LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV090823\
Data File : VV031982.D
Acq On : 08 Sep 2023 13:53
Operator : SY/MD
Sample : PB155394TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB394

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\SFAMVLM082323WMA.M
Title : VOC Analysis

Signal : TIC: VV031982.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.278	68	74	89	rVB	122702	134733	13.86%	1.549%
2	1.532	146	153	174	rVB	99385	122775	12.63%	1.412%
3	2.059	309	317	330	rVB	197641	279600	28.75%	3.215%
4	2.449	429	438	451	rVB2	10689	18200	1.87%	0.209%
5	2.568	463	475	480	rBV7	1629	3150	0.32%	0.036%
6	2.651	499	501	505	rVB3	470	292	0.03%	0.003%
7	2.838	557	559	562	rBV3	548	274	0.03%	0.003%
8	2.867	566	568	570	rBV2	464	269	0.03%	0.003%
9	3.027	616	618	619	rBV2	310	105	0.01%	0.001%
10	3.243	681	685	687	rBV3	315	293	0.03%	0.003%
11	3.301	699	703	706	rBV2	444	326	0.03%	0.004%
12	3.342	713	716	720	rBB3	488	337	0.03%	0.004%
13	3.375	725	726	731	rVB3	434	223	0.02%	0.003%
14	3.410	733	737	739	rBV	661	426	0.04%	0.005%
15	3.442	744	747	748	rVB2	313	115	0.01%	0.001%
16	3.468	753	755	756	rBV	163	58	0.01%	0.001%
17	3.526	766	773	775	rBV4	513	471	0.05%	0.005%
18	3.539	775	777	779	rBV2	238	67	0.01%	0.001%
19	3.548	779	780	781	rBV2	139	50	0.01%	0.001%
20	3.571	781	787	790	rVV3	251	304	0.03%	0.003%
21	3.635	805	807	810	rVB	395	177	0.02%	0.002%
22	3.735	835	838	840	rBV2	335	255	0.03%	0.003%
23	3.793	845	856	896	rBV	84355	242573	24.95%	2.789%
24	4.256	985	1000	1027	rBV	140950	359897	37.01%	4.138%
25	4.625	1113	1115	1117	rBV3	425	213	0.02%	0.002%
26	4.686	1132	1134	1136	rVB3	280	93	0.01%	0.001%
27	4.706	1136	1140	1142	rBV3	413	340	0.03%	0.004%
28	4.754	1151	1155	1156	rBV2	344	275	0.03%	0.003%
29	4.780	1161	1163	1164	rBV	361	162	0.02%	0.002%
30	4.844	1181	1183	1184	rVB2	295	92	0.01%	0.001%
31	4.863	1186	1189	1192	rBV2	350	312	0.03%	0.004%
32	4.895	1197	1199	1200	rBV2	384	167	0.02%	0.002%
33	4.960	1203	1219	1244	rBV2	371019	972362	100.00%	11.180%
34	5.538	1387	1399	1422	rBV	331275	680703	70.01%	7.827%
35	5.783	1472	1475	1479	rBV4	545	552	0.06%	0.006%
36	5.831	1479	1490	1508	rVB	10110	23233	2.39%	0.267%

LSC Area Percent Report

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Sample : PB155394TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB394

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\SFAMVLM082323WMA.M
Title : VOC Analysis

