LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV040424\
Data File : VV034967.D
Acq On : 04 Apr 2024 10:47
Operator : SY/MD
Sample : PB159941TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB941

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_V\Method\SFAMVLM032624WMA.M
Title : VOC Analysis

Signal : TIC: VV034967.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.214	50	54	57	rBV2	1791	1906	0.11%	0.014%
2	1.281	68	75	92	rVB	240461	257522	14.76%	1.887%
3	1.535	146	154	170	rBV	225045	268271	15.38%	1.966%
4	2.060	307	317	333	rBV	424429	617955	35.42%	4.529%
5	2.259	377	379	382	rVB4	668	348	0.02%	0.003%
6	2.449	429	438	453	rVB2	8151	14603	0.84%	0.107%
7	2.507	453	456	459	rVB5	486	339	0.02%	0.002%
8	2.526	459	462	467	rBV3	555	448	0.03%	0.003%
9	2.709	515	519	525	rVB7	568	688	0.04%	0.005%
10	2.815	548	552	554	rBV	459	334	0.02%	0.002%
11	2.879	568	572	575	rBV3	622	455	0.03%	0.003%
12	2.905	578	580	586	rVB3	454	430	0.02%	0.003%
13	2.950	590	594	595	rBV	622	335	0.02%	0.002%
14	3.040	617	622	625	rVB4	506	379	0.02%	0.003%
15	3.069	625	631	632	rBV3	541	460	0.03%	0.003%
16	3.127	642	649	650	rBV3	386	365	0.02%	0.003%
17	3.137	650	652	656	rVV	660	470	0.03%	0.003%
18	3.195	668	670	674	rVB4	725	511	0.03%	0.004%
19	3.220	674	678	681	rBV3	425	389	0.02%	0.003%
20	3.294	697	701	704	rBV3	508	410	0.02%	0.003%
21	3.349	711	718	723	rVB3	432	568	0.03%	0.004%
22	3.539	774	777	783	rVB2	510	480	0.03%	0.004%
23	3.584	788	791	796	rVB3	421	338	0.02%	0.002%
24	3.796	846	857	911	rBV	90573	314049	18.00%	2.302%
25	4.246	981	997	1034	rBV	270471	705875	40.46%	5.173%
26	4.484	1067	1071	1076	rVB5	856	949	0.05%	0.007%
27	4.519	1079	1082	1085	rVB3	592	380	0.02%	0.003%
28	4.658	1121	1125	1128	rBV2	785	720	0.04%	0.005%
29	4.735	1145	1149	1153	rVB3	455	442	0.03%	0.003%
30	4.767	1153	1159	1164	rBV5	719	751	0.04%	0.006%
31	4.828	1171	1178	1180	rBV3	423	414	0.02%	0.003%
32	4.953	1201	1217	1261	rBV2	651994	1744657	100.00%	12.786%
33	5.214	1290	1298	1311	rBV3	7727	17331	0.99%	0.127%
34	5.304	1324	1326	1328	rBV2	867	386	0.02%	0.003%
35	5.532	1386	1397	1422	rBV	483621	996954	57.14%	7.307%
36	5.719	1453	1455	1458	rVB4	957	448	0.03%	0.003%

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Instrument :
MSVOA_V
ClientSampleId :
VLEB941

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_V\Method\SFAMVLM032624WMA.M
Title : VOC Analysis

