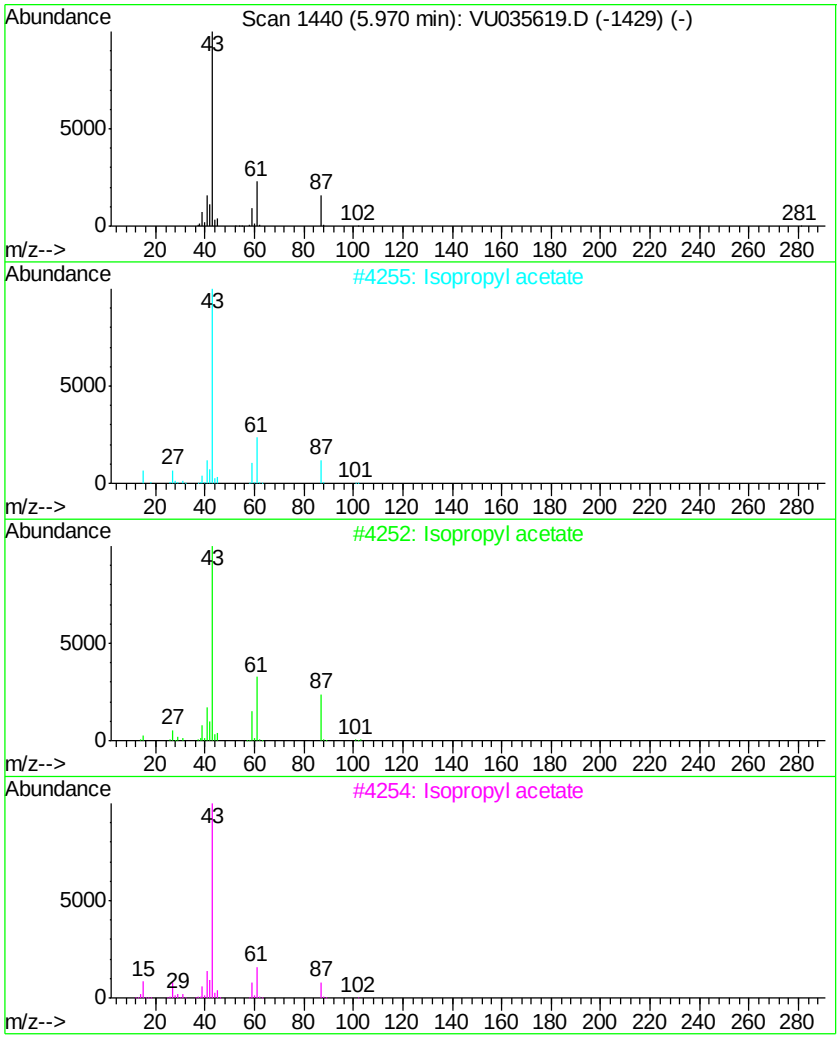
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

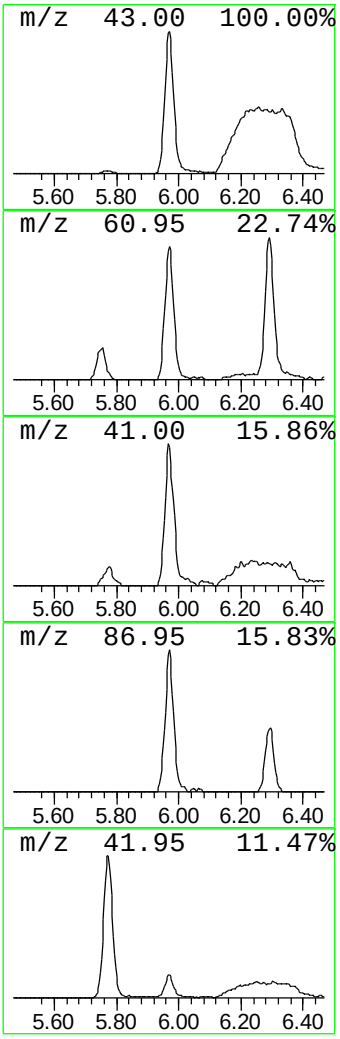
****

Peak Number 1 Isopropyl acetate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.97	4.21 ug/L	165764	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	78
3	Isopropyl acetate	102	C5H10O2	000108-21-4	56
4	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	25
5	Thiocyanic acid, ethyl ester	87	C3H5NS	000542-90-5	9





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU110519\
Data File : VU035619.D
Acq On : 05 Nov 2019 10:48
Operator : JC/SP
Sample : PB124534TB
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : VLEB01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM103119WMA.M
Quant Title : VOC Analysis

