LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121922\
Data File : VV029718.D
Acq On : 19 Dec 2022 13:52
Operator : SY/MD
Sample : N6075-08 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BGSM3

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\SFAMVLM120722WMA.M
Title : VOC Analysis

Signal : TIC: VV029718.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.304	76	82	95	rVB	213497	219723	15.25%	1.765%
2	1.555	154	160	182	rVB	158955	185111	12.84%	1.487%
3	2.101	319	330	343	rBV	351766	501117	34.77%	4.026%
4	2.282	383	386	389	rBV4	607	567	0.04%	0.005%
5	2.375	413	415	422	rVB4	335	439	0.03%	0.004%
6	2.407	422	425	428	rBV	278	207	0.01%	0.002%
7	2.500	446	454	471	rVB2	10103	16581	1.15%	0.133%
8	2.616	478	490	504	rVB	3906	7904	0.55%	0.063%
9	2.764	532	536	538	rBV	237	182	0.01%	0.001%
10	2.896	573	577	585	rBV2	212	255	0.02%	0.002%
11	3.034	618	620	626	rVB	145	118	0.01%	0.001%
12	3.066	626	630	633	rBV2	275	208	0.01%	0.002%
13	3.169	660	662	663	rBV	278	115	0.01%	0.001%
14	3.236	680	683	687	rBV	221	159	0.01%	0.001%
15	3.281	694	697	702	rBV	187	127	0.01%	0.001%
16	3.310	702	706	708	rVV3	173	118	0.01%	0.001%
17	3.536	772	776	779	rBV3	329	228	0.02%	0.002%
18	3.571	784	787	791	rBV2	120	114	0.01%	0.001%
19	3.722	826	834	838	rVB2	155	206	0.01%	0.002%
20	3.793	852	856	860	rBV2	222	160	0.01%	0.001%
21	3.876	872	882	929	rBV	89610	286283	19.86%	2.300%
22	4.339	1009	1026	1066	rBV	222398	555271	38.53%	4.461%
23	4.597	1103	1106	1108	rBV	220	124	0.01%	0.001%
24	4.638	1114	1119	1123	rBV2	175	187	0.01%	0.002%
25	4.661	1123	1126	1130	rBV3	220	237	0.02%	0.002%
26	4.712	1138	1142	1143	rBV3	158	111	0.01%	0.001%
27	4.777	1157	1162	1165	rVV2	139	121	0.01%	0.001%
28	4.841	1177	1182	1184	rBV2	205	176	0.01%	0.001%
29	5.037	1223	1243	1276	rBV2	555595	1441144	100.00%	11.577%
30	5.285	1311	1320	1335	rBV2	9545	22021	1.53%	0.177%
31	5.468	1373	1377	1379	rBV2	270	214	0.01%	0.002%
32	5.558	1400	1405	1407	rBV3	264	255	0.02%	0.002%
33	5.609	1408	1421	1458	rVV	498815	1021091	70.85%	8.203%
34	5.899	1501	1511	1524	rBV2	5110	10226	0.71%	0.082%
35	6.063	1548	1562	1585	rBV	306698	636354	44.16%	5.112%
36	6.291	1630	1633	1642	rVB4	473	541	0.04%	0.004%

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Operator : SY/MD
Sample : N6075-08 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BGSM3

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\SFAMVLM120722WMA.M
Title : VOC Analysis

