LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101023\
Data File : VU055721.D
Acq On : 10 Oct 2023 15:10
Operator : MD/SY
Sample : PB156229TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB229

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\SFAMULM101023WMA.M
Title : VOC Analysis

Signal : TIC: VU055721.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.599	88	96	112	rBV	215263	263549	14.37%	1.732%
2	1.885	178	185	202	rVB	176313	256696	13.99%	1.687%
3	2.557	382	394	411	rBV	376466	614792	33.51%	4.040%
4	2.624	411	415	420	rVB5	2900	3527	0.19%	0.023%
5	2.682	430	433	437	rVB5	854	589	0.03%	0.004%
6	2.885	494	496	498	rBV2	537	360	0.02%	0.002%
7	2.914	502	505	508	rBV3	692	470	0.03%	0.003%
8	3.036	533	543	556	rVB3	11325	20169	1.10%	0.133%
9	3.181	574	588	602	rBV2	15862	38115	2.08%	0.250%
10	3.345	634	639	646	rVB5	1384	1781	0.10%	0.012%
11	3.512	685	691	697	rVB2	617	546	0.03%	0.004%
12	3.547	697	702	707	rBV3	458	622	0.03%	0.004%
13	3.583	707	713	716	rBV2	394	400	0.02%	0.003%
14	3.840	790	793	797	rVB2	684	545	0.03%	0.004%
15	4.068	856	864	867	rBV2	404	598	0.03%	0.004%
16	4.312	935	940	942	rBV2	510	444	0.02%	0.003%
17	4.425	972	975	979	rVB2	444	301	0.02%	0.002%
18	4.447	979	982	984	rBV3	481	307	0.02%	0.002%
19	4.464	984	987	994	rVB2	435	510	0.03%	0.003%
20	4.505	994	1000	1003	rBV2	343	407	0.02%	0.003%
21	4.544	1008	1012	1017	rBV2	435	496	0.03%	0.003%
22	4.615	1017	1034	1080	rBV	167158	456472	24.88%	2.999%
23	4.972	1139	1145	1154	rVB5	757	927	0.05%	0.006%
24	5.055	1154	1171	1195	rBV	330602	733567	39.99%	4.820%
25	5.325	1250	1255	1269	rVB4	3239	5711	0.31%	0.038%
26	5.560	1320	1328	1331	rBV2	335	431	0.02%	0.003%
27	5.718	1357	1377	1402	rBV2	667505	1834474	100.00%	12.053%
28	5.910	1430	1437	1456	rVB3	12774	27048	1.47%	0.178%
29	6.042	1475	1478	1487	rVB3	1089	1121	0.06%	0.007%
30	6.132	1504	1506	1512	rBV2	388	384	0.02%	0.003%
31	6.245	1527	1541	1564	rBV	480842	930324	50.71%	6.113%
32	6.528	1619	1629	1644	rBV4	11756	24277	1.32%	0.160%
33	6.582	1644	1646	1648	rBV2	487	350	0.02%	0.002%
34	6.602	1648	1652	1654	rBV4	817	569	0.03%	0.004%
35	6.685	1664	1678	1698	rBV	419515	823529	44.89%	5.411%
36	6.849	1726	1729	1732	rVB2	900	539	0.03%	0.004%

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Sample : PB156229TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB229

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\SFAMULM101023WMA.M
Title : VOC Analysis

