LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101623\
Data File : VU055774.D
Acq On : 16 Oct 2023 16:01
Operator : MD/SY
Sample : 04824-01 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : JYCA4

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: VU055774.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	219873	262508	13.87%	1.766%
2	1.779	138	152	154	rBV4	21825	42996	2.27%	0.289%
3	1.888	179	186	207	rVB	182704	267607	14.14%	1.800%
4	2.239	293	295	298	rBV3	1071	640	0.03%	0.004%
5	2.557	381	394	408	rBV	377928	625410	33.04%	4.206%
6	2.705	436	440	443	rBV3	1170	980	0.05%	0.007%
7	2.763	452	458	461	rVB5	1001	918	0.05%	0.006%
8	2.788	461	466	472	rBV4	1031	1424	0.08%	0.010%
9	2.882	492	495	497	rBV2	385	315	0.02%	0.002%
10	2.894	497	499	505	rVB4	739	547	0.03%	0.004%
11	2.956	510	518	521	rBV2	949	1090	0.06%	0.007%
12	3.039	532	544	556	rBV3	11337	21743	1.15%	0.146%
13	3.177	573	587	601	rVV2	8069	18132	0.96%	0.122%
14	3.293	619	623	627	rVV2	315	346	0.02%	0.002%
15	3.377	640	649	654	rBV2	1125	1475	0.08%	0.010%
16	3.531	693	697	702	rVB2	377	355	0.02%	0.002%
17	3.628	722	727	730	rBV2	394	329	0.02%	0.002%
18	3.705	748	751	755	rVB2	519	343	0.02%	0.002%
19	3.743	759	763	765	rVV2	452	327	0.02%	0.002%
20	3.833	789	791	794	rBV2	623	393	0.02%	0.003%
21	3.865	799	801	804	rVV4	498	335	0.02%	0.002%
22	4.036	849	854	859	rVB	531	505	0.03%	0.003%
23	4.238	912	917	922	rBV2	393	410	0.02%	0.003%
24	4.615	1022	1034	1076	rBV	132815	371166	19.61%	2.496%
25	4.827	1098	1100	1106	rVB3	1098	556	0.03%	0.004%
26	5.055	1153	1171	1194	rBV	349222	781992	41.31%	5.260%
27	5.621	1342	1347	1352	rBV2	293	338	0.02%	0.002%
28	5.717	1356	1377	1398	rBV2	689690	1892893	100.00%	12.731%
29	5.910	1430	1437	1456	rVB2	10170	22415	1.18%	0.151%
30	6.116	1498	1501	1503	rBV3	487	342	0.02%	0.002%
31	6.245	1523	1541	1560	rBV	532854	1041677	55.03%	7.006%
32	6.451	1602	1605	1609	rVB4	411	360	0.02%	0.002%
33	6.528	1617	1629	1642	rBV2	18213	36233	1.91%	0.244%
34	6.685	1664	1678	1706	rBV	430854	860685	45.47%	5.789%
35	6.856	1729	1731	1741	rVB5	893	1006	0.05%	0.007%
36	6.898	1741	1744	1745	rBV	665	367	0.02%	0.002%

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ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : JYCA4