37	5.831	1478	1490	1506	rBV3	20937	47636	2.73%	0.349%
38	5.985	1525	1538	1574	rVV	385619	803336	46.05%	5.888%
39	6.207	1605	1607	1610	rBV3	764	406	0.02%	0.003%
40	6.304	1633	1637	1640	rBV5	1951	1748	0.10%	0.013%
41	6.394	1657	1665	1710	rBV	109340	235809	13.52%	1.728%
42	6.686	1754	1756	1761	rVB3	1038	713	0.04%	0.005%
43	6.776	1781	1784	1787	rVB3	489	364	0.02%	0.003%
44	6.911	1816	1826	1853	rBV	192254	371588	21.30%	2.723%
45	7.120	1883	1891	1904	rBV	25465	46458	2.66%	0.340%
46	7.239	1917	1928	1956	rBV	771985	1357885	77.83%	9.952%
47	7.458	1994	1996	1999	rBV3	594	355	0.02%	0.003%
48	7.551	2016	2025	2058	rBV	158371	310737	17.81%	2.277%
49	7.863	2109	2122	2136	rBV	37503	68023	3.90%	0.499%
50	7.947	2146	2148	2151	rBV3	635	419	0.02%	0.003%
51	7.979	2151	2158	2162	rVV4	7852	10957	0.63%	0.080%
52	8.027	2163	2173	2198	rVV2	298762	696272	39.91%	5.103%
53	8.130	2200	2205	2231	rVV2	66163	131680	7.55%	0.965%
54	8.249	2234	2242	2270	rVB2	29718	61658	3.53%	0.452%
55	8.487	2314	2316	2319	rVB2	682	344	0.02%	0.003%
56	8.619	2347	2357	2375	rBV	108115	182418	10.46%	1.337%
57	8.783	2397	2408	2437	rBV	779677	1272497	72.94%	9.326%
58	9.056	2491	2493	2496	rBV3	747	370	0.02%	0.003%
59	9.159	2522	2525	2530	rVB3	516	401	0.02%	0.003%
60	9.249	2549	2553	2557	rBV3	541	488	0.03%	0.004%
61	9.381	2591	2594	2599	rBV3	479	451	0.03%	0.003%
62	9.452	2611	2616	2622	rVB7	654	763	0.04%	0.006%
63	9.500	2622	2631	2639	rBV4	4510	8755	0.50%	0.064%
64	9.616	2663	2667	2672	rVB2	547	570	0.03%	0.004%
65	9.667	2679	2683	2686	rVV4	456	395	0.02%	0.003%
66	9.812	2724	2728	2731	rBV3	631	534	0.03%	0.004%
67	9.898	2753	2755	2760	rVB5	524	376	0.02%	0.003%
68	9.972	2772	2778	2780	rBV3	608	652	0.04%	0.005%
69	10.101	2813	2818	2821	rBV2	449	390	0.02%	0.003%
70	10.149	2821	2833	2855	rBV	497070	781450	44.79%	5.727%
71	10.435	2918	2922	2925	rBV2	483	458	0.03%	0.003%
72	10.683	2996	2999	3004	rVB2	407	441	0.03%	0.003%
73	10.783	3027	3030	3033	rVB4	529	421	0.02%	0.003%
74	10.870	3054	3057	3064	rVB3	388	392	0.02%	0.003%
75	11.127	3134	3137	3138	rBV	905	543	0.03%	0.004%
76	11.185	3144	3155	3182	rBV	704900	1104316	63.30%	8.093%

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ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
VLEB941

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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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM032624WMA.M
Title : VOC Analysis

77	11.558	3259	3271	3296	rBV	743177	1169260	67.02%	8.569%
78	12.011	3409	3412	3419	rVB4	381	362	0.02%	0.003%
79	12.191	3465	3468	3474	rVB3	569	553	0.03%	0.004%
80	12.361	3516	3521	3526	rVV5	509	506	0.03%	0.004%
81	12.792	3650	3655	3657	rBV3	565	479	0.03%	0.004%
82	12.924	3694	3696	3702	rVB2	560	558	0.03%	0.004%
83	13.095	3747	3749	3752	rVB3	549	333	0.02%	0.002%
84	13.210	3776	3785	3792	rVV8	3709	6408	0.37%	0.047%
85	13.326	3819	3821	3828	rVB	778	636	0.04%	0.005%
86	13.458	3852	3862	3868	rBV5	2700	4086	0.23%	0.030%
87	13.529	3880	3884	3890	rVB3	578	469	0.03%	0.003%
88	13.615	3909	3911	3916	rBV4	471	368	0.02%	0.003%
89	13.680	3927	3931	3932	rBV2	665	507	0.03%	0.004%
90	13.927	4003	4008	4010	rBV3	615	603	0.03%	0.004%
91	13.992	4025	4028	4031	rBV3	500	330	0.02%	0.002%
92	14.066	4048	4051	4055	rBV2	587	509	0.03%	0.004%
93	14.162	4078	4081	4085	rVB3	820	545	0.03%	0.004%
94	14.377	4146	4148	4154	rVB4	1026	780	0.04%	0.006%
95	14.422	4159	4162	4163	rBV	637	342	0.02%	0.003%
96	14.480	4178	4180	4186	rVB4	711	491	0.03%	0.004%
97	14.647	4229	4232	4236	rVB4	629	386	0.02%	0.003%
98	14.943	4322	4324	4329	rBV2	468	426	0.02%	0.003%
99	15.024	4345	4349	4351	rVV3	600	421	0.02%	0.003%
100	15.319	4439	4441	4443	rBV2	608	343	0.02%	0.003%

