

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101623\
 Data File : VU055770.D
 Acq On : 16 Oct 2023 14:25
 Operator : MD/SY
 Sample : PB156345TB 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VLEB345

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: VU055770.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	110	rVB	193350	224533	12.23%	1.585%
2	1.894	180	188	204	rVB	169742	240390	13.09%	1.697%
3	2.560	383	395	410	rBV	333473	549481	29.93%	3.878%
4	2.718	442	444	449	rVB3	888	539	0.03%	0.004%
5	2.869	486	491	494	rBV3	395	345	0.02%	0.002%
6	2.885	494	496	501	rVB3	477	300	0.02%	0.002%
7	3.039	533	544	557	rBV4	11478	21809	1.19%	0.154%
8	3.177	572	587	606	rBV2	17976	44011	2.40%	0.311%
9	3.300	622	625	631	rVB	496	398	0.02%	0.003%
10	3.332	631	635	640	rBV2	519	502	0.03%	0.004%
11	3.492	681	685	690	rVB2	354	316	0.02%	0.002%
12	3.528	693	696	700	rBV3	408	371	0.02%	0.003%
13	3.615	720	723	727	rVV2	459	433	0.02%	0.003%
14	3.840	787	793	796	rBV3	1047	1174	0.06%	0.008%
15	4.094	865	872	877	rVB2	290	325	0.02%	0.002%
16	4.296	932	935	940	rVB2	427	316	0.02%	0.002%
17	4.348	947	951	954	rBV2	401	329	0.02%	0.002%
18	4.396	962	966	970	rBV2	375	296	0.02%	0.002%
19	4.554	1011	1015	1019	rBV3	384	415	0.02%	0.003%
20	4.615	1022	1034	1066	rBV	139134	368754	20.09%	2.603%
21	4.939	1130	1135	1139	rVB4	492	429	0.02%	0.003%
22	5.055	1156	1171	1196	rBV	339885	751666	40.94%	5.306%
23	5.309	1246	1250	1251	rBV2	642	404	0.02%	0.003%
24	5.721	1357	1378	1403	rBV3	649869	1835919	100.00%	12.959%
25	5.914	1429	1438	1451	rVB3	11647	23417	1.28%	0.165%
26	6.110	1497	1499	1505	rVB4	690	585	0.03%	0.004%
27	6.145	1505	1510	1513	rBV4	642	648	0.04%	0.005%
28	6.164	1513	1516	1521	rBV4	381	316	0.02%	0.002%
29	6.245	1528	1541	1569	rBV	466960	908675	49.49%	6.414%
30	6.415	1592	1594	1602	rVB4	963	688	0.04%	0.005%
31	6.528	1618	1629	1643	rVB2	19062	37769	2.06%	0.267%
32	6.592	1645	1649	1652	rBV3	869	707	0.04%	0.005%
33	6.685	1664	1678	1698	rBV	423086	842078	45.87%	5.944%
34	6.875	1734	1737	1743	rVB4	731	703	0.04%	0.005%
35	6.930	1743	1754	1773	rBV2	6456	17028	0.93%	0.120%
36	7.036	1776	1787	1809	rBV	142821	265087	14.44%	1.871%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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

37	7.190	1826	1835	1850	rVB4	7369	15099	0.82%	0.107%
38	7.245	1850	1852	1856	rVB2	627	370	0.02%	0.003%
39	7.360	1883	1888	1893	rVB2	659	553	0.03%	0.004%
40	7.393	1893	1898	1901	rVB2	626	444	0.02%	0.003%
41	7.479	1921	1925	1928	rBV2	488	294	0.02%	0.002%
42	7.560	1938	1950	1968	rBV	218759	395122	21.52%	2.789%
43	7.698	1988	1993	1995	rBV3	2946	2664	0.15%	0.019%
44	7.733	1996	2004	2016	rVB2	31248	51529	2.81%	0.364%
45	7.894	2040	2054	2077	rBV	773270	1356052	73.86%	9.572%
46	8.174	2120	2141	2170	rBV2	169893	349392	19.03%	2.466%
47	8.415	2213	2216	2220	rBV2	361	301	0.02%	0.002%
48	8.463	2220	2231	2247	rBV	39205	66918	3.64%	0.472%
49	8.573	2247	2265	2272	rBV8	7635	16912	0.92%	0.119%
50	8.634	2272	2284	2306	rBV4	346526	829309	45.17%	5.854%
51	8.724	2306	2312	2331	rVB	75025	130466	7.11%	0.921%
52	8.833	2338	2346	2365	rVB2	40090	69134	3.77%	0.488%
53	9.209	2448	2463	2478	rBV	113998	185536	10.11%	1.310%
54	9.322	2496	2498	2500	rVB2	686	316	0.02%	0.002%
55	9.364	2507	2511	2514	rBV2	2122	2105	0.11%	0.015%
56	9.415	2514	2527	2552	rVV	694380	1176336	64.07%	8.303%
57	9.618	2588	2590	2592	rBV2	519	332	0.02%	0.002%
58	9.650	2592	2600	2604	rVV4	1001	1510	0.08%	0.011%
59	9.695	2610	2614	2616	rBV3	572	412	0.02%	0.003%
60	9.930	2679	2687	2690	rBV5	1576	1706	0.09%	0.012%
61	10.074	2724	2732	2748	rVV3	7787	13748	0.75%	0.097%
62	10.290	2795	2799	2802	rBV2	627	398	0.02%	0.003%
63	10.415	2834	2838	2841	rBV	458	284	0.02%	0.002%
64	10.647	2908	2910	2916	rVV2	359	402	0.02%	0.003%
65	10.753	2929	2943	2968	rBV	635055	1048620	57.12%	7.402%
66	10.865	2976	2978	2983	rVB2	621	392	0.02%	0.003%
67	10.897	2983	2988	2991	rBV3	504	473	0.03%	0.003%
68	10.939	2998	3001	3007	rBV2	428	301	0.02%	0.002%
69	11.116	3050	3056	3061	rVB4	487	564	0.03%	0.004%
70	11.225	3087	3090	3093	rVB2	452	289	0.02%	0.002%
71	11.277	3104	3106	3111	rVB2	625	424	0.02%	0.003%
72	11.589	3198	3203	3205	rBV2	367	295	0.02%	0.002%
73	11.614	3205	3211	3216	rVB3	391	416	0.02%	0.003%
74	11.669	3221	3228	3231	rBV3	340	587	0.03%	0.004%
75	11.720	3240	3244	3250	rVB2	370	419	0.02%	0.003%
76	11.746	3250	3252	3255	rBV2	480	340	0.02%	0.002%