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

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

37	6.926	1745	1753	1756	rBV2	5075	6335	0.33%	0.043%
38	7.036	1777	1787	1810	rBV	98050	185626	9.81%	1.248%
39	7.190	1828	1835	1854	rVB7	6546	15555	0.82%	0.105%
40	7.290	1863	1866	1869	rBV2	749	516	0.03%	0.003%
41	7.312	1869	1873	1876	rVV3	862	747	0.04%	0.005%
42	7.328	1876	1878	1883	rVB2	507	336	0.02%	0.002%
43	7.399	1893	1900	1903	rBV3	576	600	0.03%	0.004%
44	7.560	1938	1950	1969	rBV	221631	401089	21.19%	2.698%
45	7.698	1985	1993	1995	rVV5	2714	3497	0.18%	0.024%
46	7.733	1997	2004	2017	rVB3	25504	43605	2.30%	0.293%
47	7.894	2039	2054	2081	rBV	818297	1453892	76.81%	9.779%
48	8.087	2111	2114	2122	rVB3	772	678	0.04%	0.005%
49	8.174	2127	2141	2158	rBV2	169081	317169	16.76%	2.133%
50	8.319	2184	2186	2190	rBV3	436	362	0.02%	0.002%
51	8.463	2220	2231	2246	rVV	32084	54396	2.87%	0.366%
52	8.573	2253	2265	2272	rBV	4899	10658	0.56%	0.072%
53	8.634	2272	2284	2306	rBV3	345604	816454	43.13%	5.491%
54	8.727	2307	2313	2325	rVB	54668	90866	4.80%	0.611%
55	8.836	2338	2347	2365	rVB2	24334	41642	2.20%	0.280%
56	9.113	2431	2433	2437	rVB2	531	363	0.02%	0.002%
57	9.209	2451	2463	2486	rBV2	86595	144401	7.63%	0.971%
58	9.338	2500	2503	2506	rVB4	590	377	0.02%	0.003%
59	9.415	2506	2527	2555	rBV	803921	1366335	72.18%	9.190%
60	9.650	2593	2600	2605	rBV6	1245	1572	0.08%	0.011%
61	9.698	2610	2615	2624	rVB3	696	993	0.05%	0.007%
62	9.737	2624	2627	2631	rBV	475	326	0.02%	0.002%
63	9.852	2658	2663	2666	rBV2	416	459	0.02%	0.003%
64	9.936	2683	2689	2690	rBV3	987	962	0.05%	0.006%
65	10.077	2724	2733	2743	rBV3	4562	7979	0.42%	0.054%
66	10.171	2757	2762	2767	rBV3	703	598	0.03%	0.004%
67	10.296	2799	2801	2807	rVB	542	403	0.02%	0.003%
68	10.325	2807	2810	2814	rBV	402	312	0.02%	0.002%
69	10.399	2820	2833	2835	rBV2	461	785	0.04%	0.005%
70	10.753	2929	2943	2965	rBV	630735	1046007	55.26%	7.035%
71	10.878	2979	2982	2987	rVB4	395	349	0.02%	0.002%
72	11.000	3015	3020	3023	rBV3	407	389	0.02%	0.003%
73	11.116	3052	3056	3061	rVB4	629	634	0.03%	0.004%
74	11.180	3073	3076	3082	rVB3	416	415	0.02%	0.003%
75	11.267	3099	3103	3108	rVB2	424	398	0.02%	0.003%
76	11.720	3242	3244	3248	rVB3	637	413	0.02%	0.003%

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ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
JYCA4

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
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Peak separation: 5

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

77	11.753	3248	3254	3257	rBV3	612	496	0.03%	0.003%
78	11.810	3259	3272	3290	rBV	763340	1248907	65.98%	8.400%
79	12.061	3346	3350	3355	rVB2	558	667	0.04%	0.004%
80	12.100	3359	3362	3365	rBV3	416	333	0.02%	0.002%
81	12.190	3376	3390	3417	rBV	787152	1329658	70.24%	8.943%
82	12.425	3461	3463	3473	rVB5	740	736	0.04%	0.005%
83	12.534	3494	3497	3501	rVB2	606	501	0.03%	0.003%
84	12.624	3522	3525	3527	rBV2	483	309	0.02%	0.002%
85	12.753	3561	3565	3567	rBV2	624	449	0.02%	0.003%
86	12.852	3592	3596	3599	rVB2	508	468	0.02%	0.003%
87	12.955	3620	3628	3630	rBV2	429	588	0.03%	0.004%
88	13.055	3653	3659	3661	rBV3	421	457	0.02%	0.003%
89	13.113	3675	3677	3681	rVB2	523	345	0.02%	0.002%
90	13.344	3745	3749	3752	rBV2	614	591	0.03%	0.004%
91	13.434	3774	3777	3782	rBV3	466	488	0.03%	0.003%
92	13.505	3796	3799	3803	rBV	568	432	0.02%	0.003%
93	13.531	3803	3807	3813	rVV	719	729	0.04%	0.005%
94	13.740	3870	3872	3878	rVB	564	361	0.02%	0.002%
95	14.097	3980	3983	3984	rBV2	525	316	0.02%	0.002%
96	14.203	4014	4016	4021	rBV	428	427	0.02%	0.003%
97	15.000	4262	4264	4266	rBV2	569	379	0.02%	0.003%
98	15.293	4353	4355	4359	rBV2	554	460	0.02%	0.003%
99	15.624	4454	4458	4460	rBV3	1678	1377	0.07%	0.009%
100	15.868	4531	4534	4538	rBV3	1087	1003	0.05%	0.007%