37	6.933	1742	1755	1768	rBV	6835	16247	0.89%	0.107%
38	7.036	1777	1787	1807	rBV	162594	301827	16.45%	1.983%
39	7.187	1829	1834	1843	rBV8	3233	4579	0.25%	0.030%
40	7.322	1875	1876	1879	rVB	936	309	0.02%	0.002%
41	7.354	1882	1886	1891	rVB2	586	461	0.03%	0.003%
42	7.390	1894	1897	1901	rBV3	601	398	0.02%	0.003%
43	7.560	1937	1950	1978	rBV	229016	420119	22.90%	2.760%
44	7.737	1996	2005	2019	rVB2	32075	53024	2.89%	0.348%
45	7.795	2019	2023	2037	rVB7	3302	5970	0.33%	0.039%
46	7.894	2041	2054	2076	rBV	808823	1420244	77.42%	9.332%
47	8.174	2125	2141	2170	rBV2	181296	361240	19.69%	2.374%
48	8.463	2218	2231	2244	rBV2	39366	67193	3.66%	0.441%
49	8.573	2253	2265	2272	rBV8	8814	17797	0.97%	0.117%
50	8.634	2272	2284	2306	rVV2	544181	1186997	64.71%	7.799%
51	8.727	2306	2313	2327	rVB	81661	141983	7.74%	0.933%
52	8.833	2338	2346	2361	rVB	47912	77132	4.20%	0.507%
53	8.923	2372	2374	2380	rVB4	1055	894	0.05%	0.006%
54	8.949	2380	2382	2385	rVB3	668	326	0.02%	0.002%
55	9.049	2408	2413	2417	rBV3	886	820	0.04%	0.005%
56	9.103	2427	2430	2436	rBV2	618	459	0.03%	0.003%
57	9.209	2452	2463	2478	rBV	113397	187207	10.20%	1.230%
58	9.322	2494	2498	2500	rBV3	659	448	0.02%	0.003%
59	9.367	2505	2512	2514	rBV3	2139	2447	0.13%	0.016%
60	9.415	2514	2527	2553	rVV	712742	1203623	65.61%	7.908%
61	9.566	2569	2574	2584	rVB5	1560	2535	0.14%	0.017%
62	9.637	2593	2596	2597	rBV3	889	563	0.03%	0.004%
63	9.688	2609	2612	2613	rBV2	801	441	0.02%	0.003%
64	9.788	2635	2643	2645	rBV3	508	703	0.04%	0.005%
65	9.930	2681	2687	2693	rBV4	1314	1659	0.09%	0.011%
66	10.078	2724	2733	2745	rBV4	8319	15026	0.82%	0.099%
67	10.216	2773	2776	2781	rVB2	459	373	0.02%	0.002%
68	10.287	2796	2798	2801	rVB	539	318	0.02%	0.002%
69	10.309	2801	2805	2813	rBV2	346	483	0.03%	0.003%
70	10.489	2854	2861	2863	rBV2	988	1247	0.07%	0.008%
71	10.659	2910	2914	2917	rBV2	289	300	0.02%	0.002%
72	10.753	2929	2943	2965	rBV	658046	1086545	59.23%	7.139%
73	11.129	3057	3060	3066	rVB2	478	468	0.03%	0.003%
74	11.164	3066	3071	3074	rBV2	480	493	0.03%	0.003%
75	11.309	3112	3116	3119	rBV	549	377	0.02%	0.002%
76	11.328	3119	3122	3128	rVV2	450	506	0.03%	0.003%

LSC Area Percent Report

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Sample : PB156229TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB229

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\SFAMULM101023WMA.M
Title : VOC Analysis

77	11.473	3159	3167	3168	rBV4	1462	1786	0.10%	0.012%
78	11.531	3179	3185	3193	rBV2	467	744	0.04%	0.005%
79	11.749	3245	3253	3260	rBV5	2191	2828	0.15%	0.019%
80	11.811	3260	3272	3291	rBV	735073	1189177	64.82%	7.814%
81	12.068	3348	3352	3357	rBV4	764	923	0.05%	0.006%
82	12.190	3377	3390	3416	rBV	807170	1350517	73.62%	8.874%
83	12.775	3567	3572	3578	rBV2	799	982	0.05%	0.006%
84	12.827	3584	3588	3593	rBV3	508	627	0.03%	0.004%
85	12.872	3599	3602	3607	rBV2	625	629	0.03%	0.004%
86	13.232	3710	3714	3719	rBV5	1863	1923	0.10%	0.013%
87	13.296	3732	3734	3737	rBV2	576	337	0.02%	0.002%
88	13.322	3738	3742	3746	rVB2	729	565	0.03%	0.004%
89	13.347	3747	3750	3754	rVV2	651	337	0.02%	0.002%
90	13.425	3771	3774	3777	rBV2	587	352	0.02%	0.002%
91	13.614	3831	3833	3837	rBV3	983	556	0.03%	0.004%
92	13.666	3846	3849	3853	rVB2	844	613	0.03%	0.004%
93	13.692	3853	3857	3860	rBV3	506	500	0.03%	0.003%
94	13.849	3896	3906	3916	rBV7	5778	8571	0.47%	0.056%
95	14.100	3975	3984	4001	rBV4	7359	16249	0.89%	0.107%
96	14.335	4049	4057	4070	rVB6	5347	10157	0.55%	0.067%
97	14.392	4070	4075	4080	rVB2	729	784	0.04%	0.005%
98	14.894	4229	4231	4236	rBV4	849	700	0.04%	0.005%
99	14.974	4254	4256	4259	rVB2	827	423	0.02%	0.003%
100	15.518	4422	4425	4428	rBV3	761	436	0.02%	0.003%