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Integration Parameters: LSCINT.P

Integrator: RTE

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

77	11.810	3259	3272	3297	rBV	654651	1067553	58.15%	7.535%
78	12.036	3339	3342	3345	rBV3	500	391	0.02%	0.003%
79	12.190	3377	3390	3410	rBV	743990	1226420	66.80%	8.657%
80	12.540	3496	3499	3502	rBV2	473	352	0.02%	0.002%
81	12.688	3542	3545	3547	rBV	491	289	0.02%	0.002%
82	12.778	3570	3573	3577	rVB2	796	640	0.03%	0.005%
83	12.807	3577	3582	3584	rBV2	334	306	0.02%	0.002%
84	12.942	3620	3624	3627	rBV2	630	508	0.03%	0.004%
85	12.965	3627	3631	3633	rBV3	523	434	0.02%	0.003%
86	13.090	3667	3670	3672	rBV	439	277	0.02%	0.002%
87	13.299	3733	3735	3738	rVB2	639	284	0.02%	0.002%
88	13.466	3784	3787	3791	rBV3	573	581	0.03%	0.004%
89	13.666	3844	3849	3852	rBV2	763	818	0.04%	0.006%
90	13.791	3885	3888	3890	rBV3	470	328	0.02%	0.002%
91	13.868	3909	3912	3916	rBV3	656	620	0.03%	0.004%
92	14.039	3962	3965	3968	rBV2	581	388	0.02%	0.003%
93	14.077	3974	3977	3979	rBV2	608	355	0.02%	0.003%
94	14.132	3991	3994	3998	rVV2	924	754	0.04%	0.005%
95	14.296	4042	4045	4048	rBV2	613	519	0.03%	0.004%
96	14.347	4058	4061	4064	rBV3	933	576	0.03%	0.004%
97	14.788	4196	4198	4202	rVB2	688	458	0.02%	0.003%
98	14.852	4216	4218	4220	rBV2	606	331	0.02%	0.002%
99	15.820	4516	4519	4526	rVB6	1545	1202	0.07%	0.008%
100	16.093	4601	4604	4607	rBV2	1479	1072	0.06%	0.008%