37	5.899	1508	1511	1514	rVB2	584	256	0.03%	0.003%
38	5.911	1514	1515	1518	rBV2	280	186	0.02%	0.002%
39	5.995	1528	1541	1562	rBV	210046	440738	45.33%	5.068%
40	6.233	1613	1615	1616	rBV	400	163	0.02%	0.002%
41	6.400	1658	1667	1705	rBV	135250	264045	27.16%	3.036%
42	6.799	1787	1791	1795	rBV3	471	479	0.05%	0.006%
43	6.918	1817	1828	1856	rBV2	124662	239247	24.60%	2.751%
44	7.127	1884	1893	1903	rBV	29044	50179	5.16%	0.577%
45	7.249	1920	1931	1961	rBV	440896	789391	81.18%	9.077%
46	7.558	2017	2027	2047	rBV	122643	221664	22.80%	2.549%
47	7.866	2113	2123	2144	rVB	44525	76942	7.91%	0.885%
48	8.030	2165	2174	2198	rBV2	259982	472220	48.56%	5.430%
49	8.136	2201	2207	2231	rVB	66376	112816	11.60%	1.297%
50	8.249	2235	2242	2260	rBV	37594	63170	6.50%	0.726%
51	8.625	2349	2359	2379	rBV	126458	202752	20.85%	2.331%
52	8.789	2398	2410	2440	rBV	516518	853428	87.77%	9.813%
53	9.426	2604	2608	2610	rBV5	495	400	0.04%	0.005%
54	9.496	2622	2630	2644	rBV3	9555	16272	1.67%	0.187%
55	9.603	2661	2663	2667	rBV3	364	245	0.03%	0.003%
56	9.622	2667	2669	2671	rBV2	353	128	0.01%	0.001%
57	9.950	2767	2771	2775	rBV5	531	457	0.05%	0.005%
58	9.992	2779	2784	2787	rBV	387	319	0.03%	0.004%
59	10.008	2787	2789	2792	rBV2	589	298	0.03%	0.003%
60	10.159	2823	2836	2858	rBV	279526	447575	46.03%	5.146%
61	10.371	2901	2902	2904	rBV2	374	193	0.02%	0.002%
62	10.432	2919	2921	2922	rBV	251	110	0.01%	0.001%
63	10.474	2933	2934	2938	rBV2	407	331	0.03%	0.004%
64	10.545	2954	2956	2960	rBV2	480	330	0.03%	0.004%
65	10.567	2960	2963	2969	rVB4	395	426	0.04%	0.005%
66	10.622	2979	2980	2985	rBV4	344	227	0.02%	0.003%
67	10.644	2985	2987	2990	rVB2	571	307	0.03%	0.004%
68	10.757	3018	3022	3025	rBV5	426	454	0.05%	0.005%
69	10.779	3027	3029	3032	rBV2	258	161	0.02%	0.002%
70	10.860	3051	3054	3056	rBV3	484	364	0.04%	0.004%
71	10.988	3091	3094	3095	rBV2	514	248	0.03%	0.003%
72	11.059	3109	3116	3121	rBV5	629	796	0.08%	0.009%
73	11.188	3144	3156	3177	rBV	560980	879680	90.47%	10.115%
74	11.416	3224	3227	3230	rBV3	419	245	0.03%	0.003%
75	11.442	3233	3235	3237	rVB2	599	292	0.03%	0.003%
76	11.461	3237	3241	3242	rBV3	453	326	0.03%	0.004%

LSC Area Percent Report

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Acq On : 08 Sep 2023 13:53
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Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB394

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\SFAMVLM082323WMA.M
Title : VOC Analysis

77	11.477	3244	3246	3250	rVV3	384	273	0.03%	0.003%
78	11.564	3262	3273	3290	rBV	452279	707160	72.73%	8.131%
79	11.783	3338	3341	3348	rBV4	839	1136	0.12%	0.013%
80	11.940	3387	3390	3395	rVB5	655	583	0.06%	0.007%
81	11.975	3398	3401	3403	rBV2	374	257	0.03%	0.003%
82	12.056	3421	3426	3428	rBV3	439	476	0.05%	0.005%
83	12.156	3455	3457	3458	rBV	232	94	0.01%	0.001%
84	12.184	3459	3466	3467	rBV4	799	793	0.08%	0.009%
85	12.278	3493	3495	3496	rBV2	470	246	0.03%	0.003%
86	12.365	3520	3522	3525	rBV4	464	361	0.04%	0.004%
87	12.503	3559	3565	3568	rBV5	571	609	0.06%	0.007%
88	12.599	3593	3595	3596	rBV2	386	151	0.02%	0.002%
89	12.754	3641	3643	3646	rBV2	561	422	0.04%	0.005%
90	12.808	3658	3660	3661	rBV	587	233	0.02%	0.003%
91	12.937	3697	3700	3704	rBV3	508	388	0.04%	0.004%
92	13.046	3731	3734	3737	rBV2	374	301	0.03%	0.003%
93	13.062	3737	3739	3744	rVV4	413	368	0.04%	0.004%
94	13.091	3744	3748	3749	rBV3	399	258	0.03%	0.003%
95	13.152	3763	3767	3768	rBV3	564	346	0.04%	0.004%
96	13.217	3782	3787	3790	rBV2	897	838	0.09%	0.010%
97	13.300	3811	3813	3818	rBV4	396	321	0.03%	0.004%