Sum of corrected areas: 15219444

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Data File : VU055721.D
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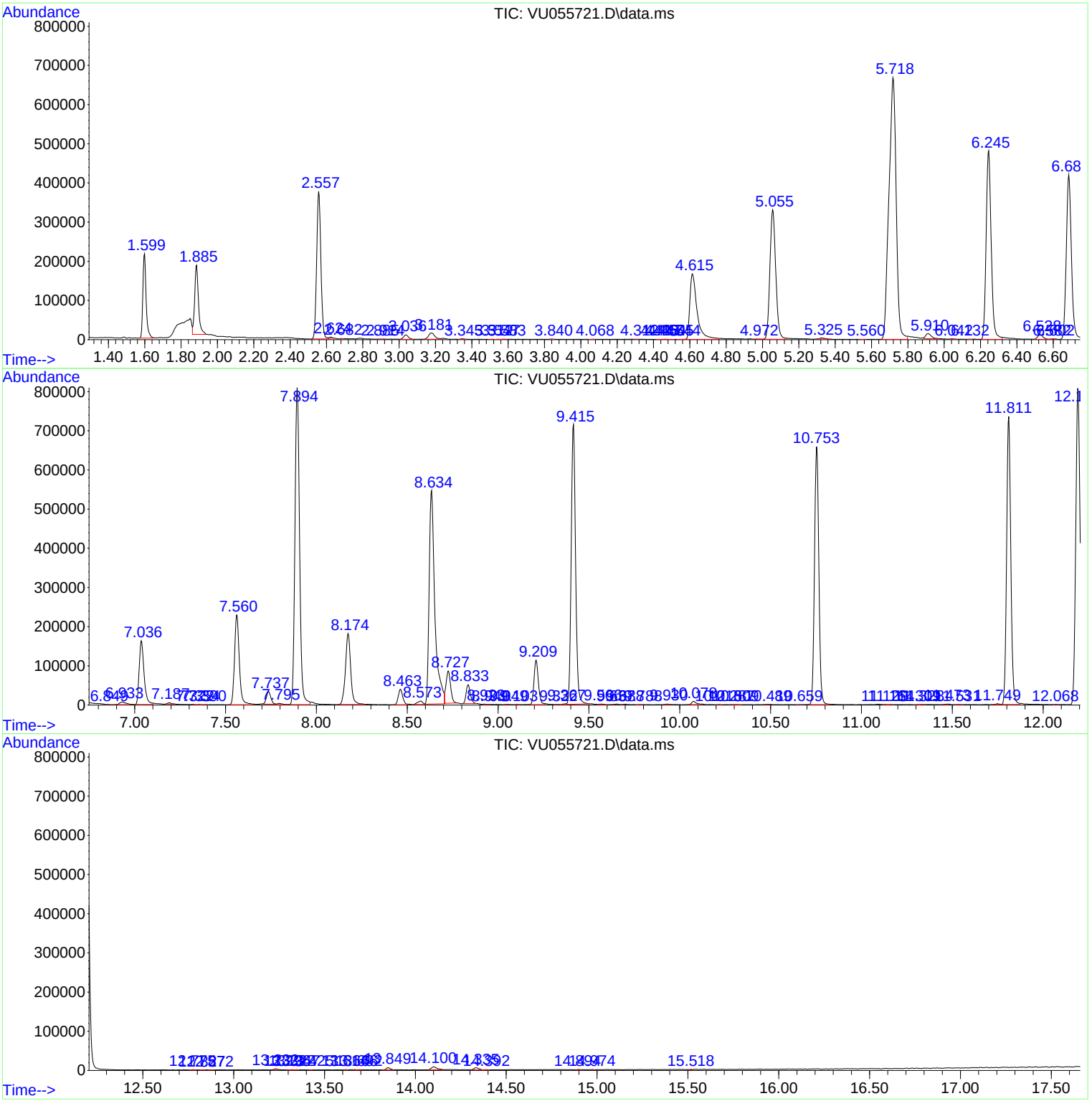
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB229

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101023\
Data File : VU055721.D
Acq On : 10 Oct 2023 15:10
Operator : MD/SY
Sample : PB156229TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB229