Sum of corrected areas: 13644530

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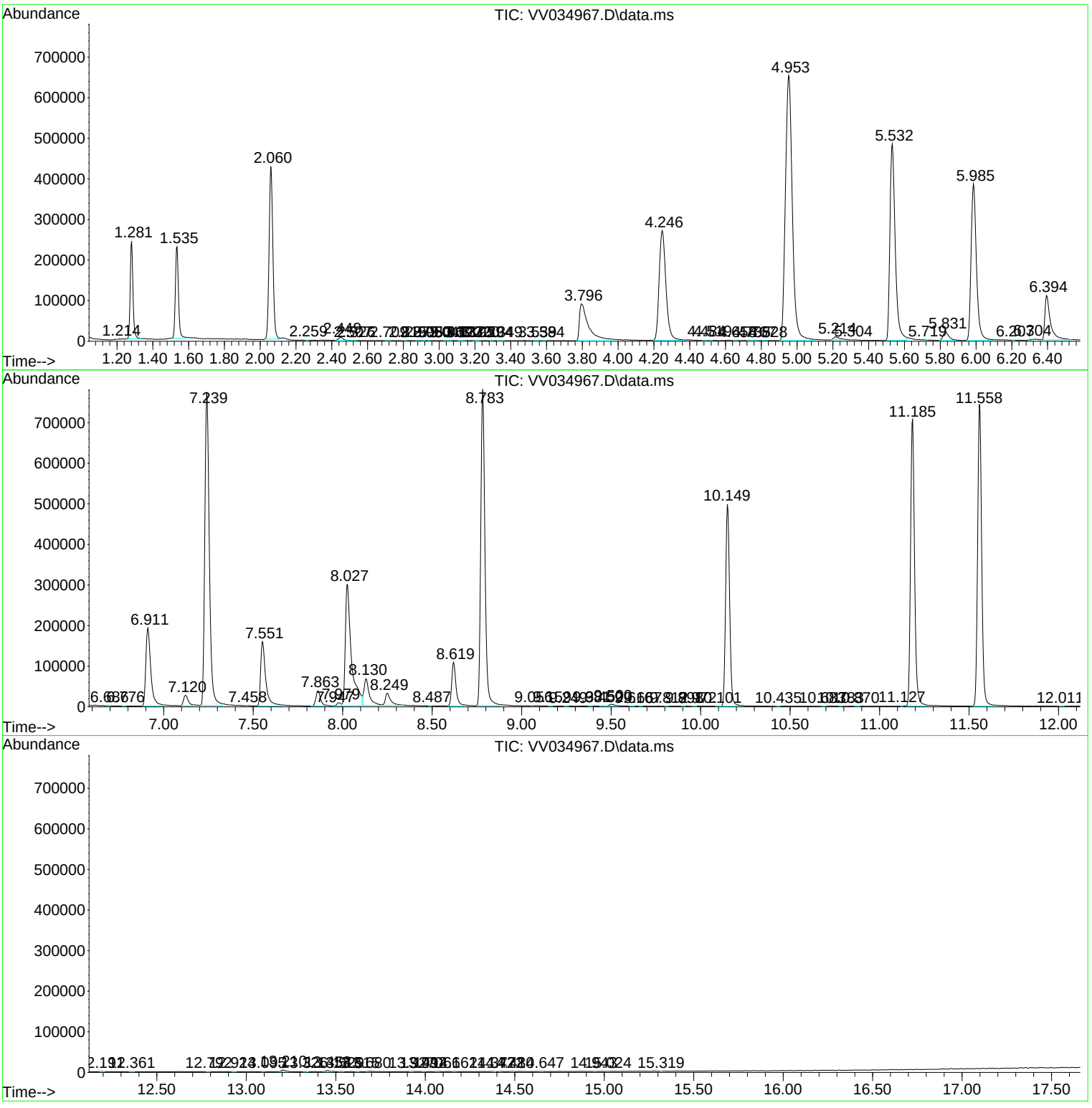
Instrument :
MSVOA_V
ClientSampleId :
VLEB941