Sum of corrected areas: 14868128

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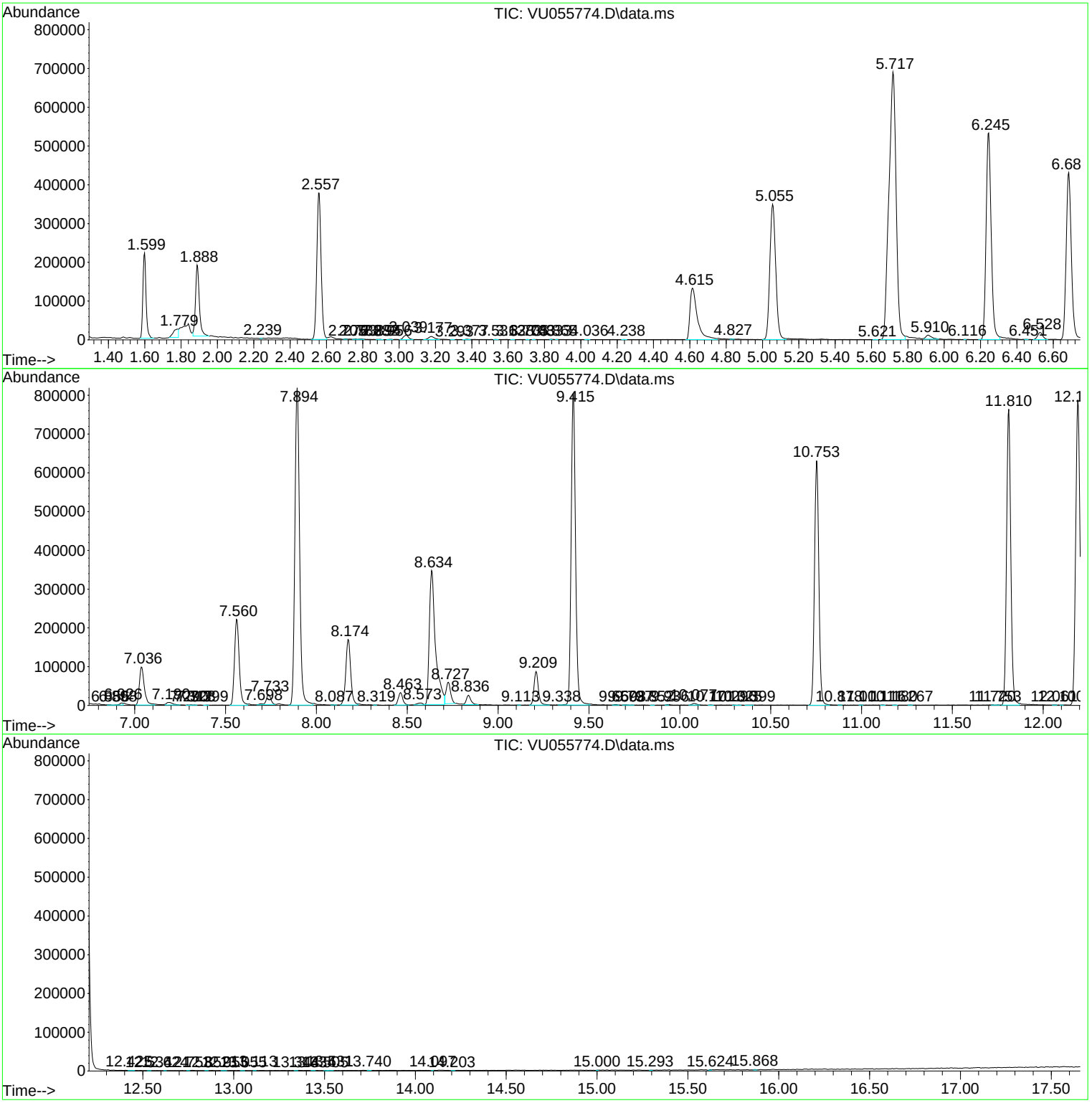
Instrument :
MSVOA_U
ClientSampleId :
JYCA4