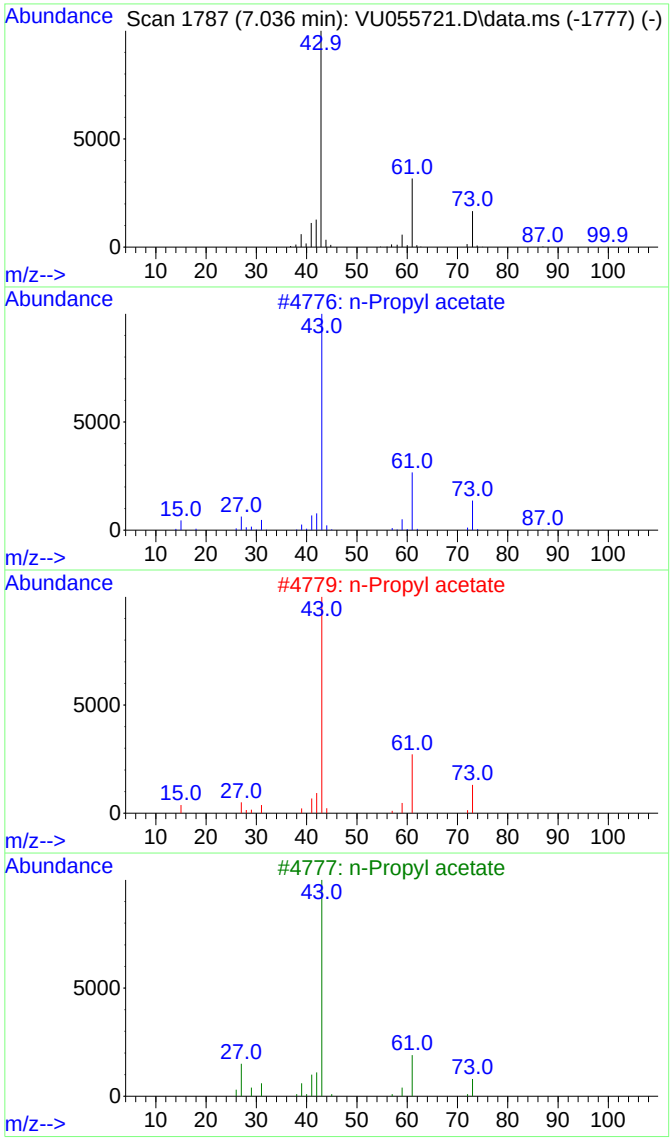
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

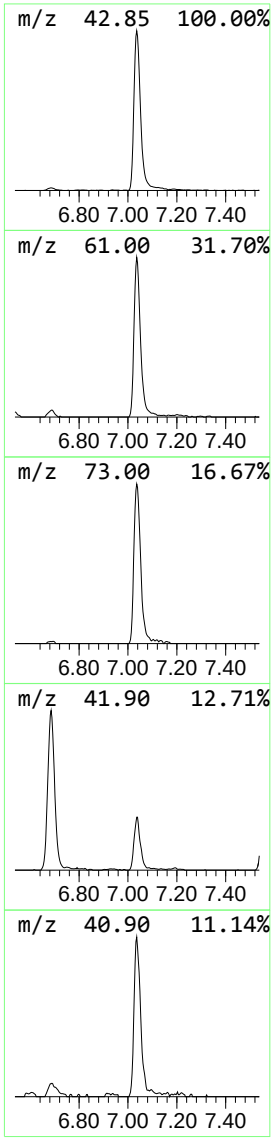
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.036	16.22 ug/L	301827	1,4-Difluorobenzene	6.245

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	72
3	n-Propyl acetate	102	C5H10O2	000109-60-4	72
4	n-Propyl acetate	102	C5H10O2	000109-60-4	64
5	n-Propyl acetate	102	C5H10O2	000109-60-4	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101023\
Data File : VU055721.D
Acq On : 10 Oct 2023 15:10
Operator : MD/SY
Sample : PB156229TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB229

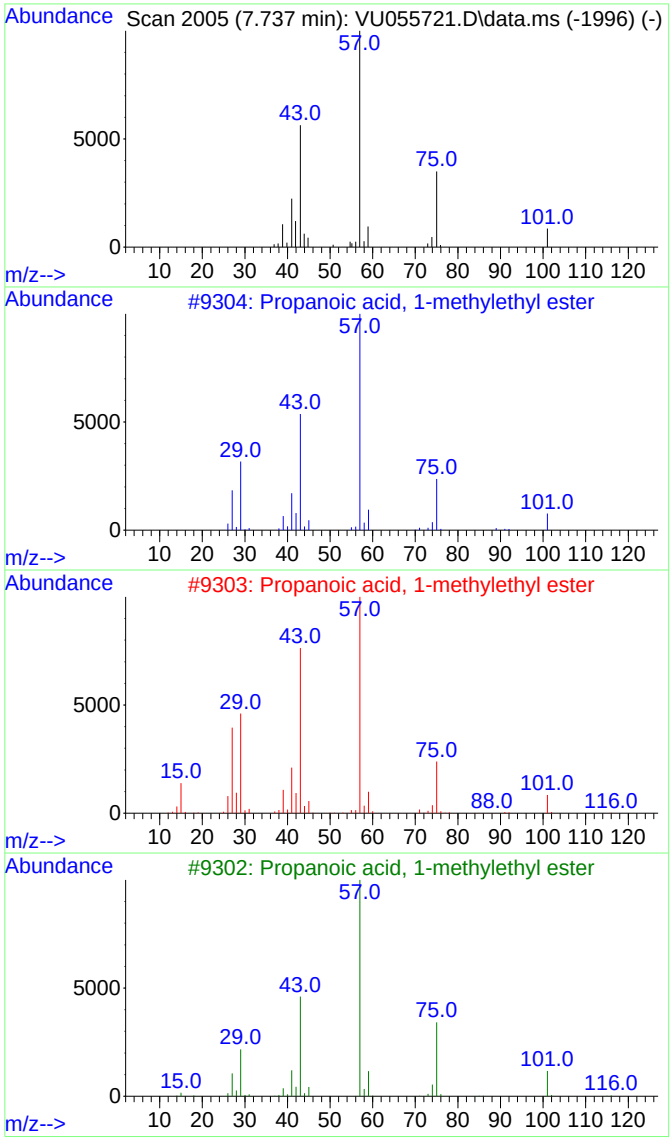
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