37	6.352	1642	1652	1665	rBV	4682	12174	0.84%	0.098%
38	6.461	1676	1686	1711	rBV	133095	257191	17.85%	2.066%
39	6.760	1777	1779	1781	rVB2	477	191	0.01%	0.002%
40	6.812	1793	1795	1799	rVB3	419	260	0.02%	0.002%
41	6.834	1799	1802	1804	rBV	299	213	0.01%	0.002%
42	6.979	1830	1847	1872	rBV	162427	297260	20.63%	2.388%
43	7.182	1900	1910	1923	rBV2	30805	55549	3.85%	0.446%
44	7.307	1936	1949	1981	rBV	681336	1202748	83.46%	9.662%
45	7.613	2033	2044	2063	rBV2	151100	268543	18.63%	2.157%
46	7.776	2091	2095	2098	rBV4	602	577	0.04%	0.005%
47	7.838	2112	2114	2116	rBV2	201	119	0.01%	0.001%
48	7.918	2126	2139	2158	rBV	40891	71505	4.96%	0.574%
49	8.030	2162	2174	2180	rBV6	7686	14091	0.98%	0.113%
50	8.085	2181	2191	2214	rVV	327043	614292	42.63%	4.935%
51	8.188	2217	2223	2241	rVB	69760	113066	7.85%	0.908%
52	8.301	2249	2258	2275	rVB	40259	68641	4.76%	0.551%
53	8.513	2323	2324	2327	rBV2	372	224	0.02%	0.002%
54	8.609	2351	2354	2357	rBV2	342	265	0.02%	0.002%
55	8.632	2358	2361	2364	rBV2	342	194	0.01%	0.002%
56	8.674	2364	2374	2393	rBV	124946	200499	13.91%	1.611%
57	8.844	2414	2427	2453	rBV	750305	1240220	86.06%	9.963%
58	9.056	2491	2493	2494	rBV	322	125	0.01%	0.001%
59	9.104	2505	2508	2509	rBV2	950	556	0.04%	0.004%
60	9.178	2527	2531	2536	rBV2	253	312	0.02%	0.003%
61	9.223	2542	2545	2546	rVB	266	113	0.01%	0.001%
62	9.336	2576	2580	2582	rBV2	237	152	0.01%	0.001%
63	9.378	2586	2593	2594	rBV3	886	681	0.05%	0.005%
64	9.542	2635	2644	2658	rBV3	9939	15979	1.11%	0.128%
65	9.690	2687	2690	2693	rBV4	242	222	0.02%	0.002%
66	9.847	2734	2739	2743	rBV2	332	324	0.02%	0.003%
67	9.908	2755	2758	2759	rBV2	267	132	0.01%	0.001%
68	9.998	2783	2786	2791	rVB2	341	284	0.02%	0.002%
69	10.030	2791	2796	2798	rBV2	272	160	0.01%	0.001%
70	10.088	2810	2814	2816	rBV2	276	224	0.02%	0.002%
71	10.165	2826	2838	2841	rBV	16508	24138	1.67%	0.194%
72	10.207	2842	2851	2867	rVB	438928	687861	47.73%	5.526%
73	10.374	2895	2903	2910	rBV4	1464	2358	0.16%	0.019%
74	10.439	2921	2923	2925	rBV	263	144	0.01%	0.001%
75	10.519	2942	2948	2949	rBV2	458	325	0.02%	0.003%
76	10.567	2955	2963	2975	rVB2	8366	13787	0.96%	0.111%

LSC Area Percent Report

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Acq On : 19 Dec 2022 13:52
Operator : SY/MD
Sample : N6075-08 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BGSM3

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\SFAMVLM120722WMA.M
Title : VOC Analysis

77	10.702	2998	3005	3010	rBV2	381	426	0.03%	0.003%
78	10.809	3035	3038	3042	rVB2	210	154	0.01%	0.001%
79	10.844	3042	3049	3055	rBB3	567	521	0.04%	0.004%
80	10.870	3055	3057	3060	rBV	269	179	0.01%	0.001%
81	10.944	3077	3080	3083	rBV3	298	215	0.01%	0.002%
82	10.956	3083	3084	3087	rVV	313	142	0.01%	0.001%
83	10.979	3090	3091	3098	rVB2	236	168	0.01%	0.001%
84	11.069	3116	3119	3123	rBV2	278	236	0.02%	0.002%
85	11.236	3159	3171	3197	rBV	816692	1263597	87.68%	10.151%
86	11.519	3255	3259	3261	rBV3	348	308	0.02%	0.002%
87	11.612	3276	3288	3307	rVV	706642	1104145	76.62%	8.870%
88	11.853	3358	3363	3364	rBV	355	269	0.02%	0.002%
89	11.905	3375	3379	3381	rBV	439	302	0.02%	0.002%
90	12.014	3411	3413	3416	rBV	293	151	0.01%	0.001%
91	12.075	3430	3432	3435	rVB2	241	110	0.01%	0.001%
92	12.098	3435	3439	3442	rBV2	360	292	0.02%	0.002%
93	12.156	3452	3457	3464	rBV3	598	737	0.05%	0.006%
94	12.426	3538	3541	3542	rBV	225	119	0.01%	0.001%
95	12.461	3549	3552	3555	rBV	284	210	0.01%	0.002%
96	12.503	3562	3565	3567	rBV2	591	334	0.02%	0.003%
97	12.683	3619	3621	3622	rBV	367	154	0.01%	0.001%
98	12.847	3668	3672	3676	rBV2	473	457	0.03%	0.004%
99	12.921	3693	3695	3698	rBV2	513	389	0.03%	0.003%
100	13.249	3795	3797	3802	rVB2	766	554	0.04%	0.004%