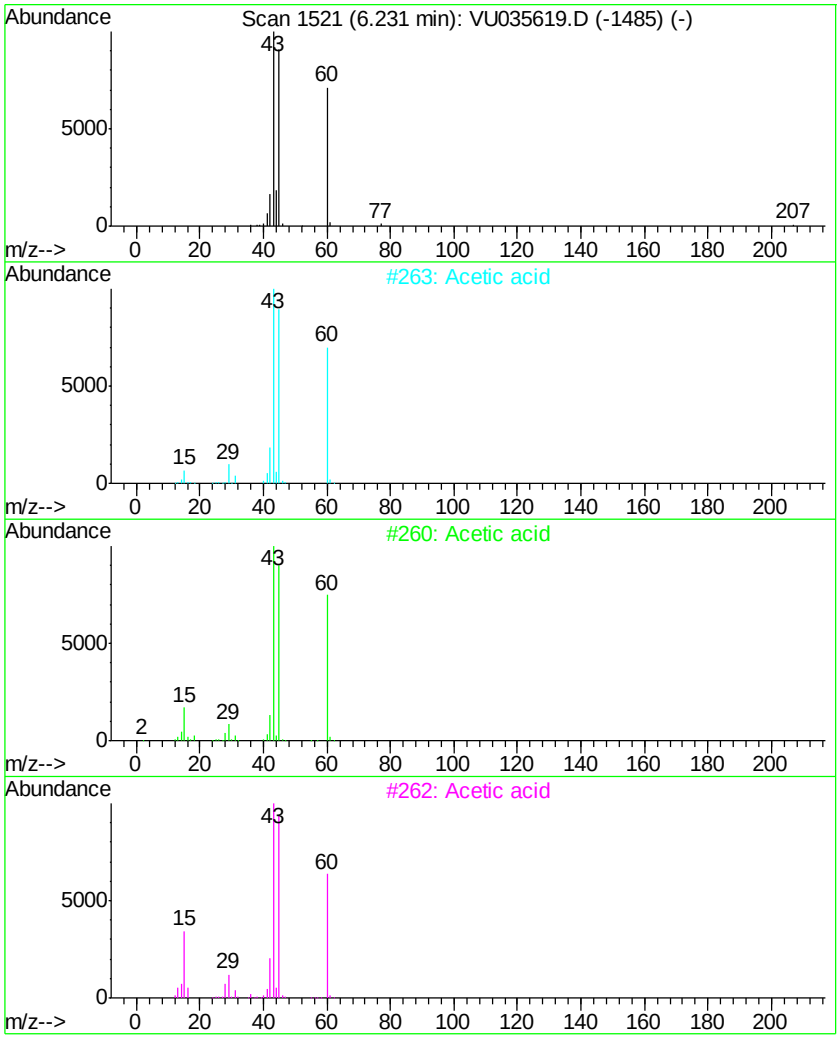
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

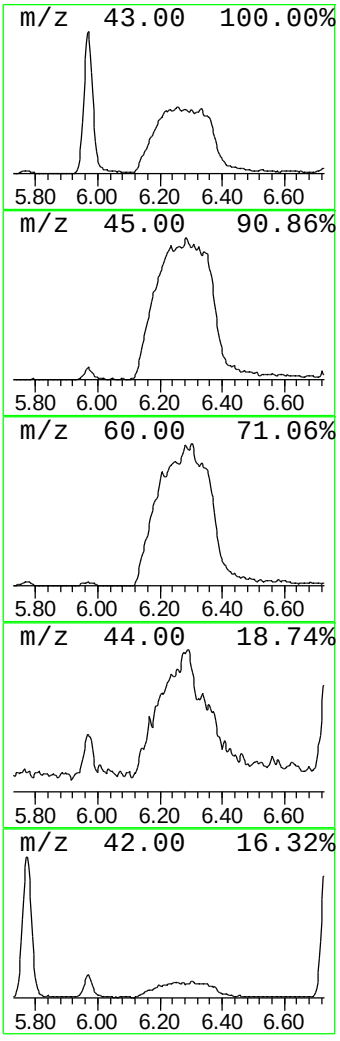
****

Peak Number 2 Acetic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.23	6.64 ug/L	261704	1,4-Difluorobenzene	6.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid	60	C2H4O2	000064-19-7	80
2	Acetic acid	60	C2H4O2	000064-19-7	80
3	Acetic acid	60	C2H4O2	000064-19-7	80
4	Acetic acid	60	C2H4O2	000064-19-7	64
5	Acetic acid	60	C2H4O2	000064-19-7	56