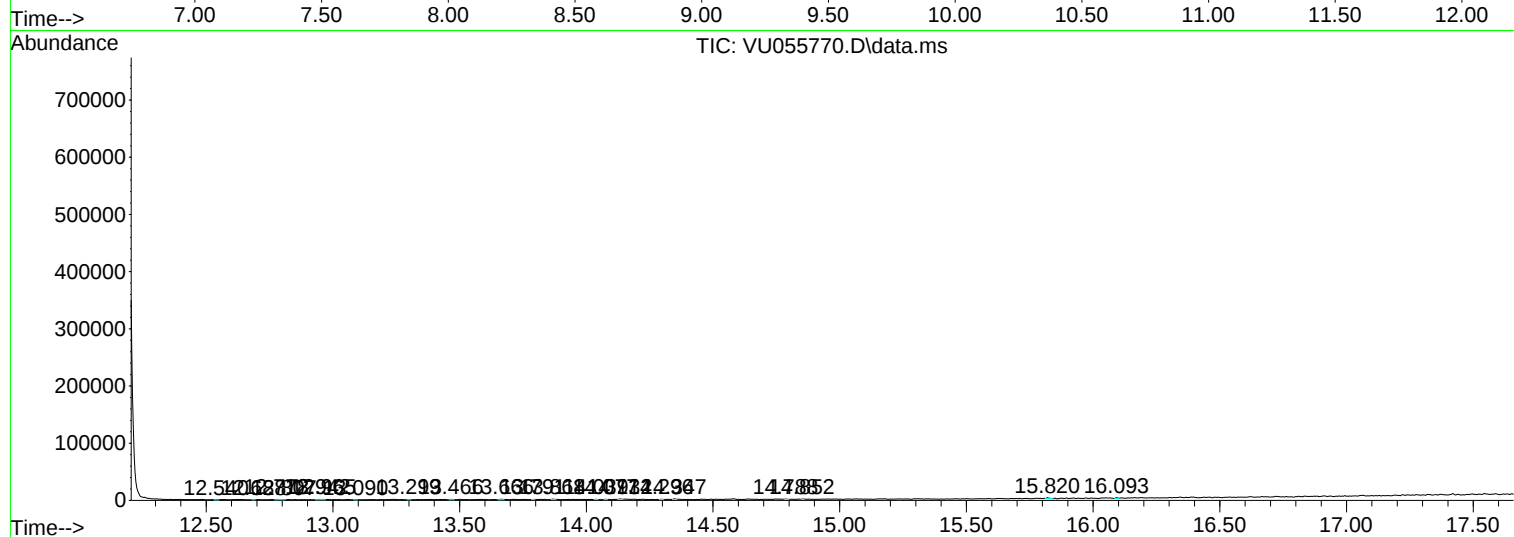
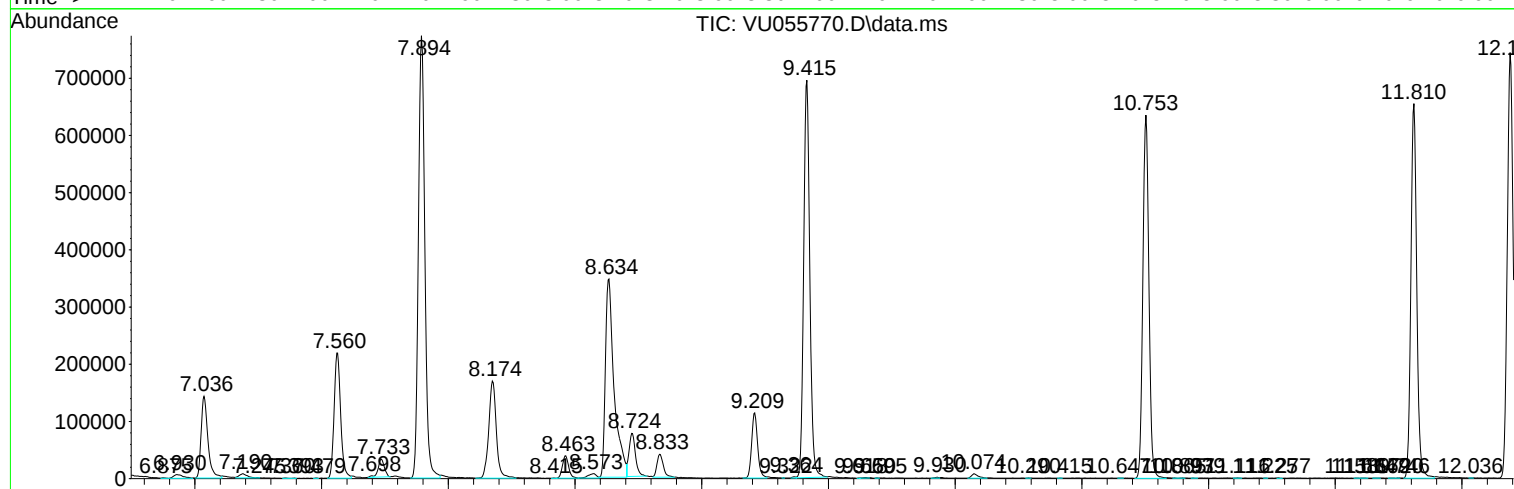
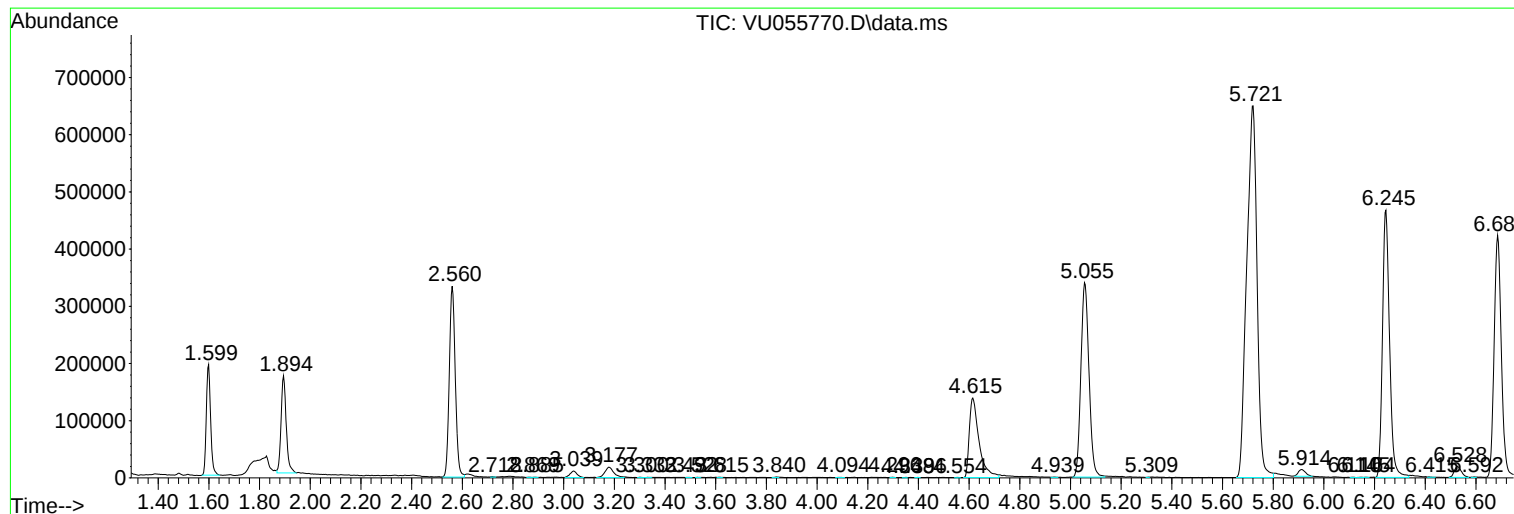
Sum of corrected areas: 14167376