Sum of corrected areas: 8696948

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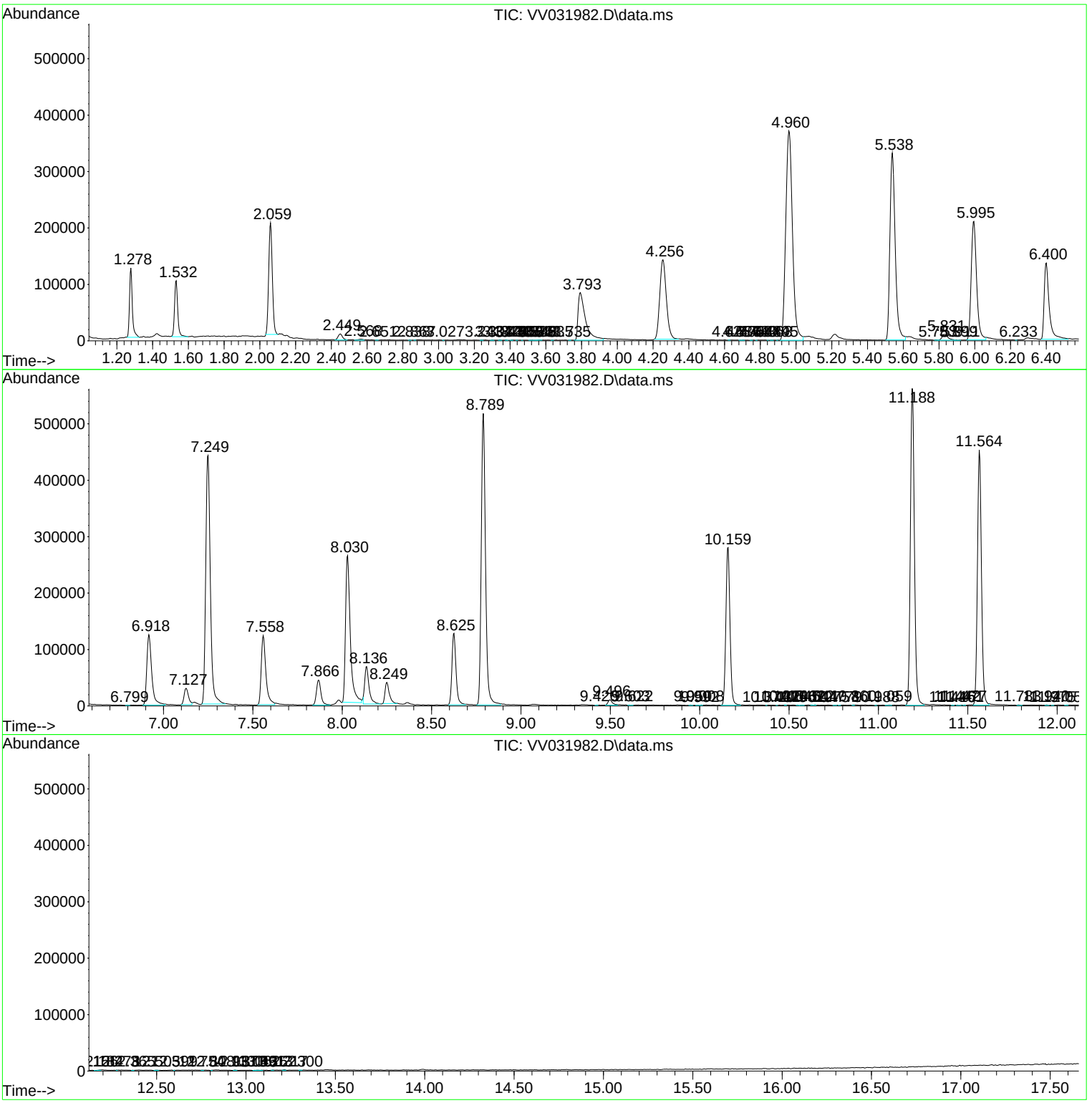
Data File : VV031982.D
Acq On : 08 Sep 2023 13:53
Operator : SY/MD
Sample : PB155394TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB394

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV090823\
Data File : VV031982.D
Acq On : 08 Sep 2023 13:53
Operator : SY/MD
Sample : PB155394TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB394