Library Search Compound Report

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ALS Vial : 5 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : VLEB01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM103119WMA.M
Quant Title : VOC Analysis

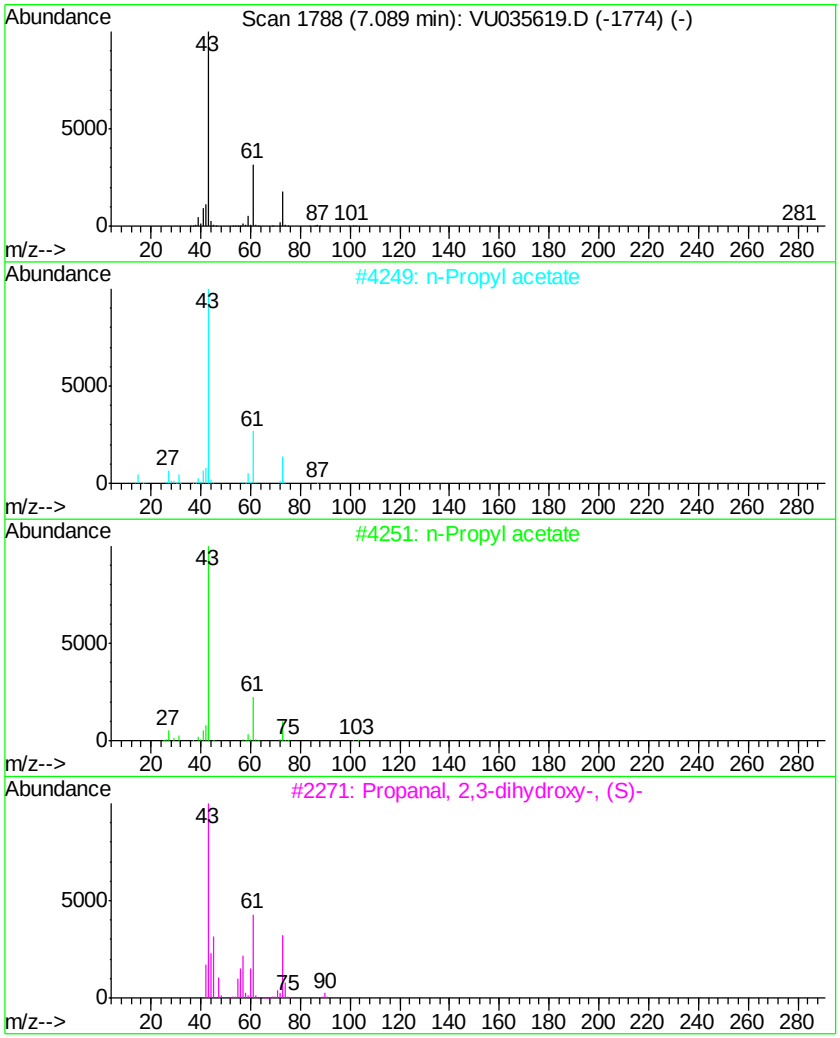
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

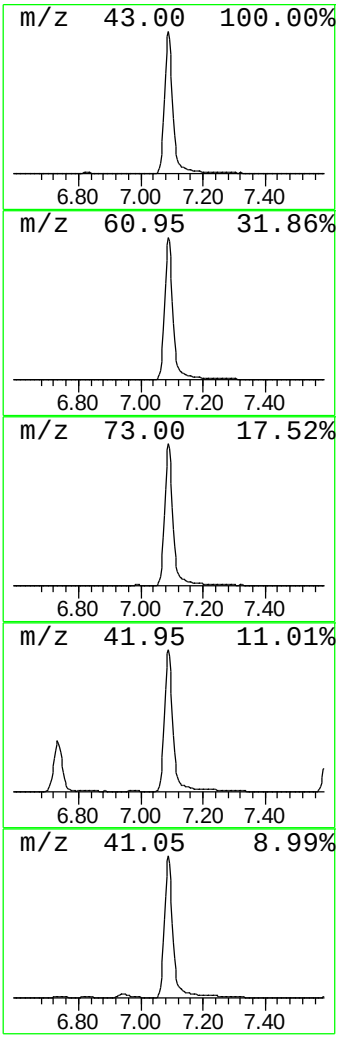
****

Peak Number 3 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.09	79.72 ug/L	3142800	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	Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	36
4	Isopropyl acetate	102	C5H10O2	000108-21-4	36
5	n-Propyl acetate	102	C5H10O2	000109-60-4	9





Library Search Compound Report

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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : VLEB01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM103119WMA.M
Quant Title : VOC Analysis