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM032624WMA.M
Quant Title : VOC Analysis

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



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM032624WMA.M
Quant Title : VOC Analysis

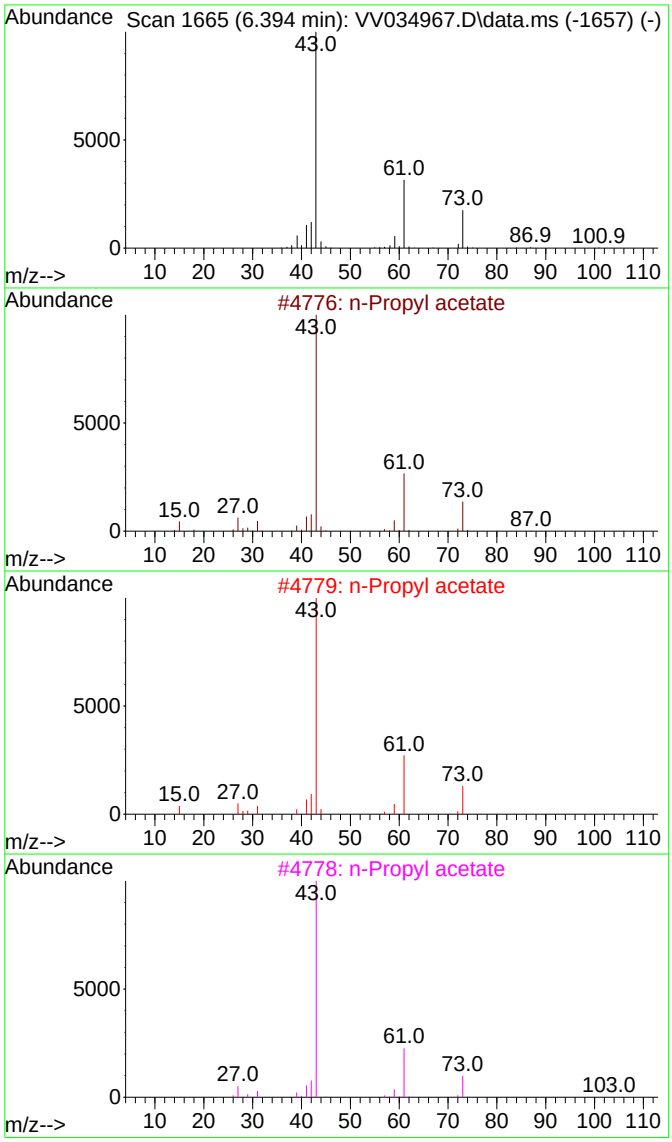
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

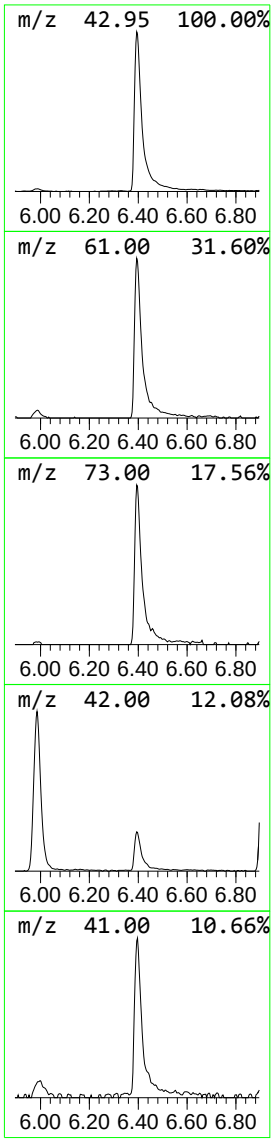
****

Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.394	11.83 ug/L	235809	1,4-Difluorobenzene	5.532