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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB345

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

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P



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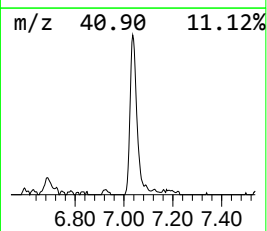
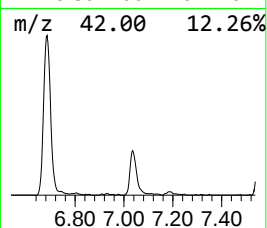
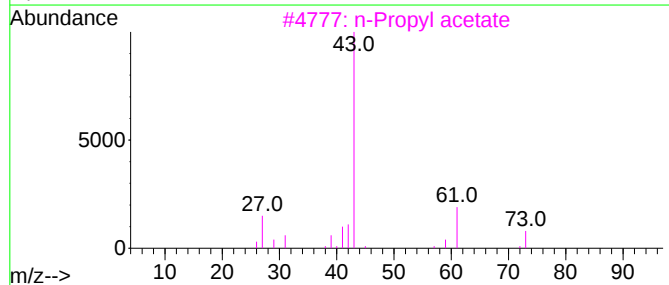
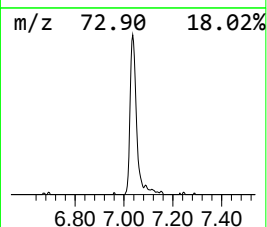
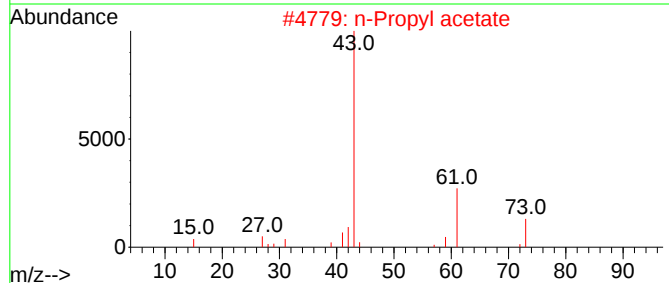
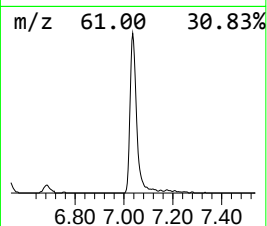
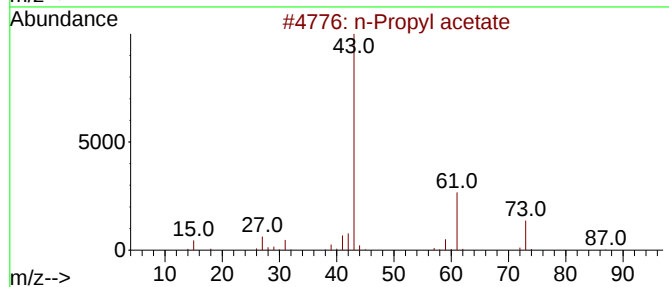
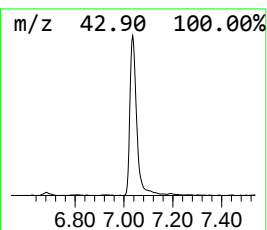
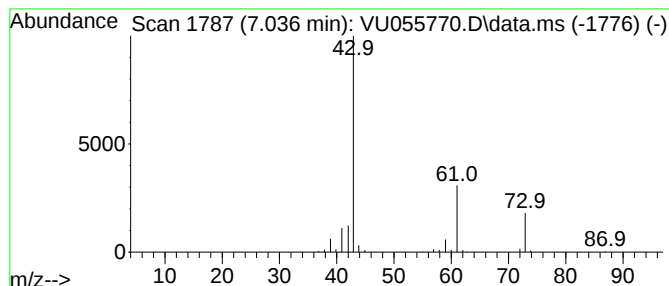
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.036	14.59 ug/L	265087	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	78
3	n-Propyl acetate			102	C5H10O2	000109-60-4	78
4	n-Propyl acetate			102	C5H10O2	000109-60-4	74
5	n-Propyl acetate			102	C5H10O2	000109-60-4	64