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



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Quant Title : VOC Analysis

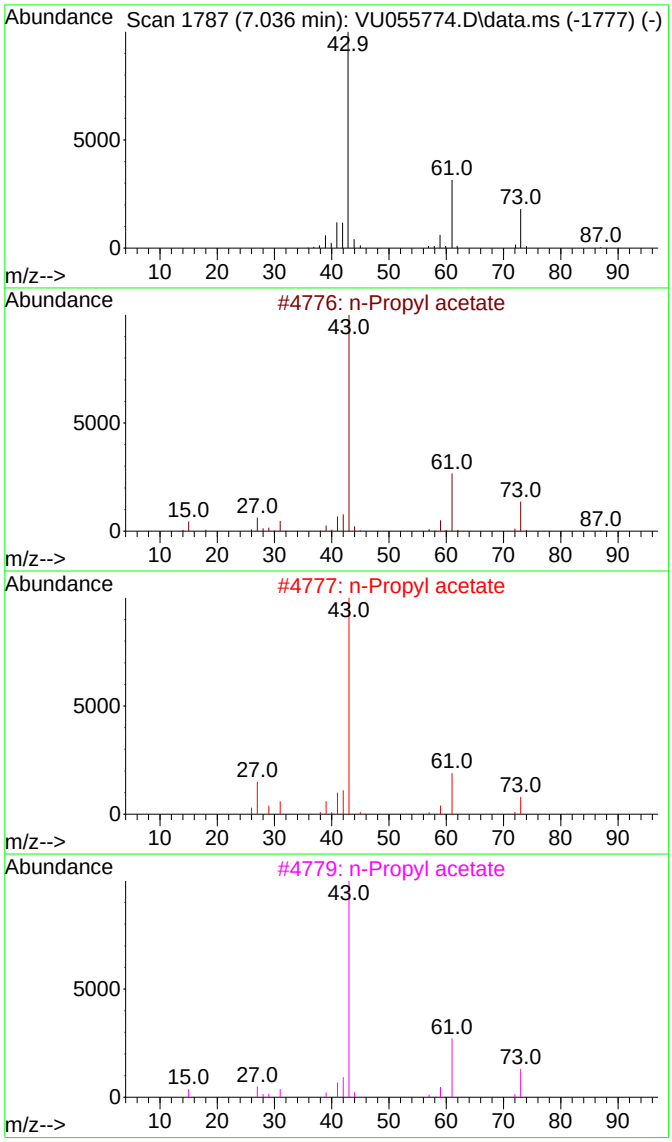
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

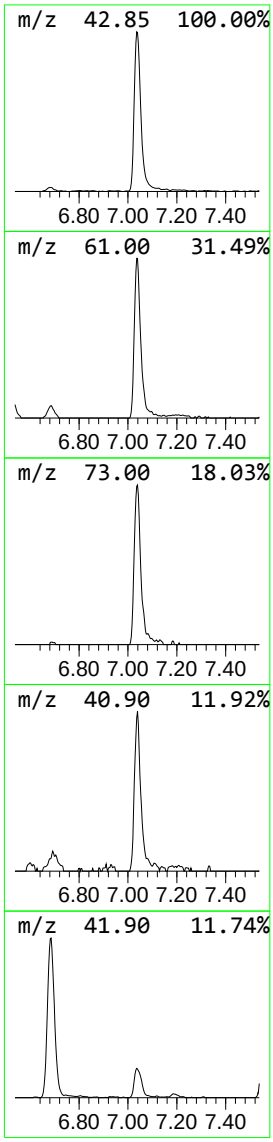
****

Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.036	8.91 ug/L	185626	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	64
4	n-Propyl acetate	102	C5H10O2	000109-60-4	56
5	n-Propyl acetate	102	C5H10O2	000109-60-4	50