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	64
5	Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	36





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Instrument :
MSVOA_V
ClientSampleId :
VLEB941

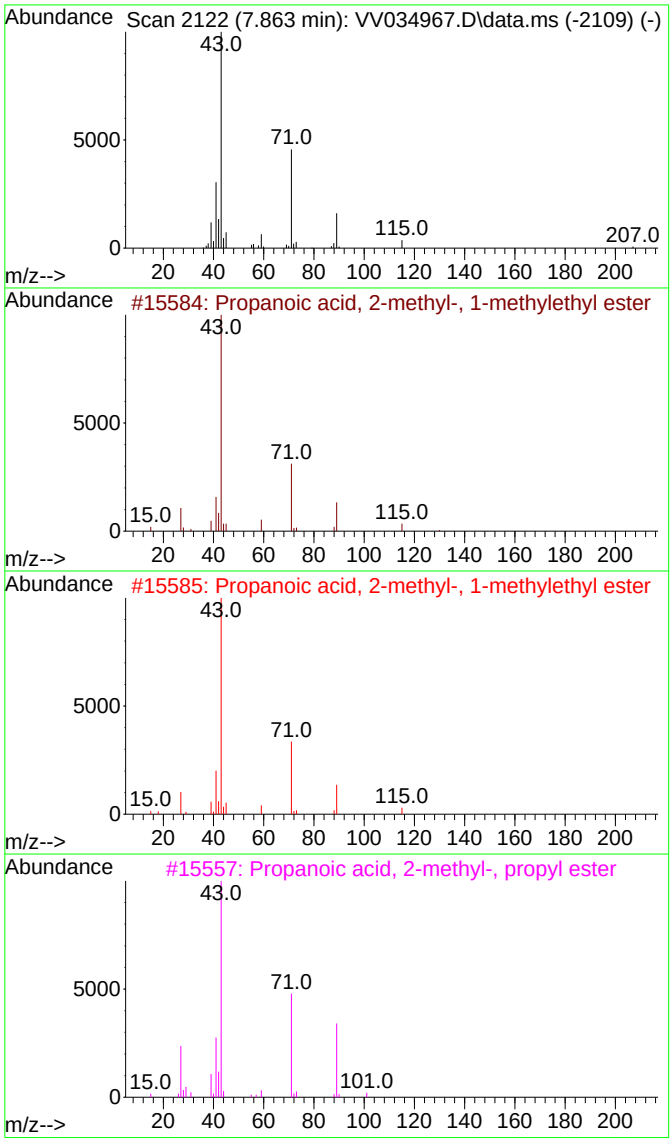
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM032624WMA.M
Quant Title : VOC Analysis

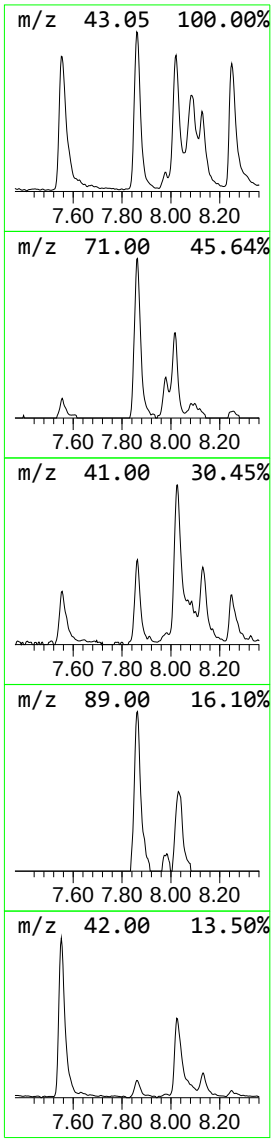
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Propanoic acid, 2-methyl-, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.863	2.67 ug/L	68023	Chlorobenzene-d5	8.783