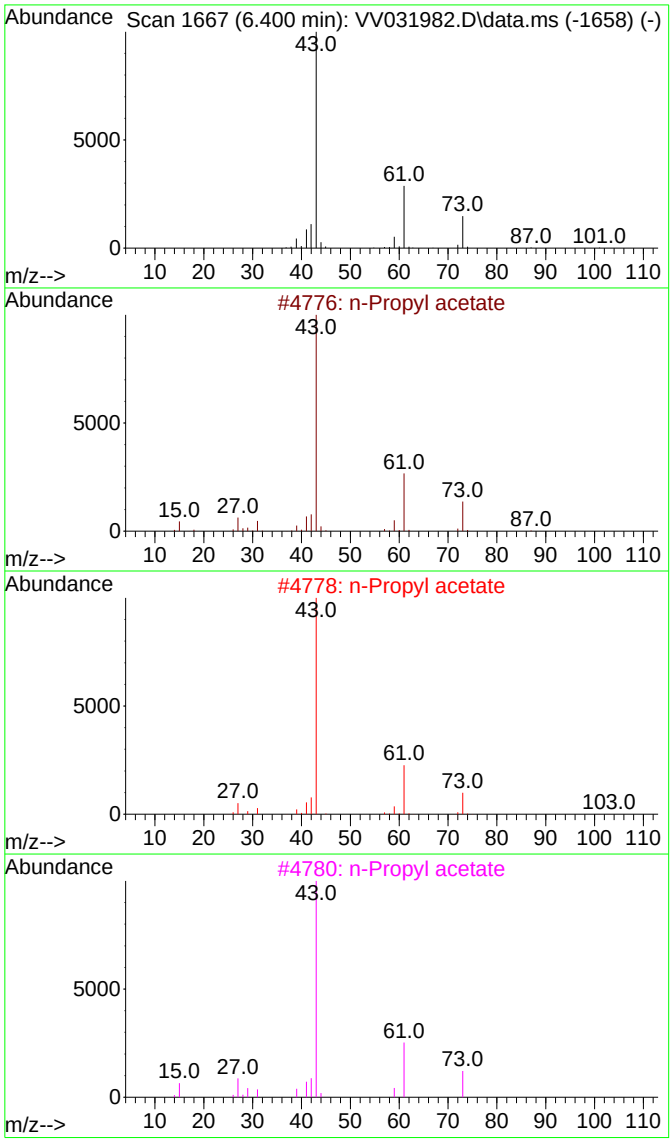
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
Quant Title : VOC Analysis

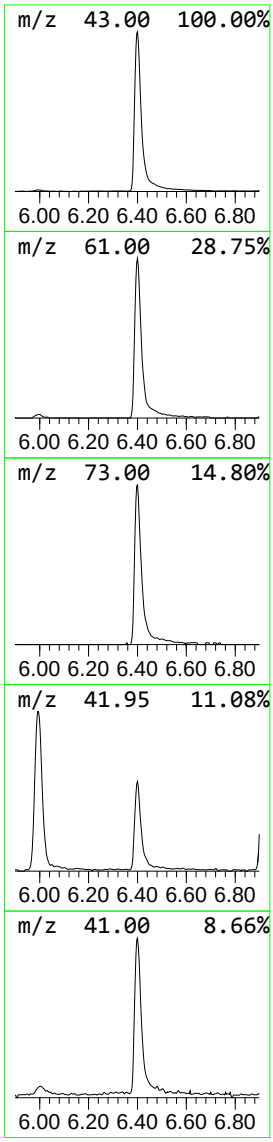
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.400	19.40 ug/L	264045	1,4-Difluorobenzene	5.538

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	78
3	n-Propyl acetate	102	C5H10O2	000109-60-4	72
4	n-Propyl acetate	102	C5H10O2	000109-60-4	64
5	Isopropyl acetate	102	C5H10O2	000108-21-4	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV090823\
Data File : VV031982.D
Acq On : 08 Sep 2023 13:53
Operator : SY/MD
Sample : PB155394TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB394

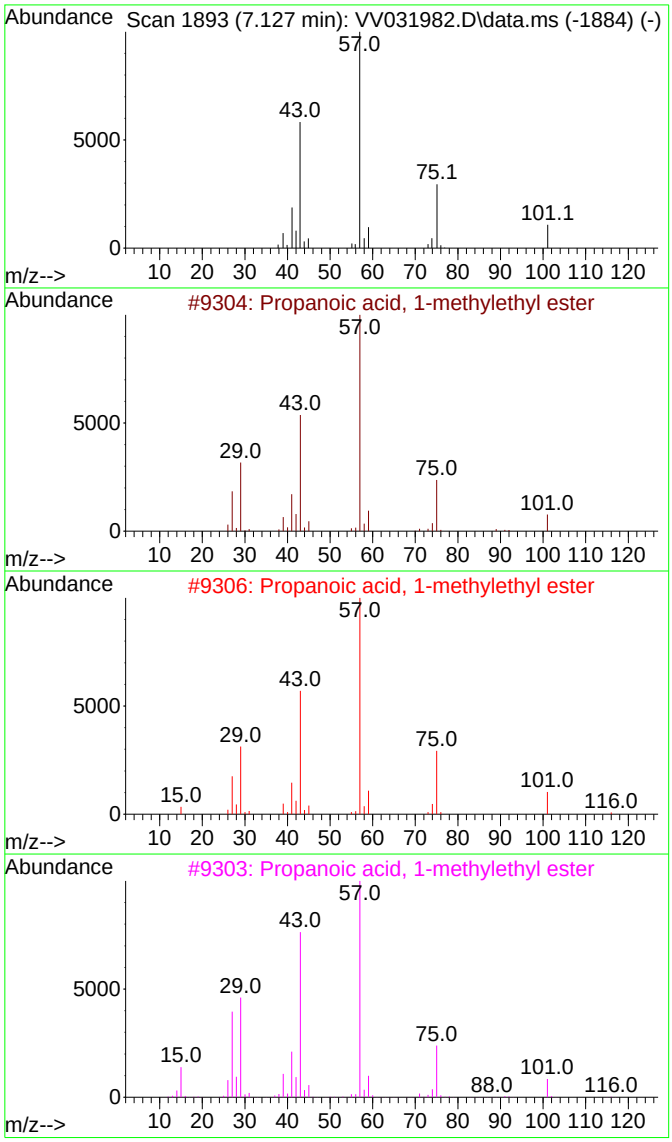
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
Quant Title : VOC Analysis