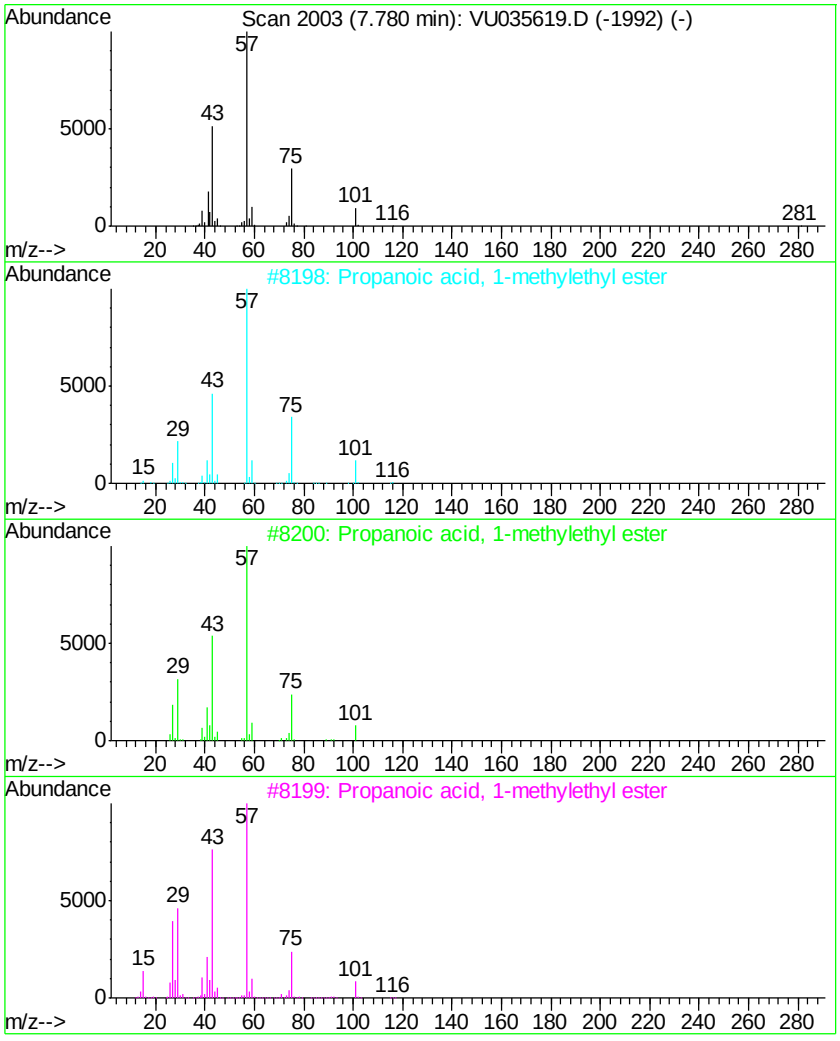
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

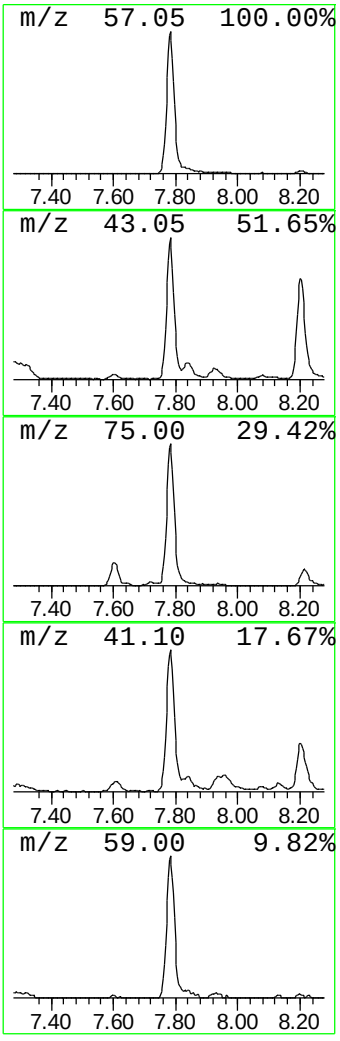
****

Peak Number 5 Propanoic acid, 1-methyleth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.78	8.74 ug/L	344595	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	83
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, propyl ester	116	C6H12O2	000106-36-5	50
5	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	50





Library Search Compound Report

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Acq On : 05 Nov 2019 10:48
Operator : JC/SP
Sample : PB124534TB
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : VLEB01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM103119WMA.M
Quant Title : VOC Analysis