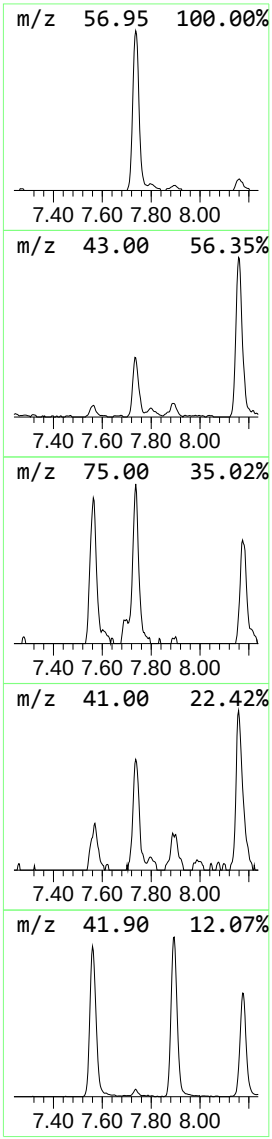
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.737	2.85 ug/L	53024	1,4-Difluorobenzene	6.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	78
2	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	64
3	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	64
4	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	50
5	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	40





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Data File : VU055721.D
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Sample : PB156229TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB229

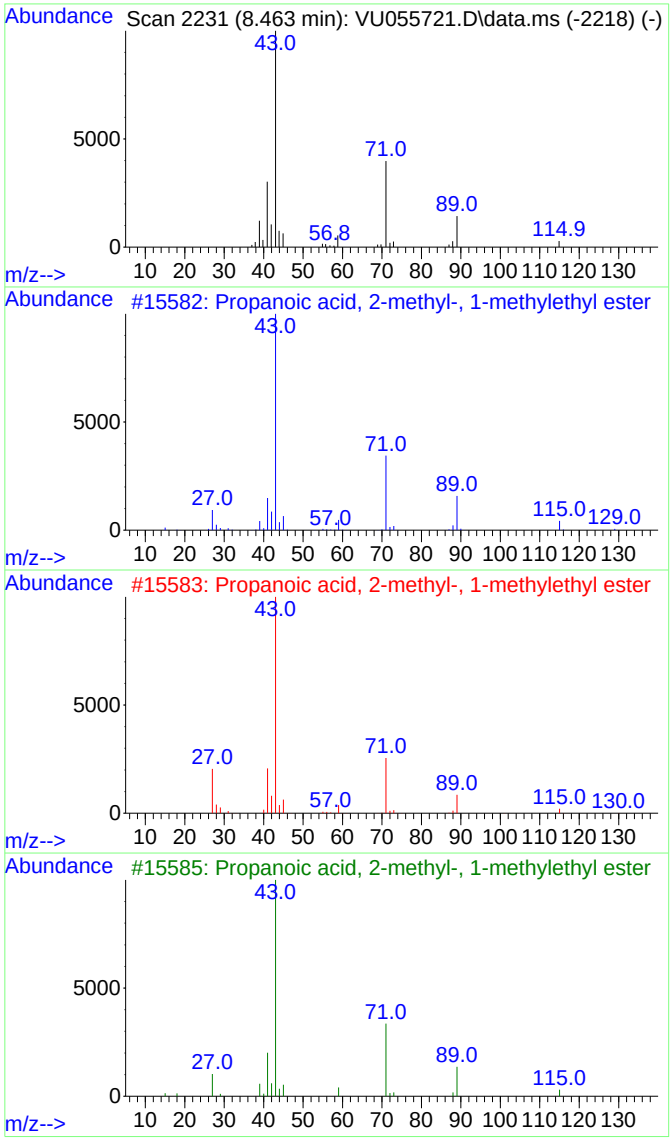
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