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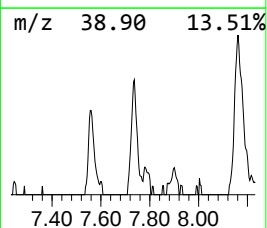
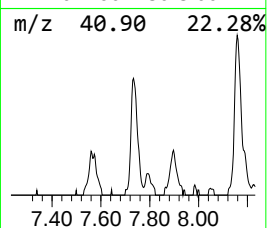
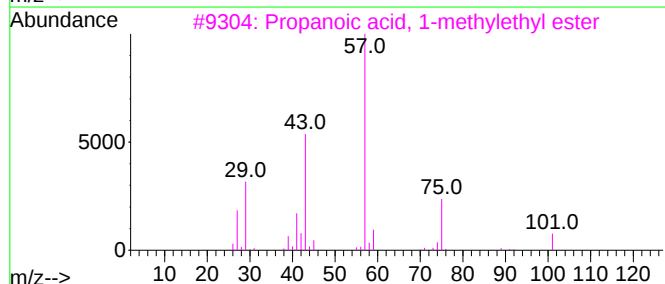
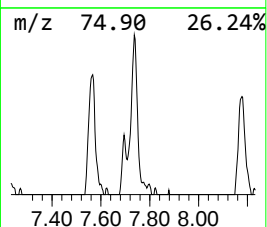
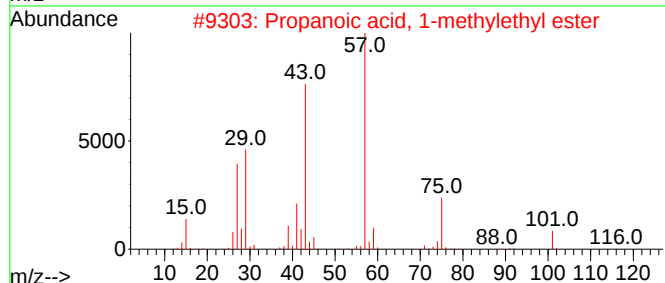
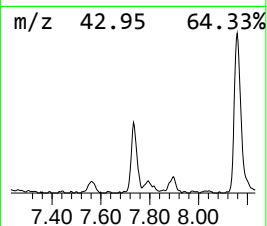
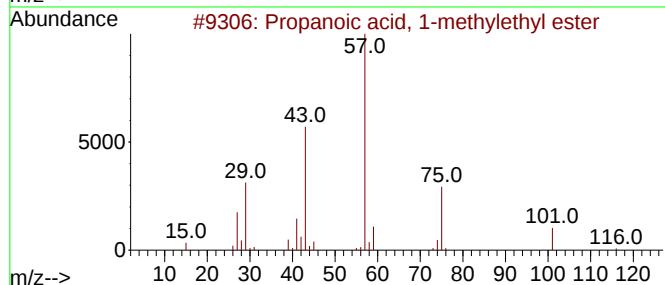
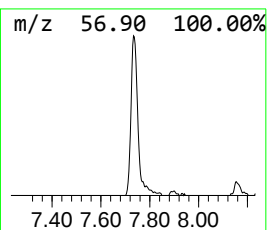
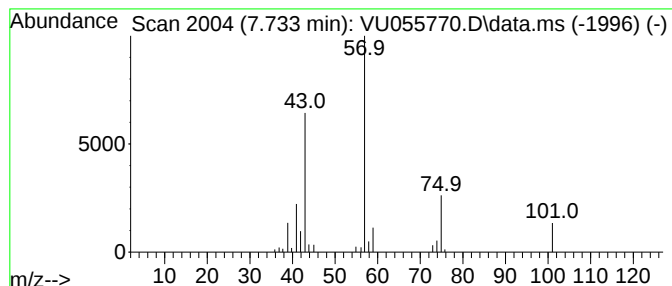
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.733	2.84 ug/L	51529	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	83
2			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	78
3			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	72
4			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	64
5			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	56