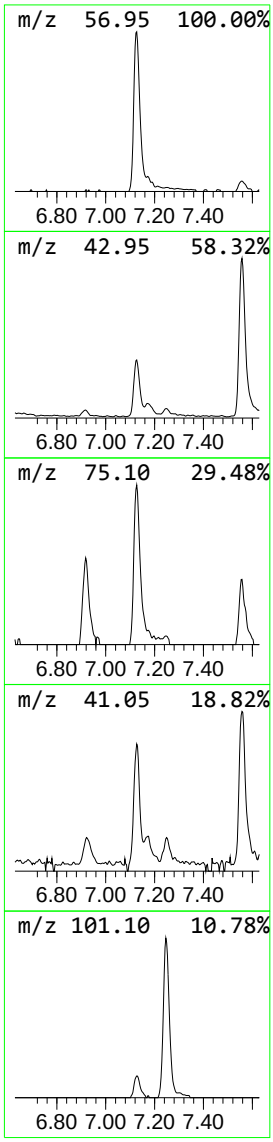
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.127	3.69 ug/L	50179	1,4-Difluorobenzene	5.538

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	64
4	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	50
5	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV090823\
Data File : VV031982.D
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Operator : SY/MD
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ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB394

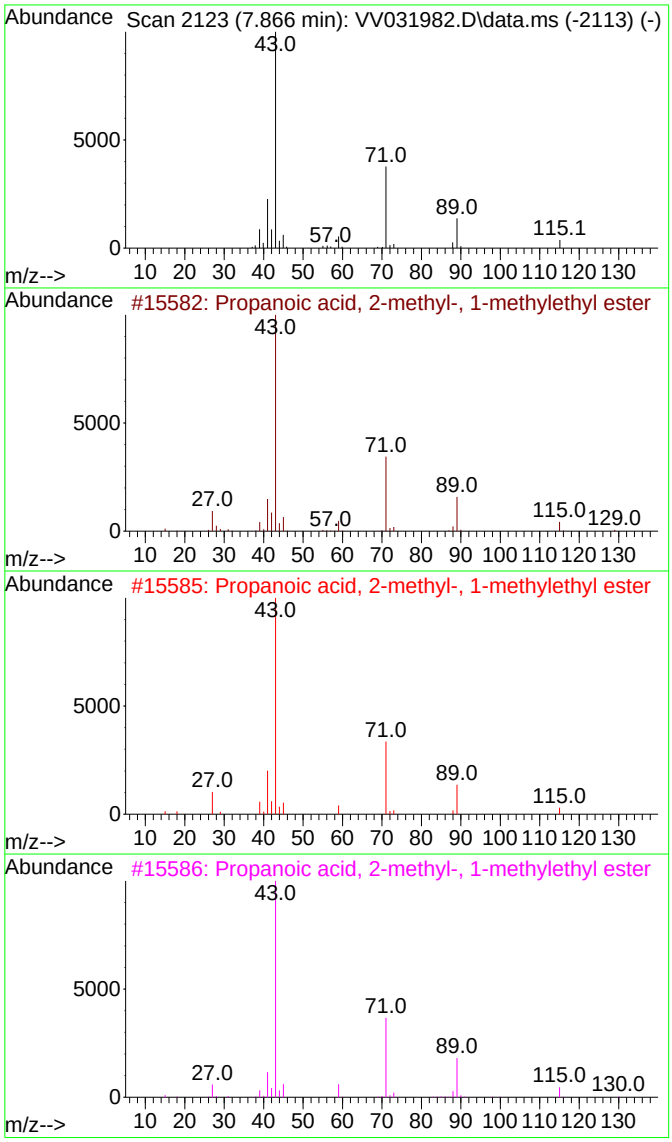
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
Quant Title : VOC Analysis