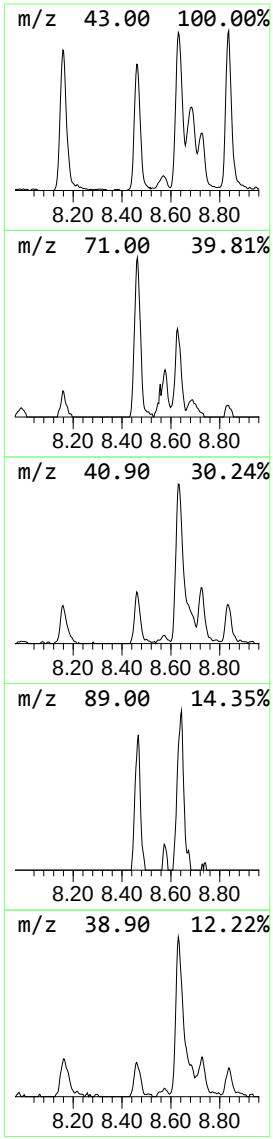
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Propanoic acid, 2-methyl-, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.463	2.79 ug/L	67193	Chlorobenzene-d5	9.415

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	78
5	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64





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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB229

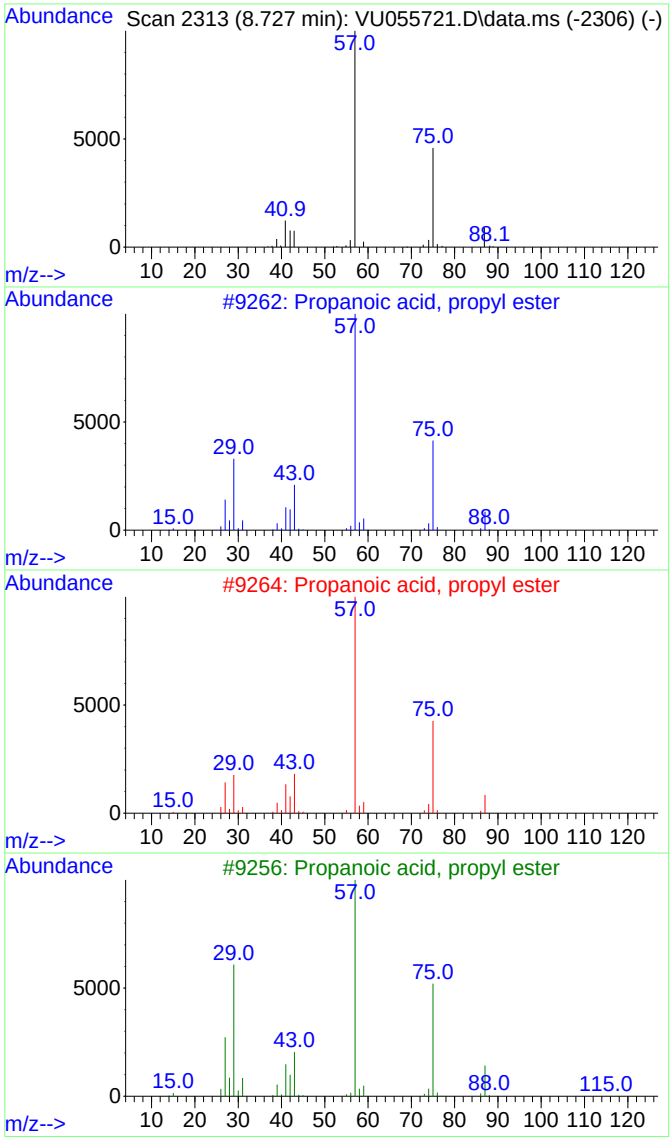
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

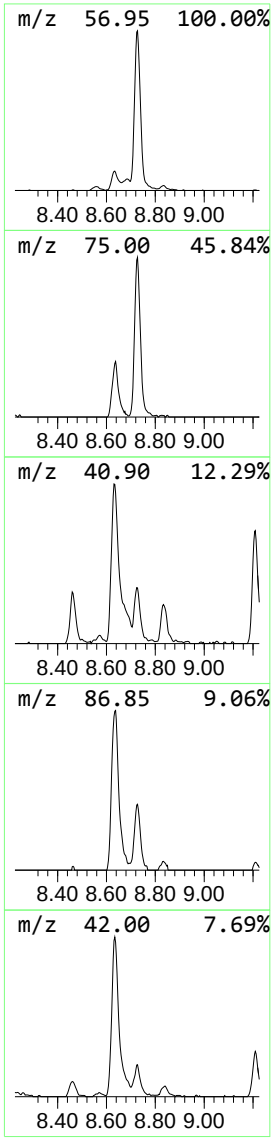
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Propanoic acid, propyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.727	5.90 ug/L	141983	Chlorobenzene-d5	9.415