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Instrument :
MSVOA_U
ClientSampleId :
JYCA4

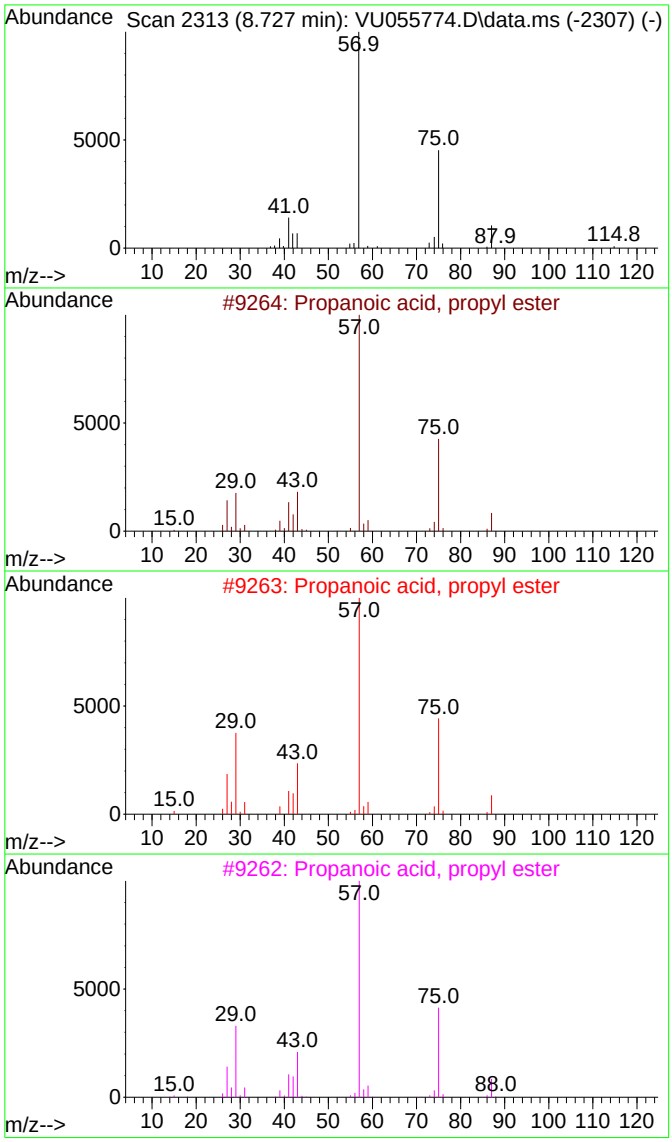
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

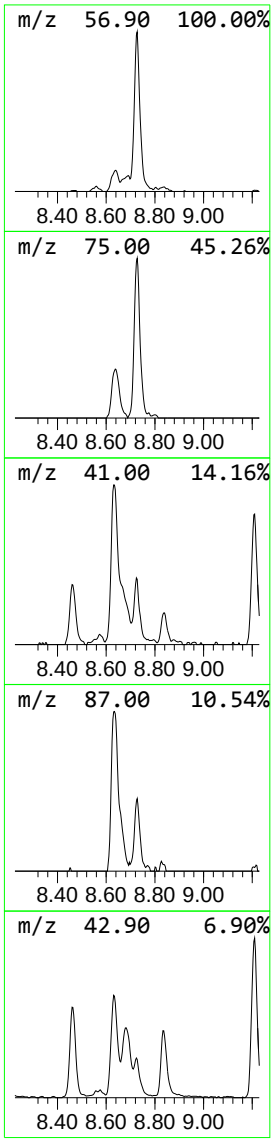
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Propanoic acid, propyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.727	3.33 ug/L	90866	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	78
3	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	64
4	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	43
5	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	43