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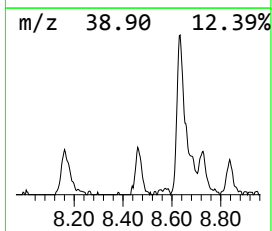
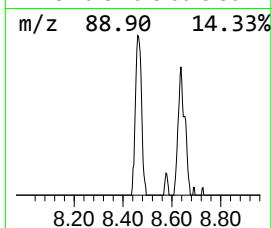
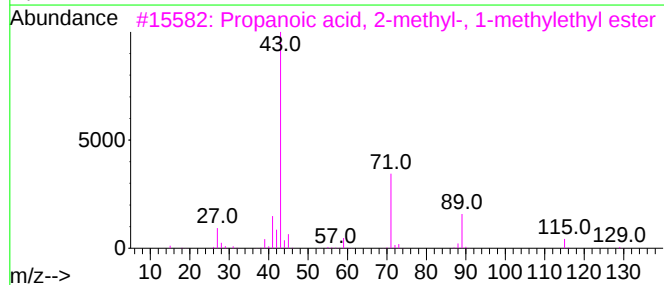
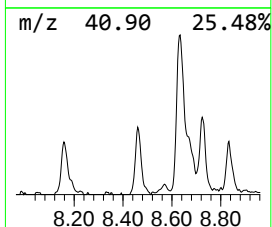
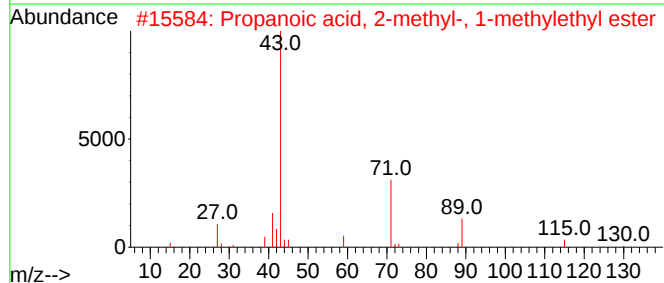
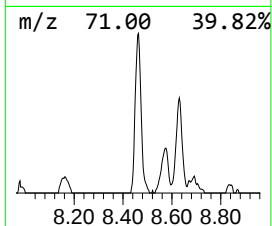
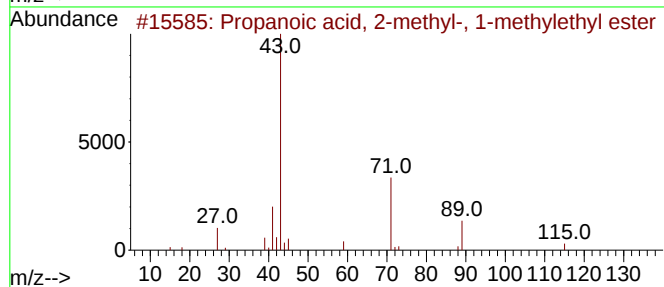
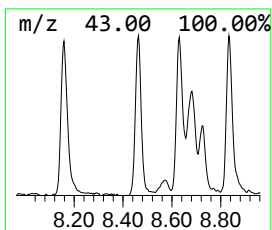
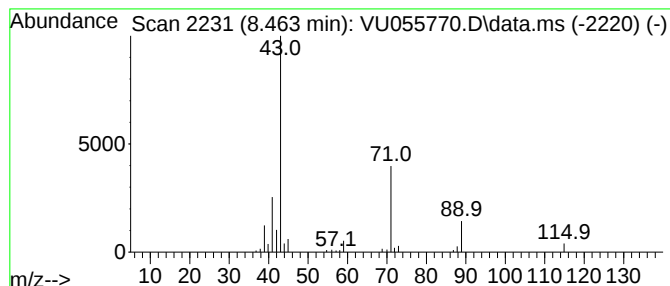
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.463	2.84 ug/L	66918	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-, 1-met...	130	C7H14O2	000617-50-5	83
5			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101623\
Data File : VU055770.D
Acq On : 16 Oct 2023 14:25
Operator : MD/SY
Sample : PB156345TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB345

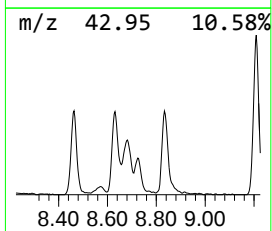
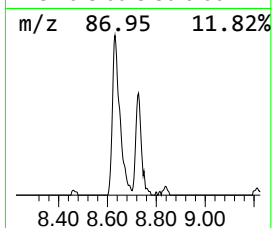
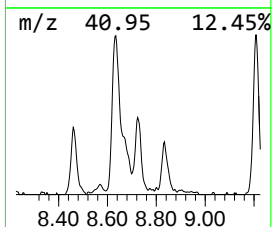
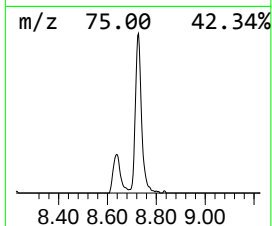
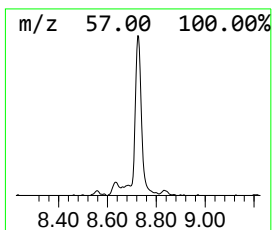
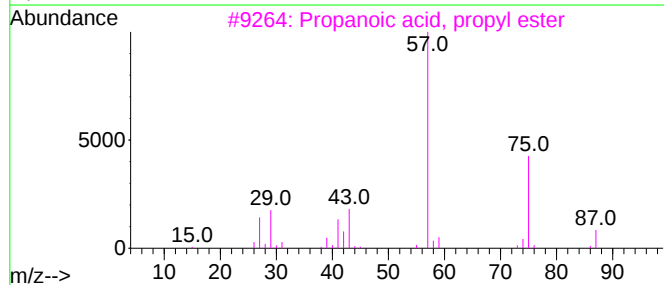
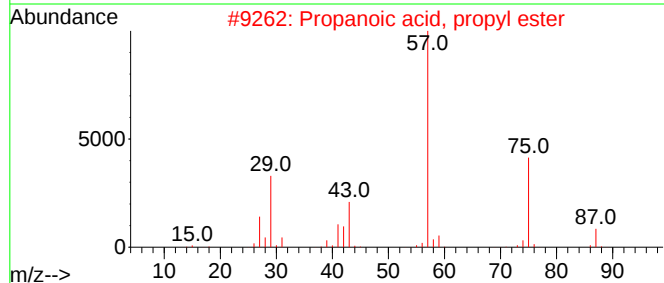
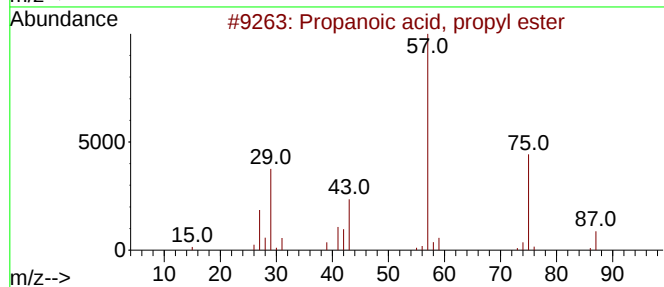
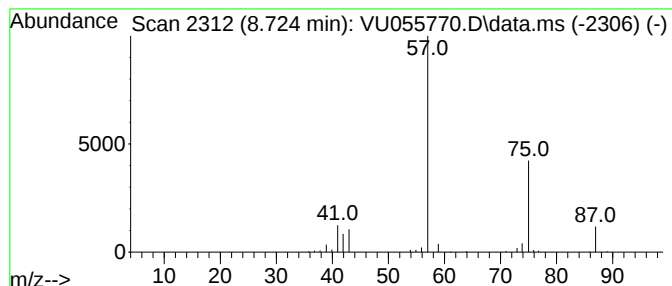
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Quant Title : VOC Analysis