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	78
2	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	64
3	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	64
4	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	56
5	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101023\
Data File : VU055721.D
Acq On : 10 Oct 2023 15:10
Operator : MD/SY
Sample : PB156229TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB229

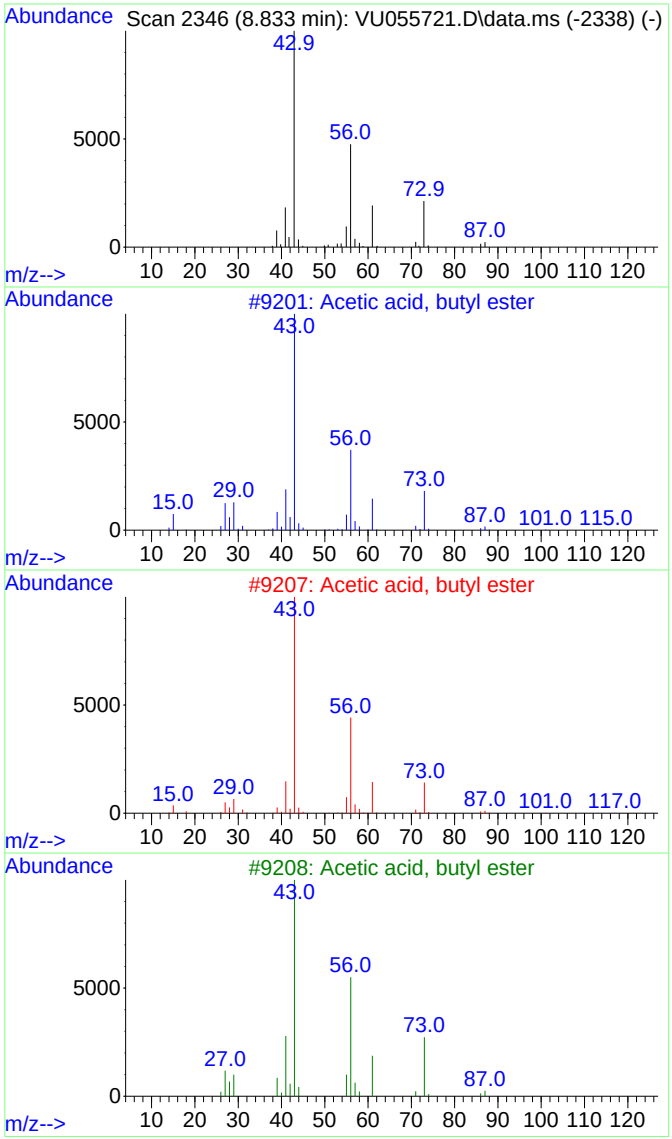
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

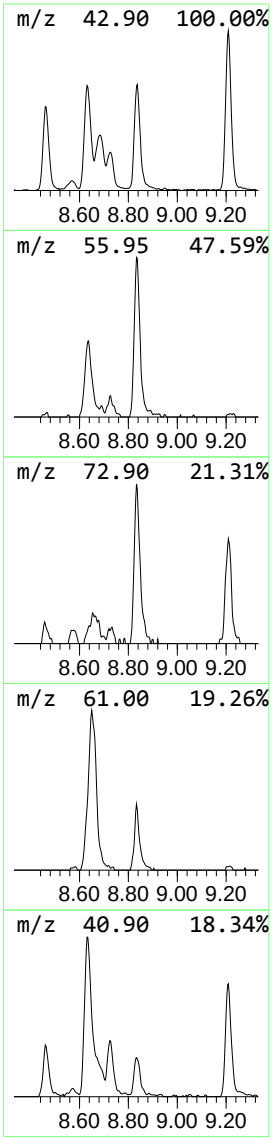
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.833	3.20 ug/L	77132	Chlorobenzene-d5	9.415

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	72
3	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	64
4	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	56
5	Isobutyl acetate	116	C6H12O2	000110-19-0	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101023\
Data File : VU055721.D
Acq On : 10 Oct 2023 15:10
Operator : MD/SY
Sample : PB156229TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB229