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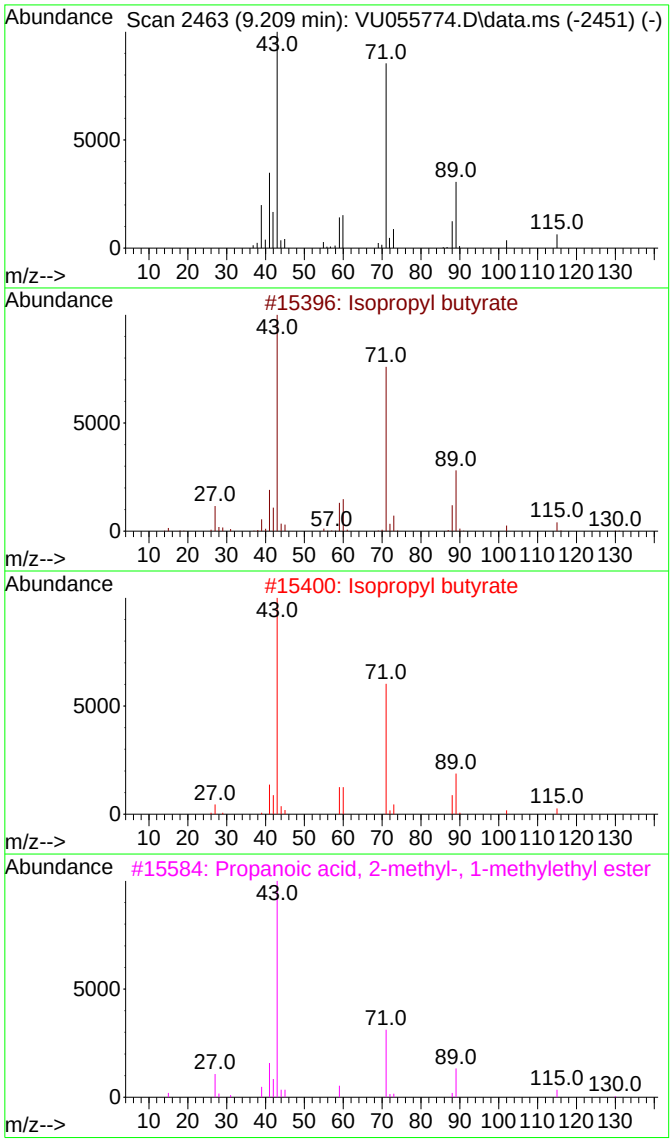
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

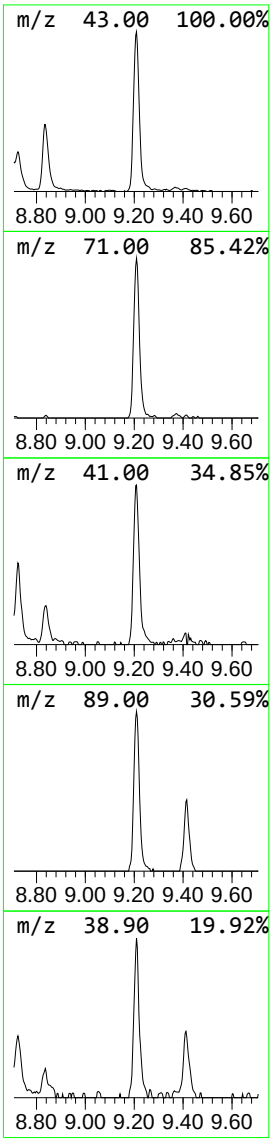
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.209	5.28 ug/L	144401	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	78
3	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
4	Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	72
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72





Tentatively Identified Compound (LSC) summary

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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	8.9	ug/L	185626	1	6.245	1041680	50.0
Propanoic acid,...	8.727	3.3	ug/L	90866	2	9.415	1366340	50.0
Isopropyl butyrate	9.209	5.3	ug/L	144401	2	9.415	1366340	50.0