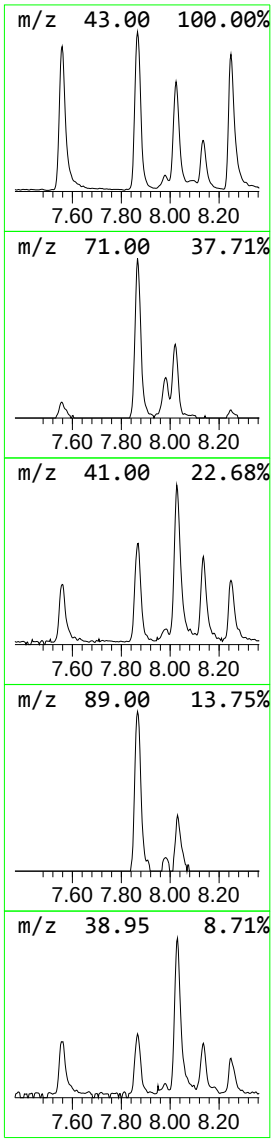
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Propanoic acid, 2-methyl-, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.866	4.51 ug/L	76942	Chlorobenzene-d5	8.789

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	78
4	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72





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Operator : SY/MD
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ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB394

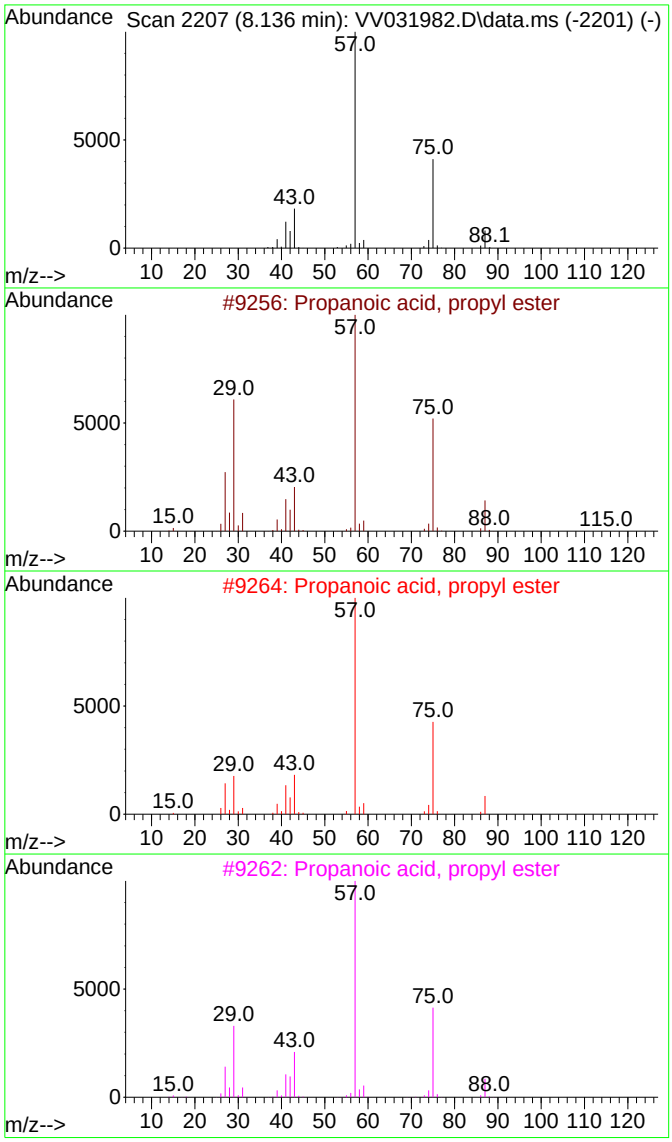
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
Quant Title : VOC Analysis