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





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ClientSampleId :
VLEB941

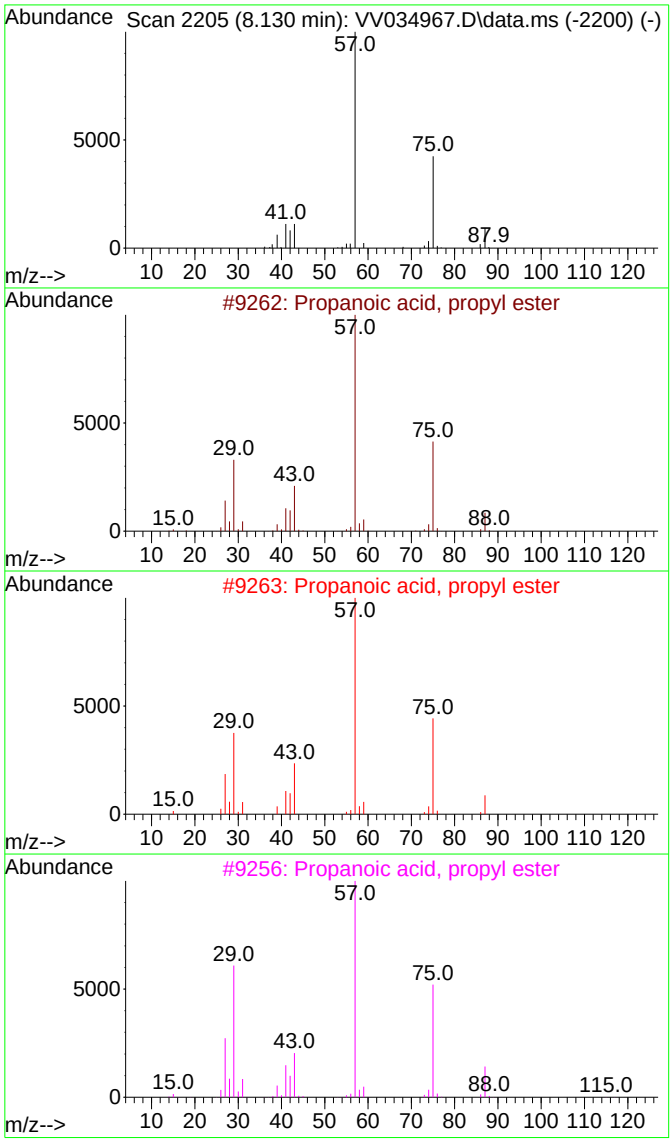
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM032624WMA.M
Quant Title : VOC Analysis

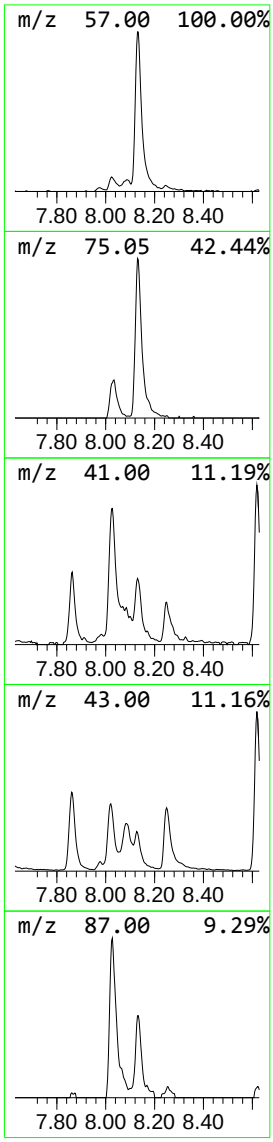
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.130	5.17 ug/L	131680	Chlorobenzene-d5	8.783

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	72
3	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	64
4	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	56
5	n-Hexane	86	C6H14	000110-54-3	9





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Instrument :
MSVOA_V
ClientSampleId :
VLEB941

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM032624WMA.M
Quant Title : VOC Analysis