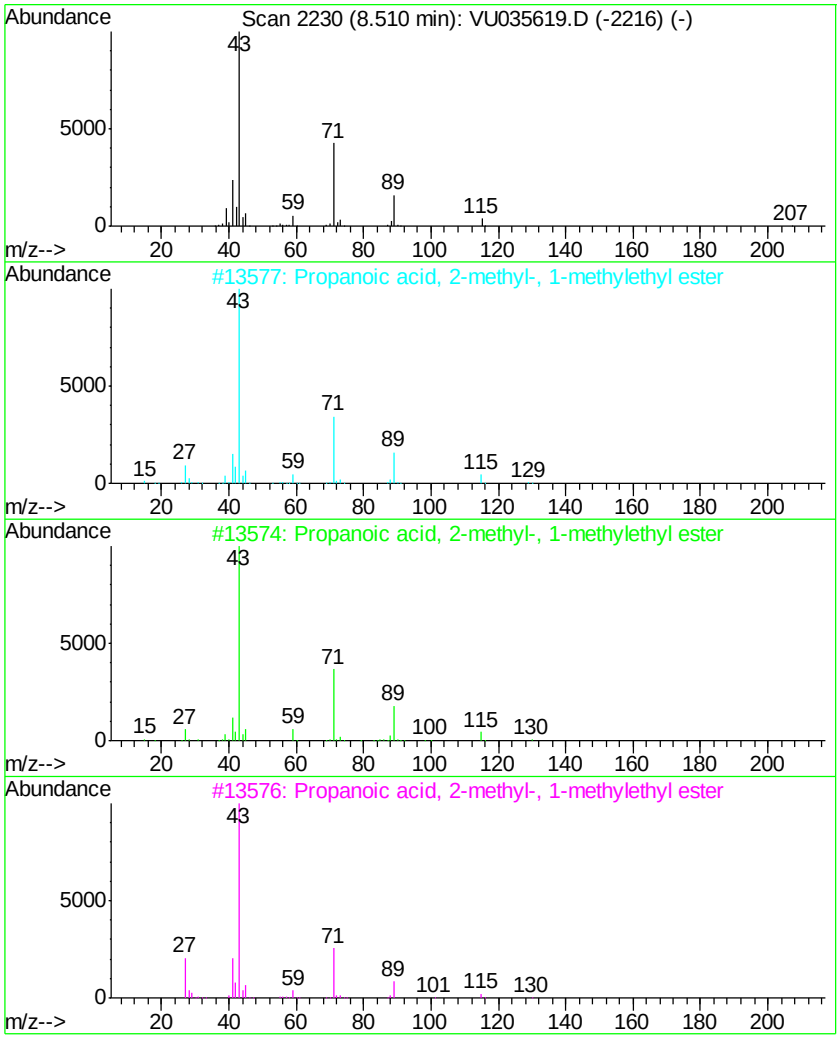
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

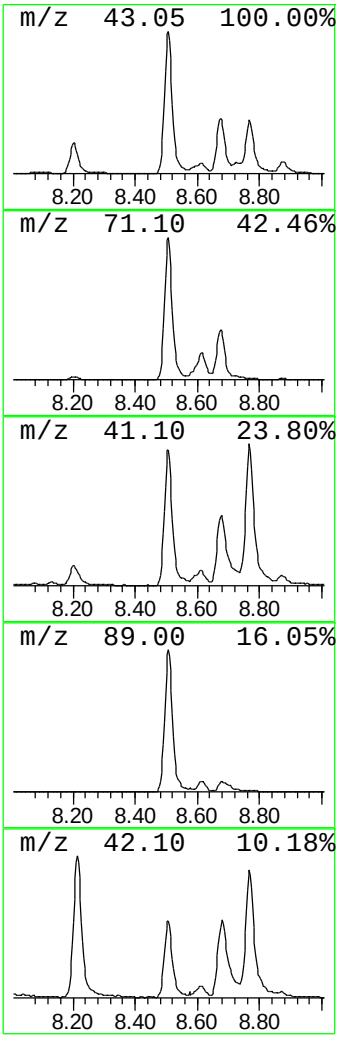
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.51	14.53 ug/L	581347	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-, 1-met...	130	C7H14O2	000617-50-5	74
4	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
5	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU110519\
Data File : VU035619.D
Acq On : 05 Nov 2019 10:48
Operator : JC/SP
Sample : PB124534TB
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : VLEB01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM103119WMA.M
Quant Title : VOC Analysis