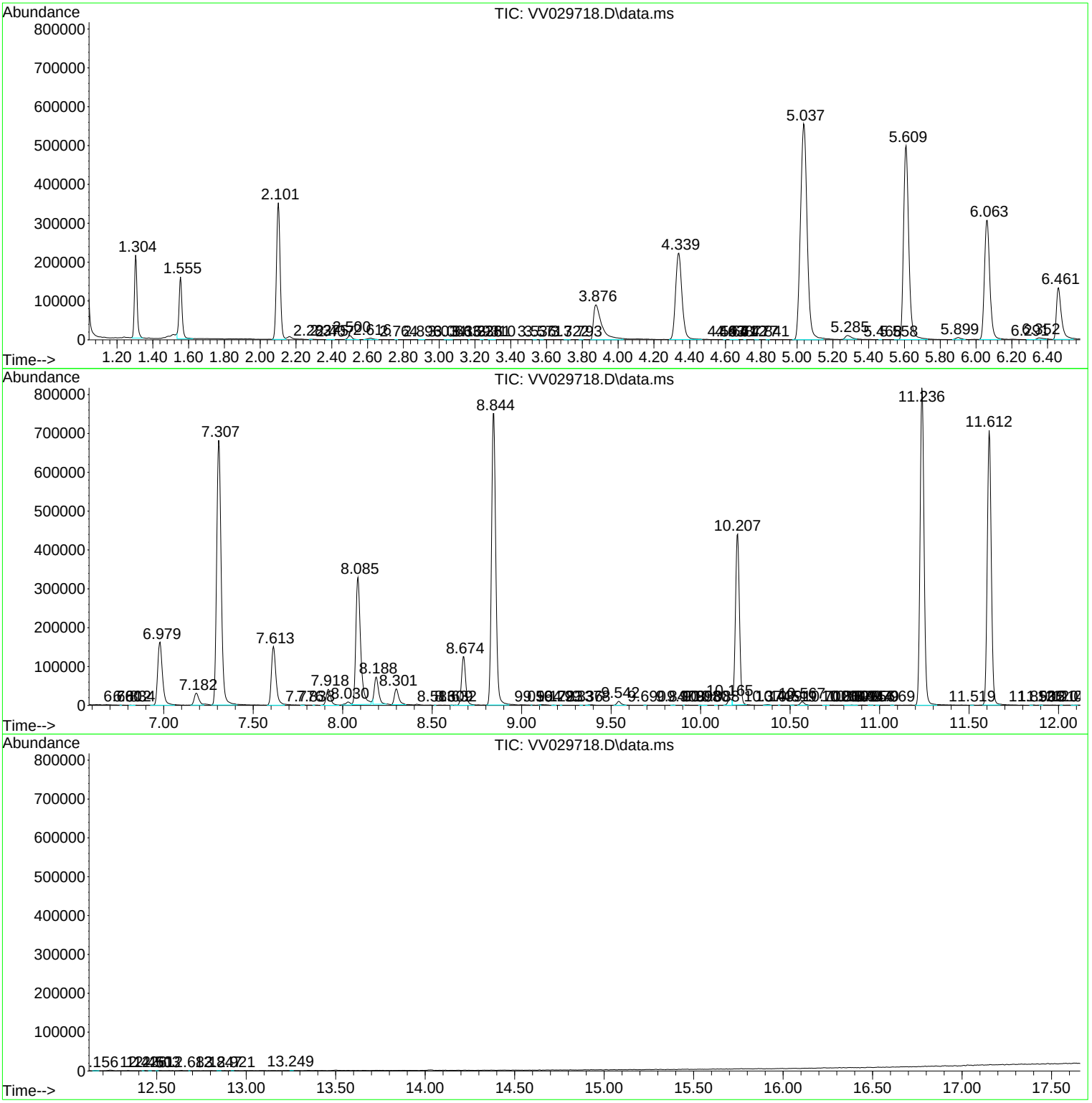
Sum of corrected areas: 12447863

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121922\
Data File : VV029718.D
Acq On : 19 Dec 2022 13:52
Operator : SY/MD
Sample : N6075-08 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BGSM3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121922\