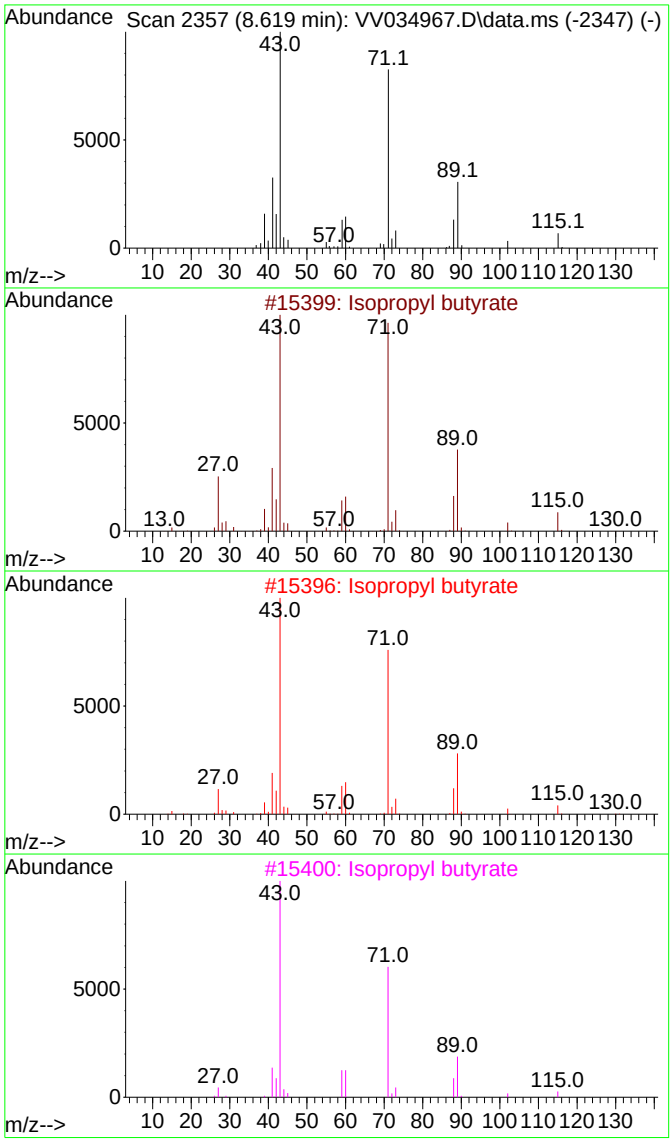
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

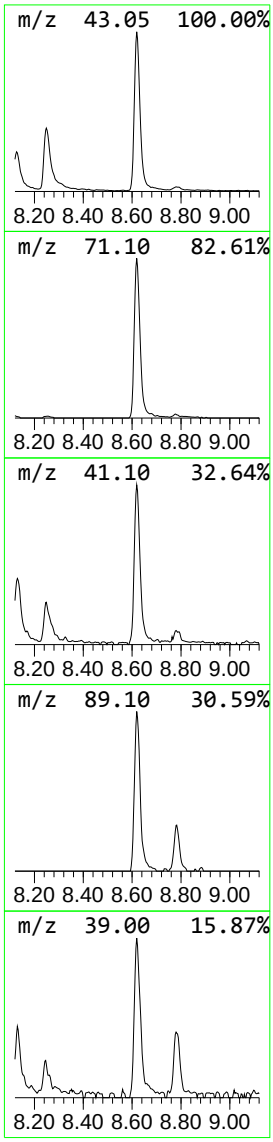
****

Peak Number 5 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.619	7.17 ug/L	182418	Chlorobenzene-d5	8.783

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl butyrate	130	C7H14O2	000638-11-9	91
2	Isopropyl butyrate	130	C7H14O2	000638-11-9	90
3	Isopropyl butyrate	130	C7H14O2	000638-11-9	83
4	Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	72
5	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72





Tentatively Identified Compound (LSC) summary

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ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB941

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM032624WMA.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	6.394	11.8	ug/L	235809	1	5.532	996954	50.0
Propanoic acid,...	7.863	2.7	ug/L	68023	2	8.783	1272500	50.0
Propanoic acid,...	8.130	5.2	ug/L	131680	2	8.783	1272500	50.0
Isopropyl butyrate	8.619	7.2	ug/L	182418	2	8.783	1272500	50.0