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

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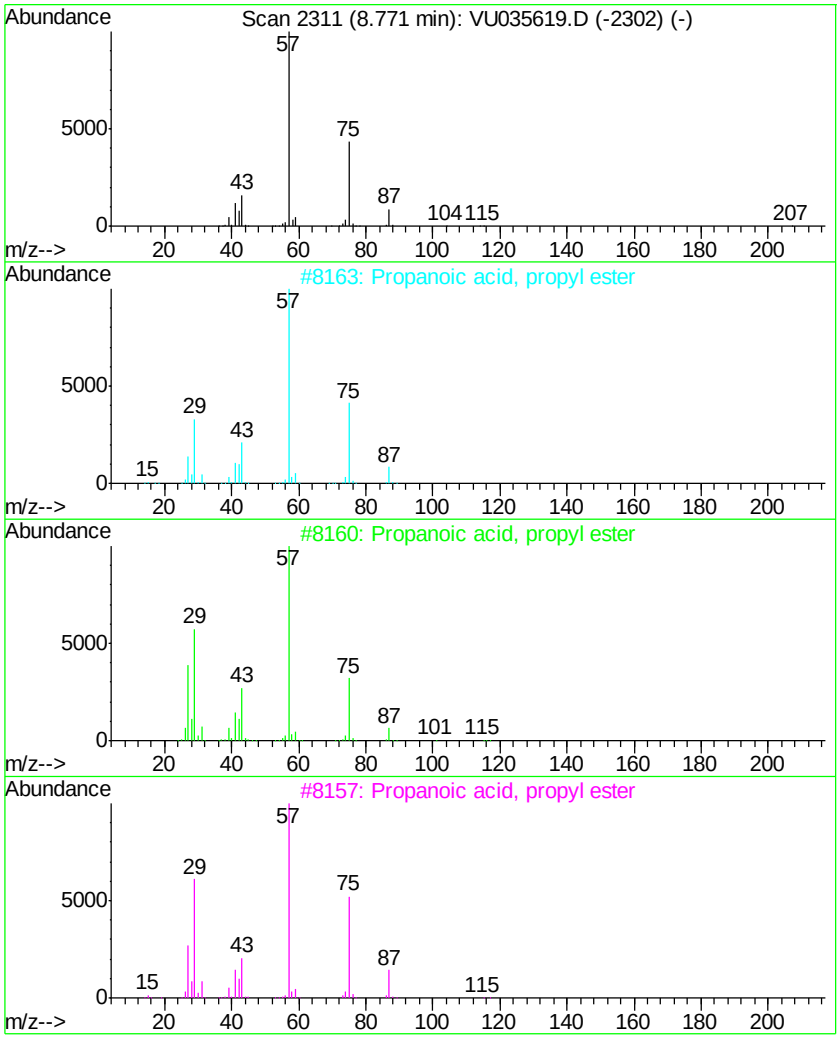
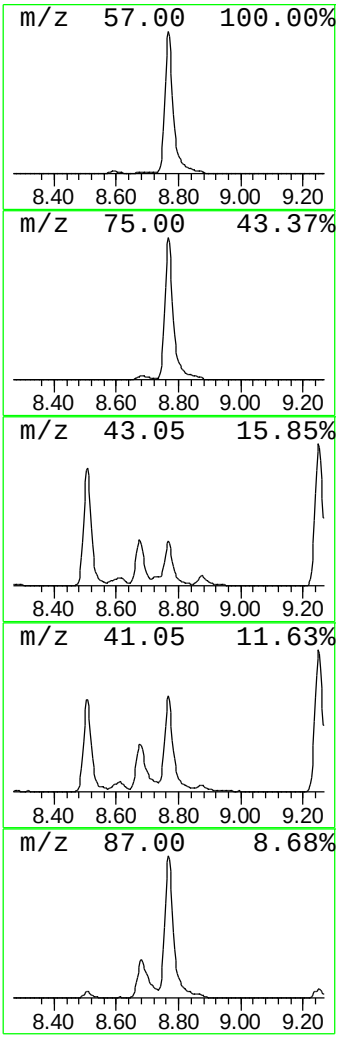
Peak Number 7 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.77	27.80 ug/L	1111990	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





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU110519\
Data File : VU035619.D
Acq On : 05 Nov 2019 10:48
Operator : JC/SP
Sample : PB124534TB
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : VLEB01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM103119WMA.M
Quant Title : VOC Analysis