Data File : VV029718.D
Acq On : 19 Dec 2022 13:52
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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BGSM3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

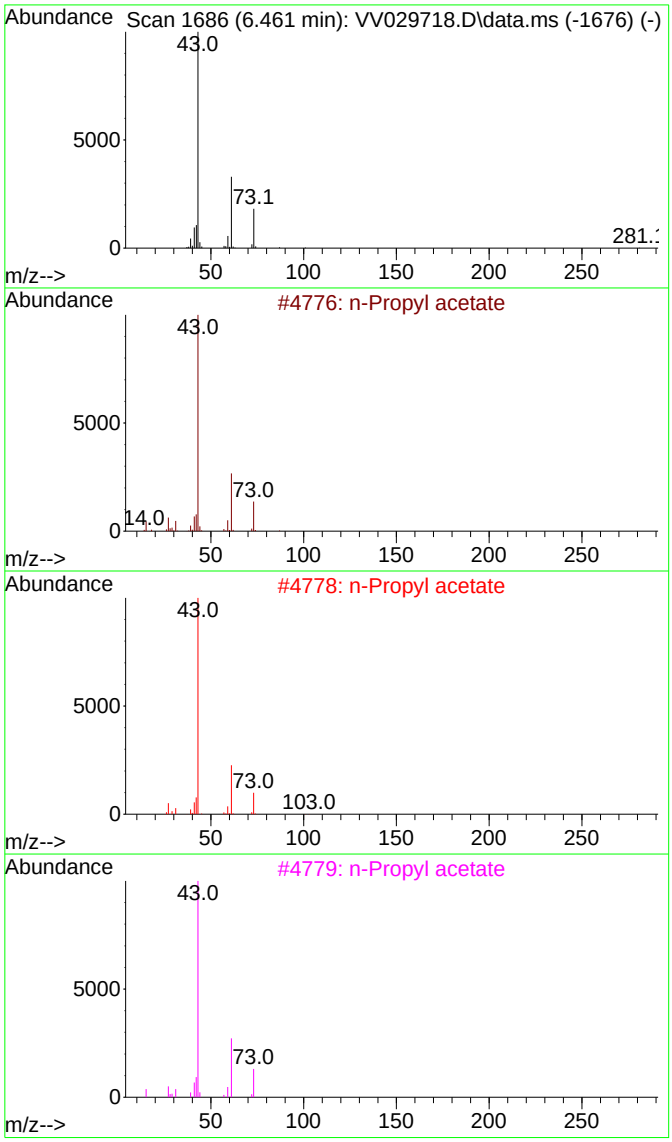
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