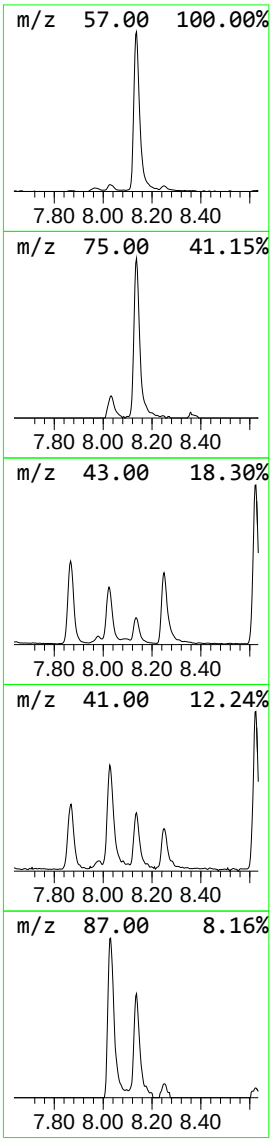
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.136	6.61 ug/L	112816	Chlorobenzene-d5	8.789

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	72
4	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	64
5	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	28





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Data File : VV031982.D
Acq On : 08 Sep 2023 13:53
Operator : SY/MD
Sample : PB155394TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB394

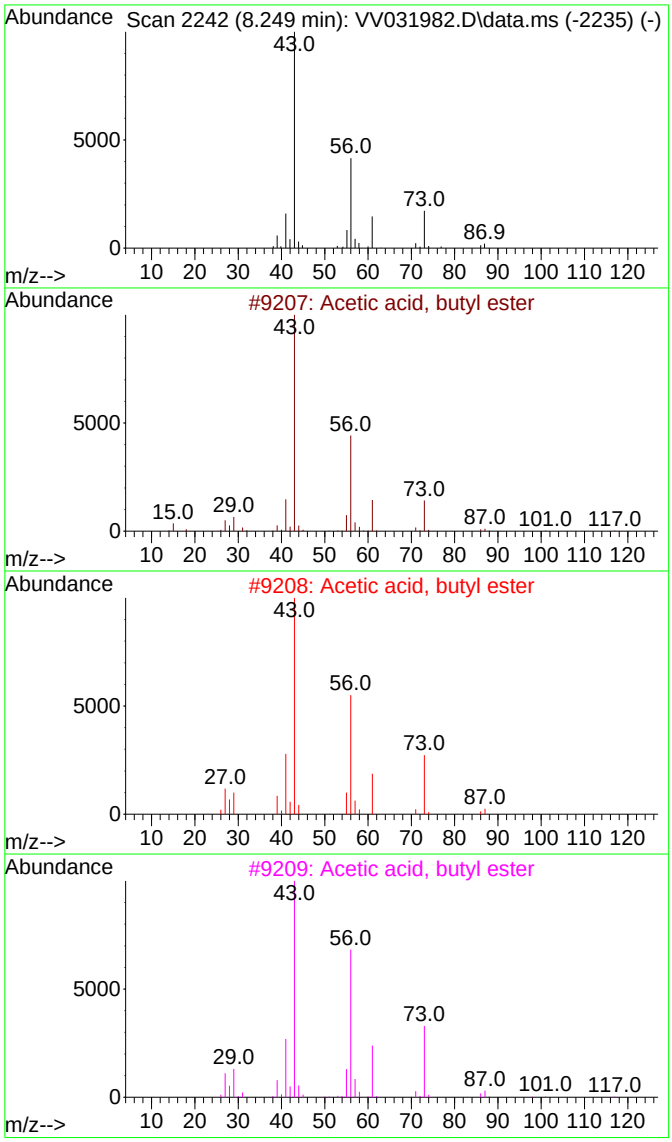
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
Quant Title : VOC Analysis

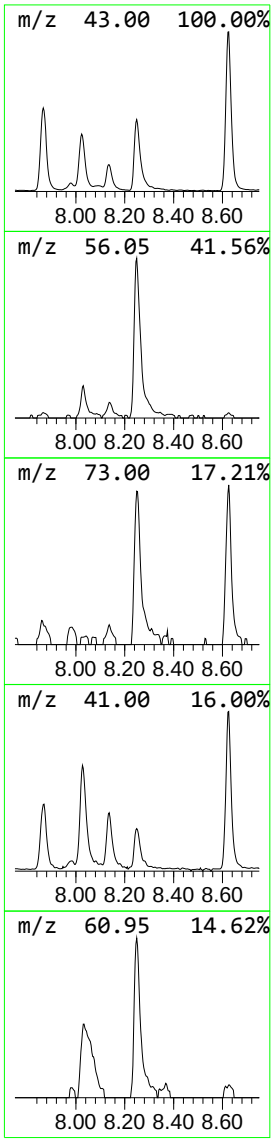
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.249	3.70 ug/L	63170	Chlorobenzene-d5	8.789

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	83
2	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
3	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
4	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	59
5	Isobutyl acetate	116	C6H12O2	000110-19-0	39