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

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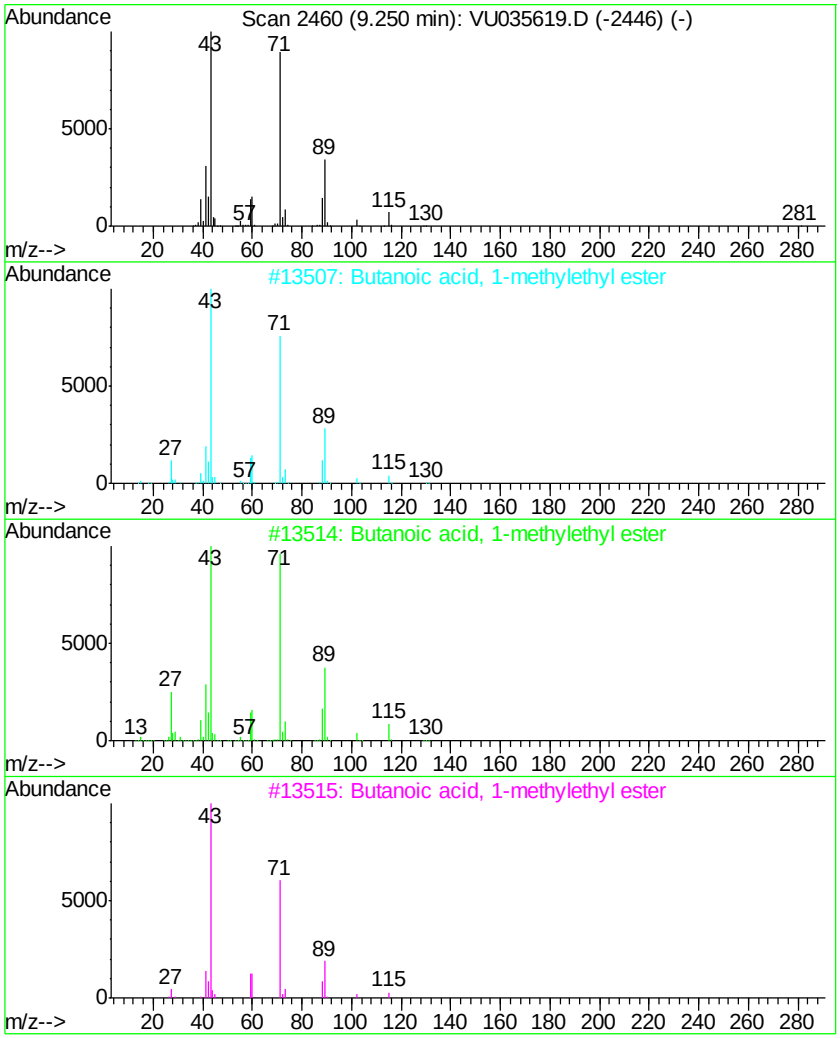
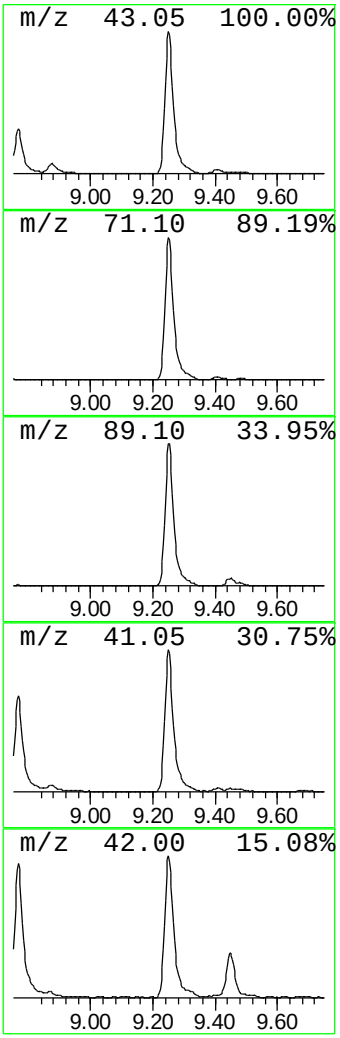
Peak Number 8 Butanoic acid, 1-methylethy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.25	30.42 ug/L	1216720	Chlorobenzene-d5	9.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	94
2	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	91
3	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	78
4	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU110519\
Data File : VU035619.D
Acq On : 05 Nov 2019 10:48
Operator : JC/SP
Sample : PB124534TB
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : VLEB01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM103119WMA.M
Quant Title : VOC Analysis