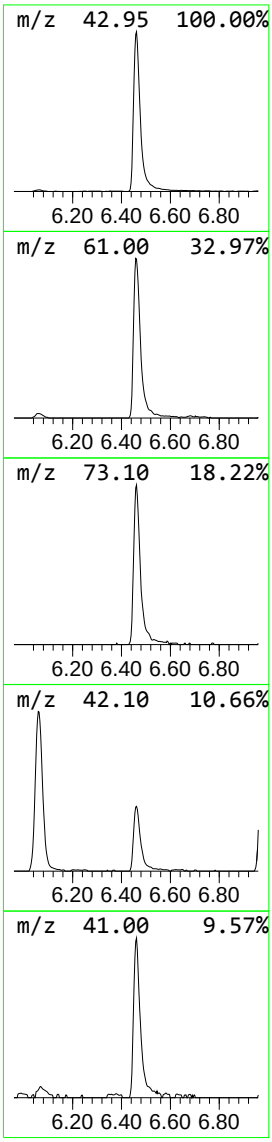
****

Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.461	12.59 ug/L	257191	1,4-Difluorobenzene	5.609

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	83
3	n-Propyl acetate	102	C5H10O2	000109-60-4	78
4	n-Propyl acetate	102	C5H10O2	000109-60-4	64
5	n-Propyl acetate	102	C5H10O2	000109-60-4	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121922\
Data File : VV029718.D
Acq On : 19 Dec 2022 13:52
Operator : SY/MD
Sample : N6075-08 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BGSM3

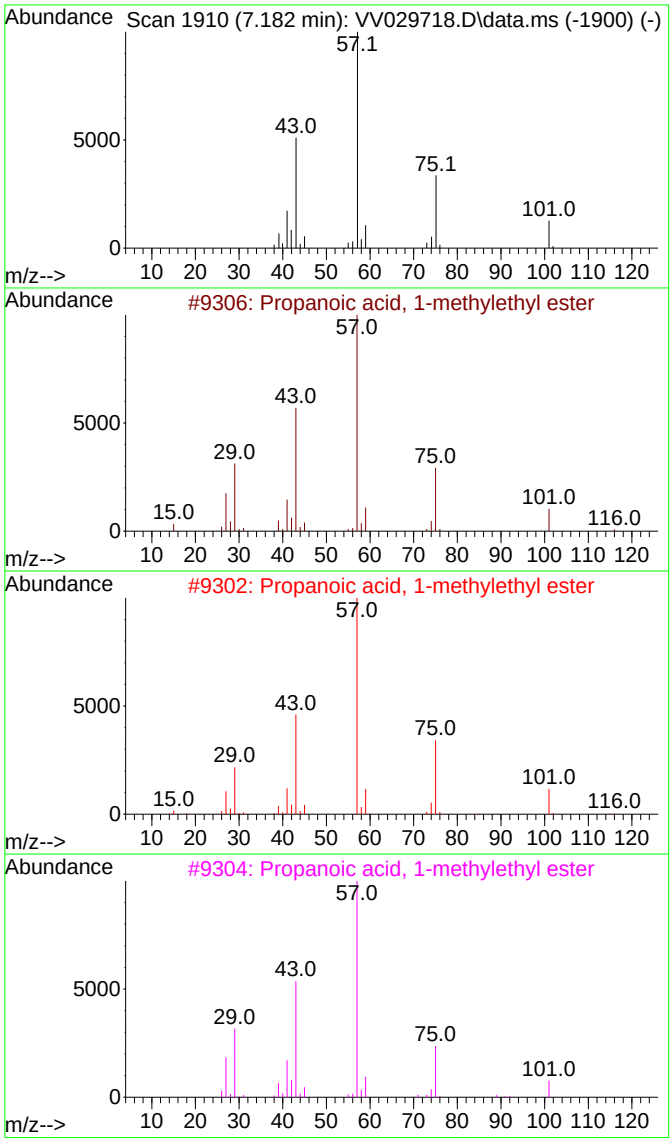
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

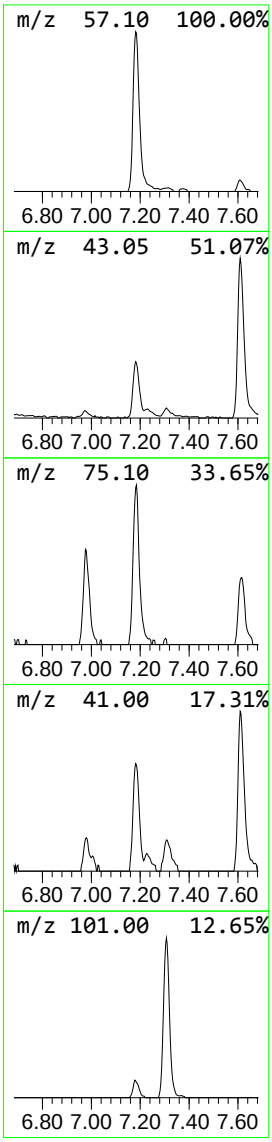
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.182	2.72 ug/L	55549	1,4-Difluorobenzene	5.609