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.
8.724	5.55 ug/L	130466	Chlorobenzene-d5	9.415

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	64
2			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	56
3			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	50
4			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	39
5			1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101623\
Data File : VU055770.D
Acq On : 16 Oct 2023 14:25
Operator : MD/SY
Sample : PB156345TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB345

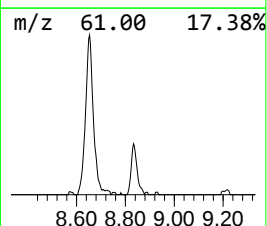
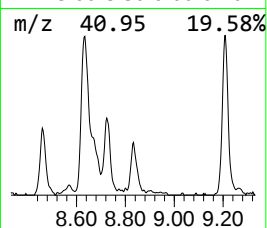
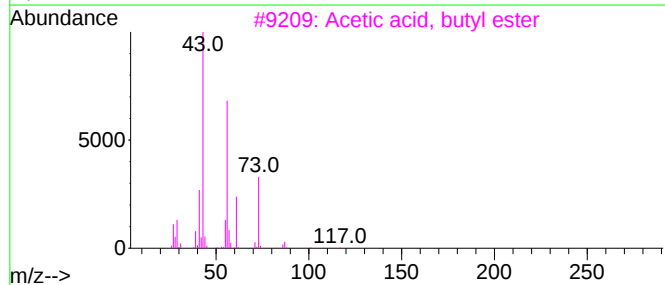
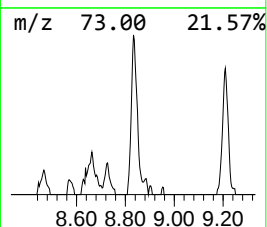
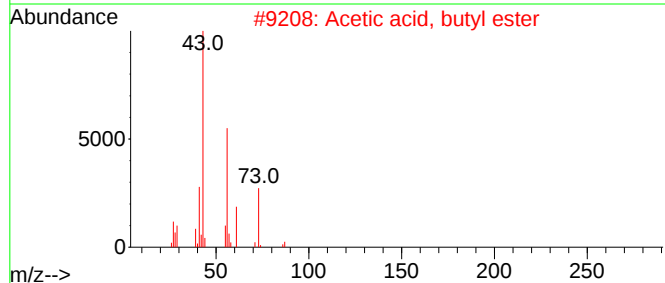
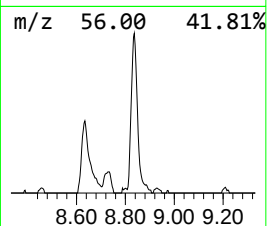
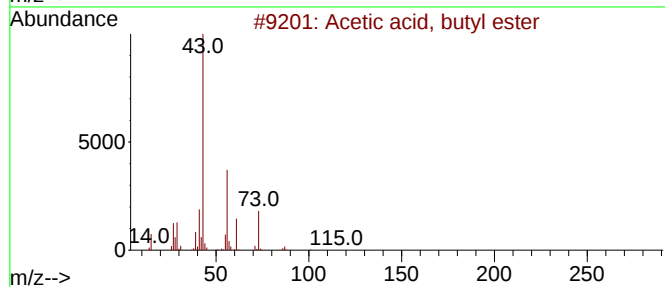
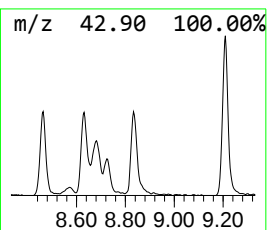
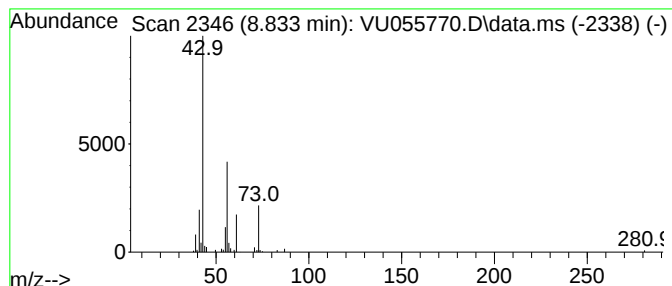
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Quant Title : VOC Analysis