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Data File : VV031982.D
Acq On : 08 Sep 2023 13:53
Operator : SY/MD
Sample : PB155394TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB394

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
Quant Title : VOC Analysis

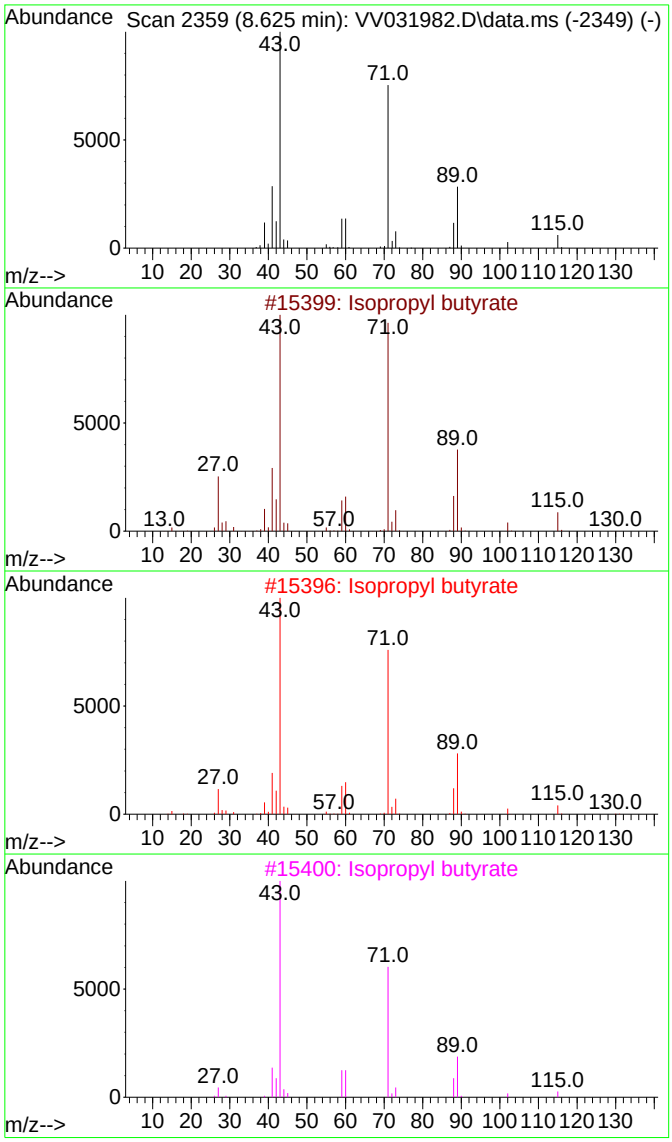
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

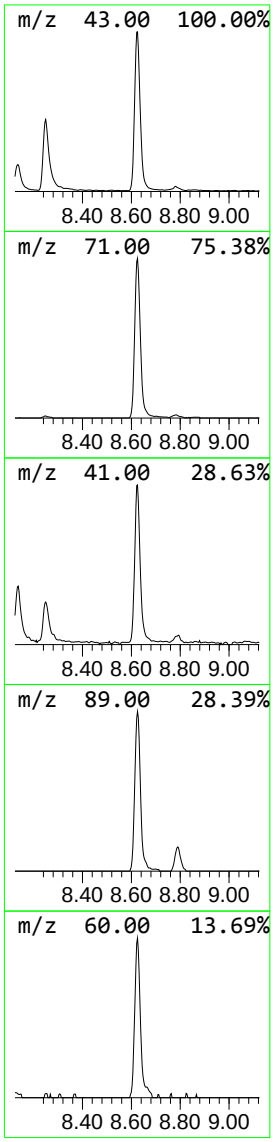
****

Peak Number 7 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.625	11.88 ug/L	202752	Chlorobenzene-d5	8.789

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	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV090823\
Data File : VV031982.D
Acq On : 08 Sep 2023 13:53
Operator : SY/MD
Sample : PB155394TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB394

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.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	6.400	19.4	ug/L	264045	1	5.538	680703	50.0
Propanoic acid,...	7.127	3.7	ug/L	50179	1	5.538	680703	50.0
Propanoic acid,...	7.866	4.5	ug/L	76942	2	8.789	853428	50.0
Propanoic acid,...	8.136	6.6	ug/L	112816	2	8.789	853428	50.0
Acetic acid, bu...	8.249	3.7	ug/L	63170	2	8.789	853428	50.0
Isopropyl butyrate	8.625	11.9	ug/L	202752	2	8.789	853428	50.0