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	83
3	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	83
4	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	74
5	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	42





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121922\
Data File : VV029718.D
Acq On : 19 Dec 2022 13:52
Operator : SY/MD
Sample : N6075-08 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BGSM3

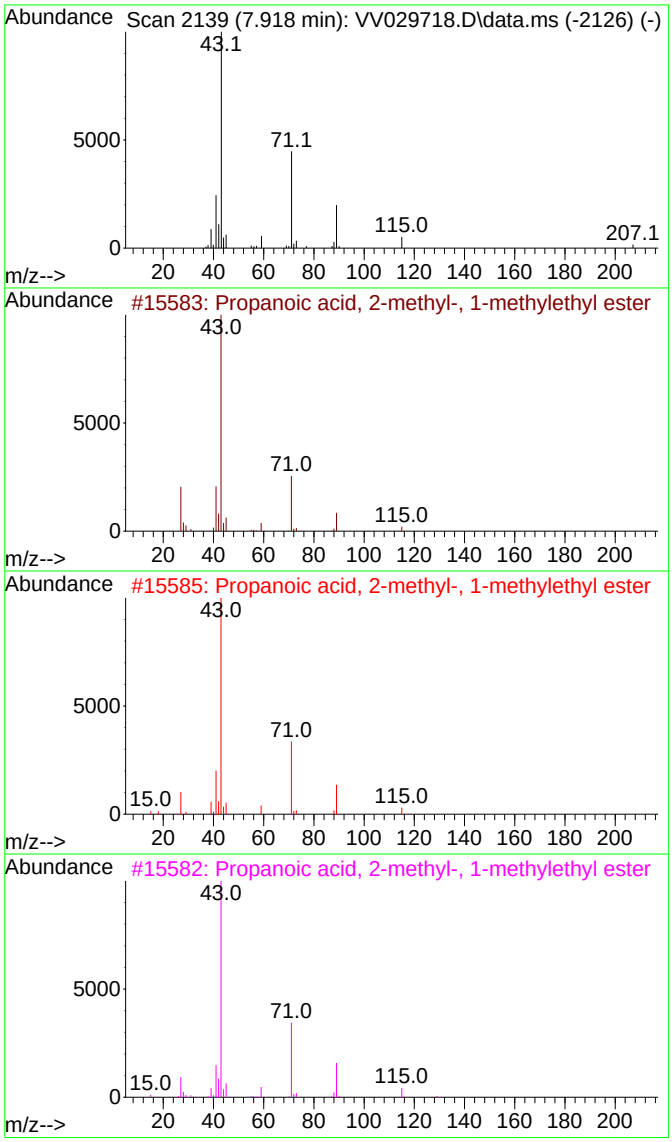
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

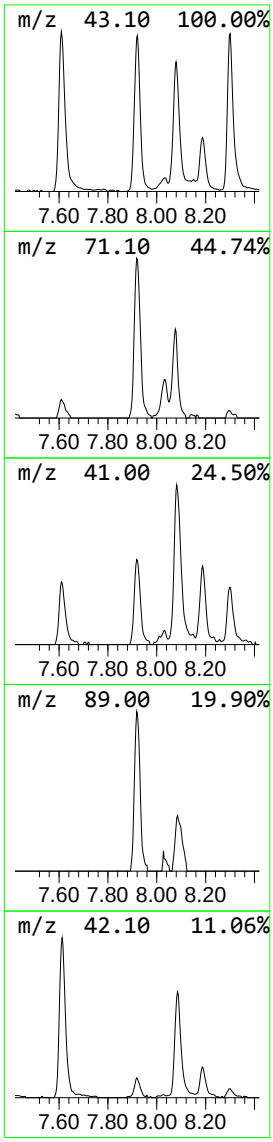
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.918	2.88 ug/L	71505	Chlorobenzene-d5	8.844