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	2.94 ug/L	69134	Chlorobenzene-d5	9.415

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72		
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	64		
5	Acetic acid, hexyl ester	144	C8H16O2	000142-92-7	36		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101623\
Data File : VU055770.D
Acq On : 16 Oct 2023 14:25
Operator : MD/SY
Sample : PB156345TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB345

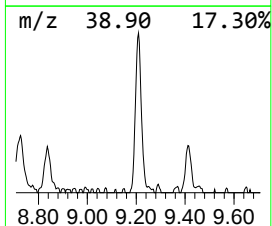
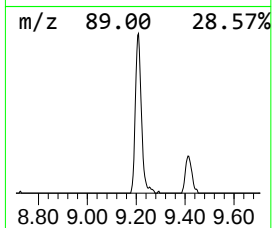
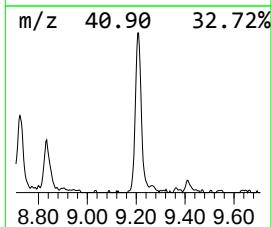
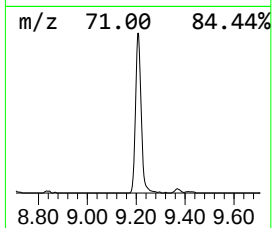
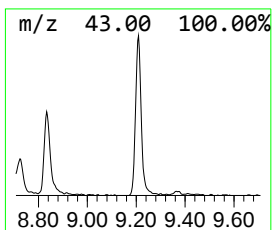
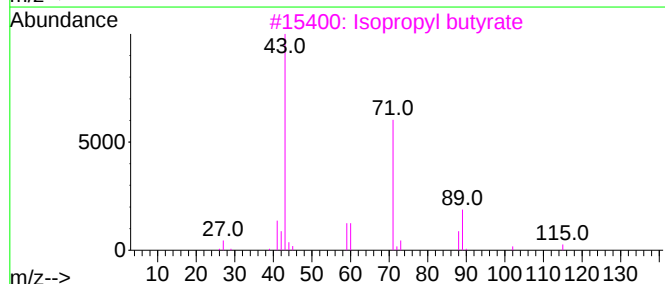
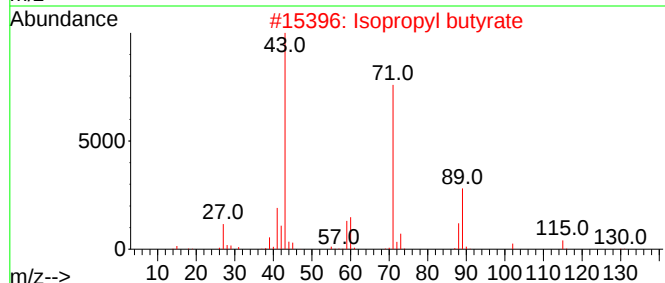
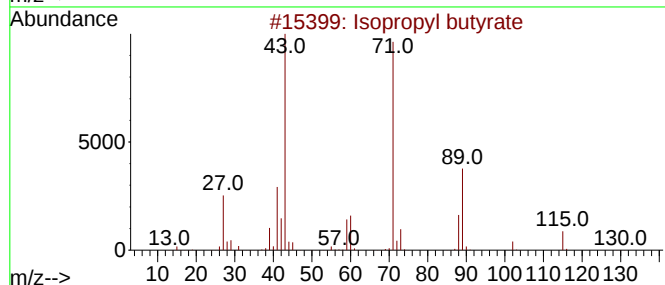
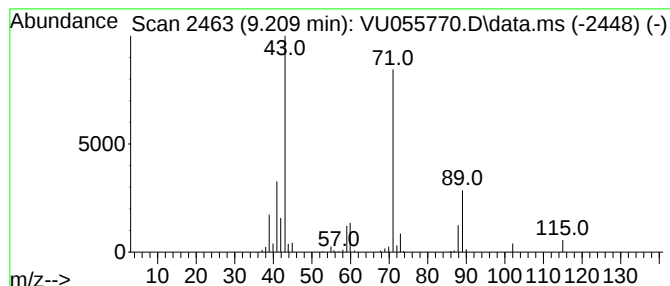
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Quant Title : VOC Analysis

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	7.89 ug/L	185536	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, 1-methylpropyl ester	144	C8H16O2	000819-97-6	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101623\
Data File : VU055770.D
Acq On : 16 Oct 2023 14:25
Operator : MD/SY
Sample : PB156345TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB345

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

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	7.036	14.6	ug/L	265087	1	6.245	908675	50.0
Propanoic acid,...	7.733	2.8	ug/L	51529	1	6.245	908675	50.0
Propanoic acid,...	8.463	2.8	ug/L	66918	2	9.415	1176340	50.0
Propanoic acid,...	8.724	5.5	ug/L	130466	2	9.415	1176340	50.0
Acetic acid, bu...	8.833	2.9	ug/L	69134	2	9.415	1176340	50.0
Isopropyl butyrate	9.209	7.9	ug/L	185536	2	9.415	1176340	50.0