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

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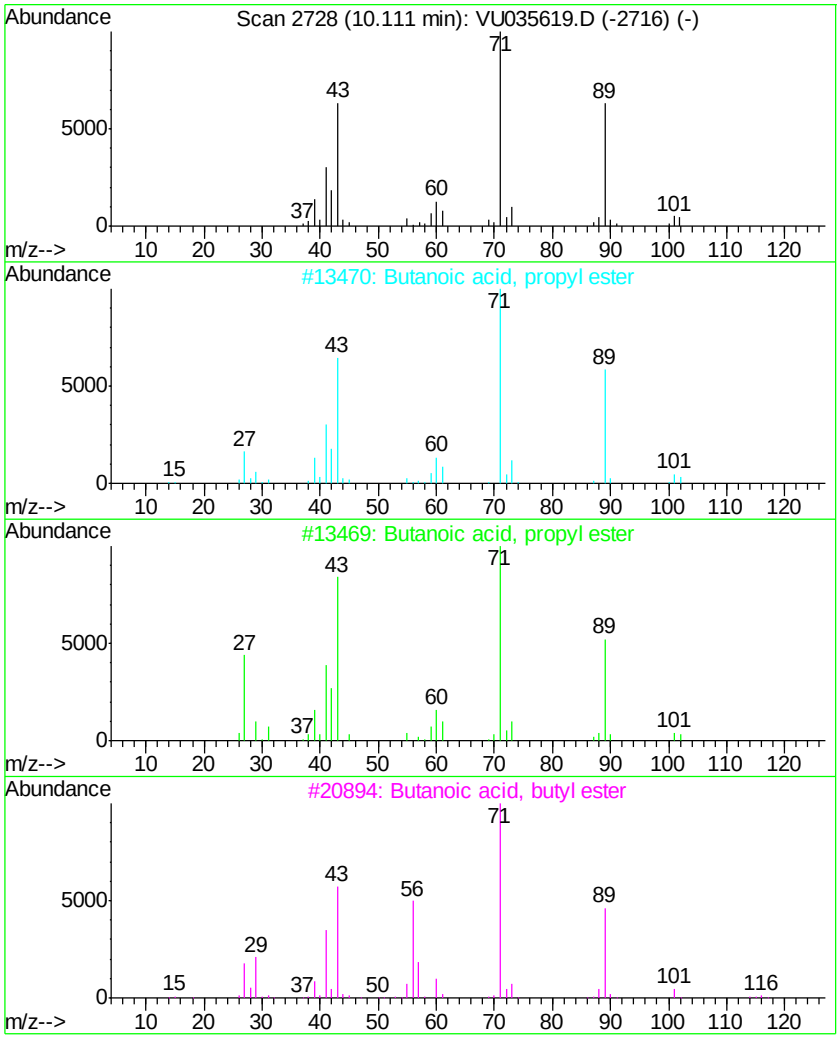
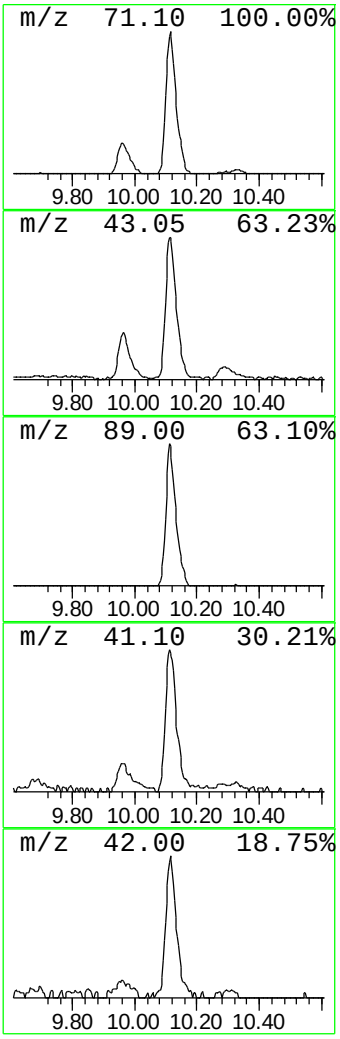
Peak Number 9 Butanoic acid, propyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.11	3.53 ug/L	141131	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, propyl ester	130	C7H14O2	000105-66-8	80
3	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	78
4	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
5	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU110519\
Data File : VU035619.D
Acq On : 05 Nov 2019 10:48
Operator : JC/SP
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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : VLEB01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM103119WMA.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	5.97	4.2	ug/L	165764	1	6.29	1971030	50.0
Acetic acid	6.23	6.6	ug/L	261704	1	6.29	1971030	50.0
n-Propyl acetate	7.09	79.7	ug/L	3142800	1	6.29	1971030	50.0
Propanoic acid, 1...	7.78	8.7	ug/L	344595	1	6.29	1971030	50.0
Propanoic acid, 2...	8.51	14.5	ug/L	581347	2	9.45	1999890	50.0
Propanoic acid, p...	8.77	27.8	ug/L	1111990	2	9.45	1999890	50.0
Butanoic acid, 1-...	9.25	30.4	ug/L	1216720	2	9.45	1999890	50.0
Butanoic acid, pr...	10.11	3.5	ug/L	141131	2	9.45	1999890	50.0