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





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121922\
Data File : VV029718.D
Acq On : 19 Dec 2022 13:52
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Sample : N6075-08 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BGSM3

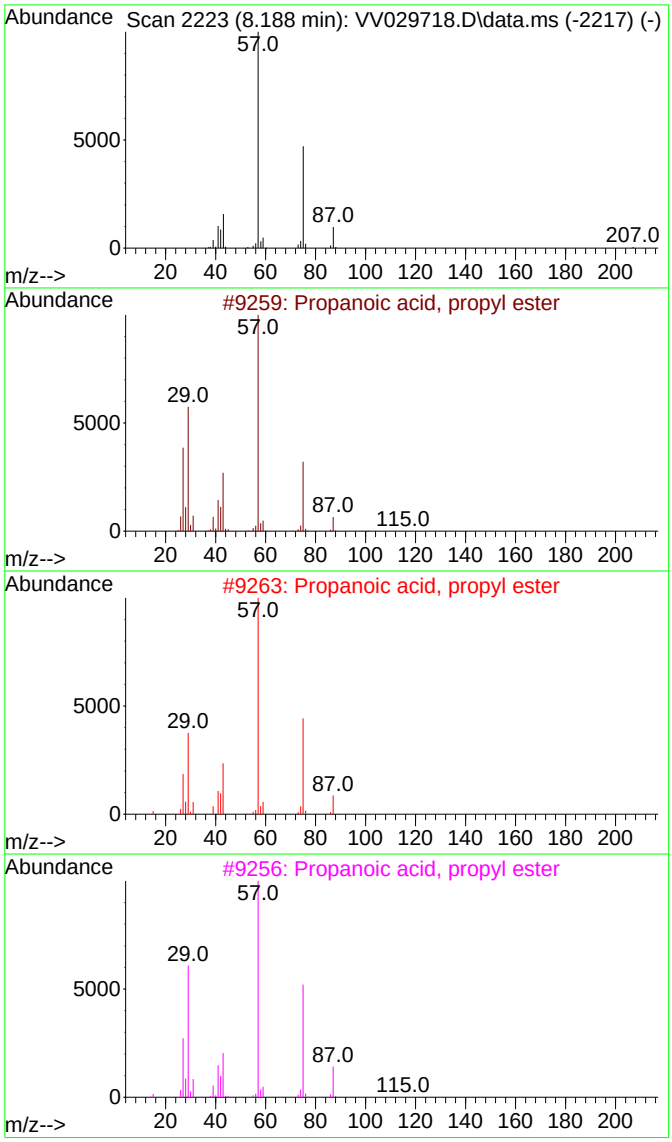
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

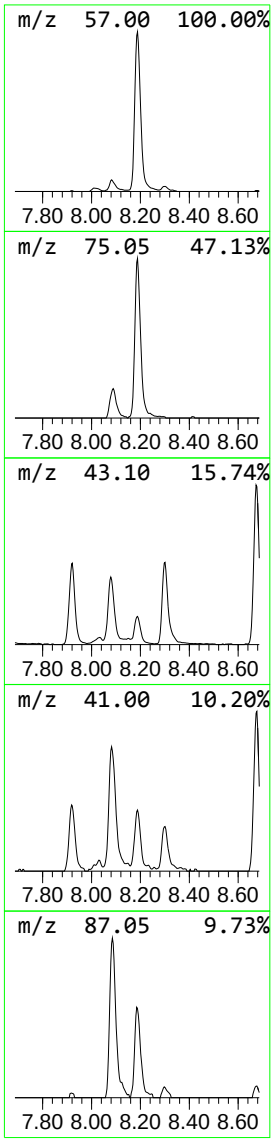
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.188	4.56 ug/L	113066	Chlorobenzene-d5	8.844