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

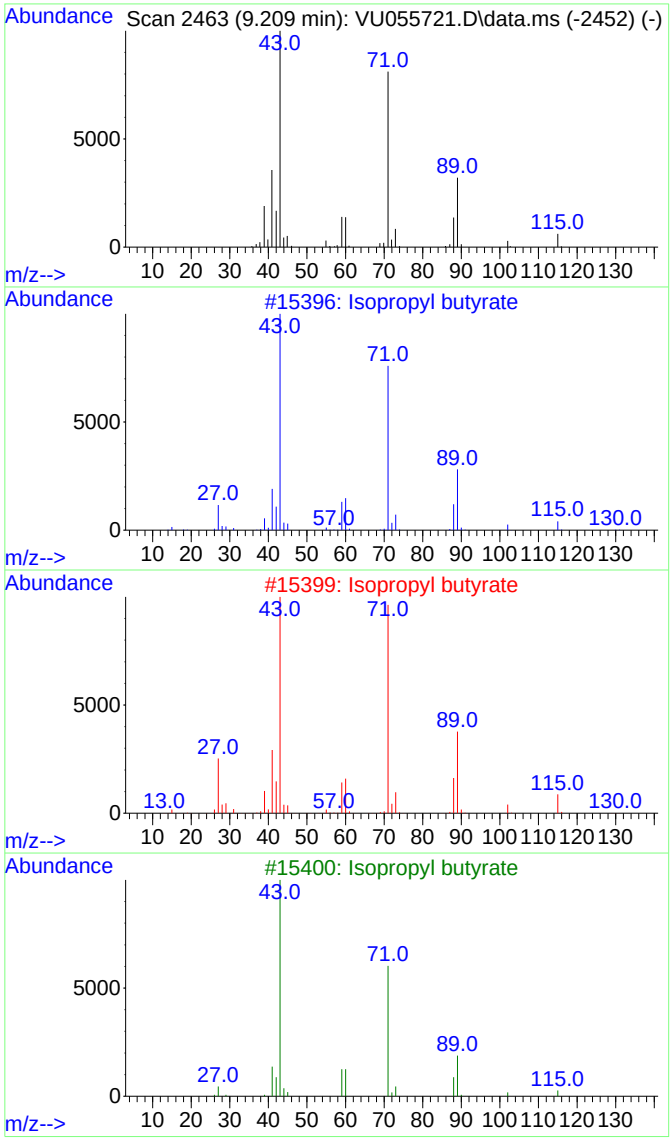
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

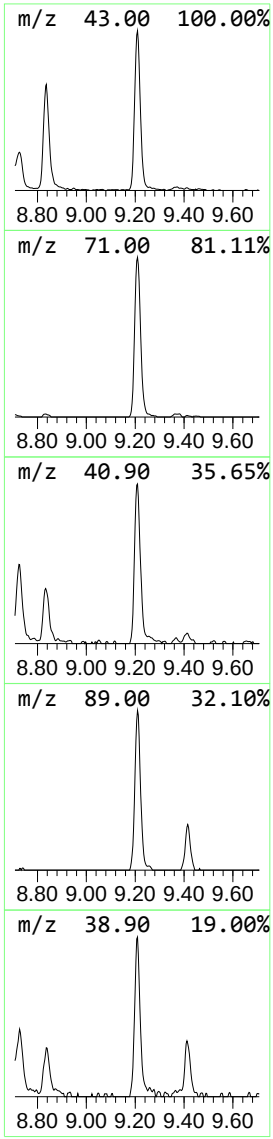
****

Peak Number 7 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.209	7.78 ug/L	187207	Chlorobenzene-d5	9.415

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl butyrate	130	C7H14O2	000638-11-9	90
2	Isopropyl butyrate	130	C7H14O2	000638-11-9	90
3	Isopropyl butyrate	130	C7H14O2	000638-11-9	83
4	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101023\
Data File : VU055721.D
Acq On : 10 Oct 2023 15:10
Operator : MD/SY
Sample : PB156229TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB229

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Propyl acetate	7.036	16.2	ug/L	301827	1	6.245	930324	50.0
Propanoic acid,...	7.737	2.9	ug/L	53024	1	6.245	930324	50.0
Propanoic acid,...	8.463	2.8	ug/L	67193	2	9.415	1203620	50.0
Propanoic acid,...	8.727	5.9	ug/L	141983	2	9.415	1203620	50.0
Acetic acid, bu...	8.833	3.2	ug/L	77132	2	9.415	1203620	50.0
Isopropyl butyrate	9.209	7.8	ug/L	187207	2	9.415	1203620	50.0