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	78
3	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	78
4	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	53
5	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121922\
Data File : VV029718.D
Acq On : 19 Dec 2022 13:52
Operator : SY/MD
Sample : N6075-08 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BGSM3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

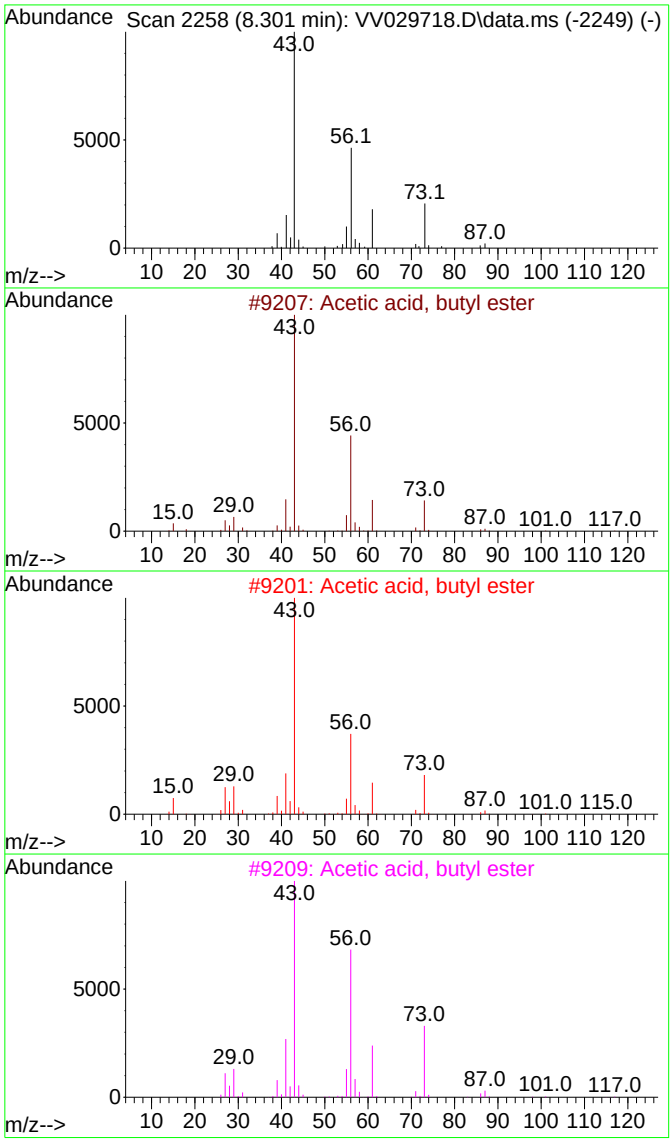
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

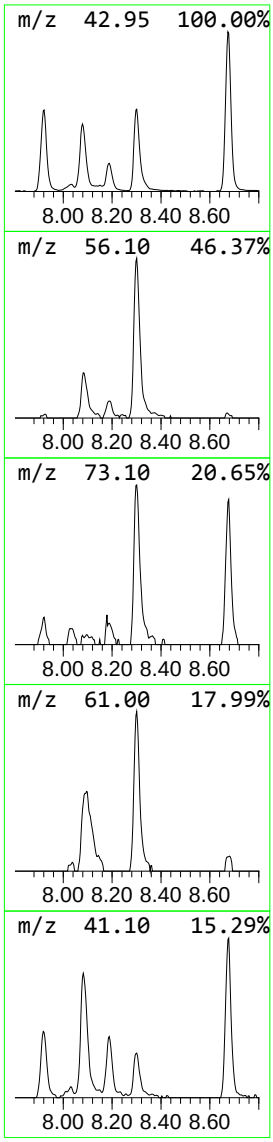
****

Peak Number 6 Acetic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.301	2.77 ug/L	68641	Chlorobenzene-d5	8.844

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	78
3	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
4	Acetic acid, hexyl ester	144	C8H16O2	000142-92-7	42
5	Isobutyl acetate	116	C6H12O2	000110-19-0	40





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121922\
Data File : VV029718.D
Acq On : 19 Dec 2022 13:52
Operator : SY/MD
Sample : N6075-08 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BGSM3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

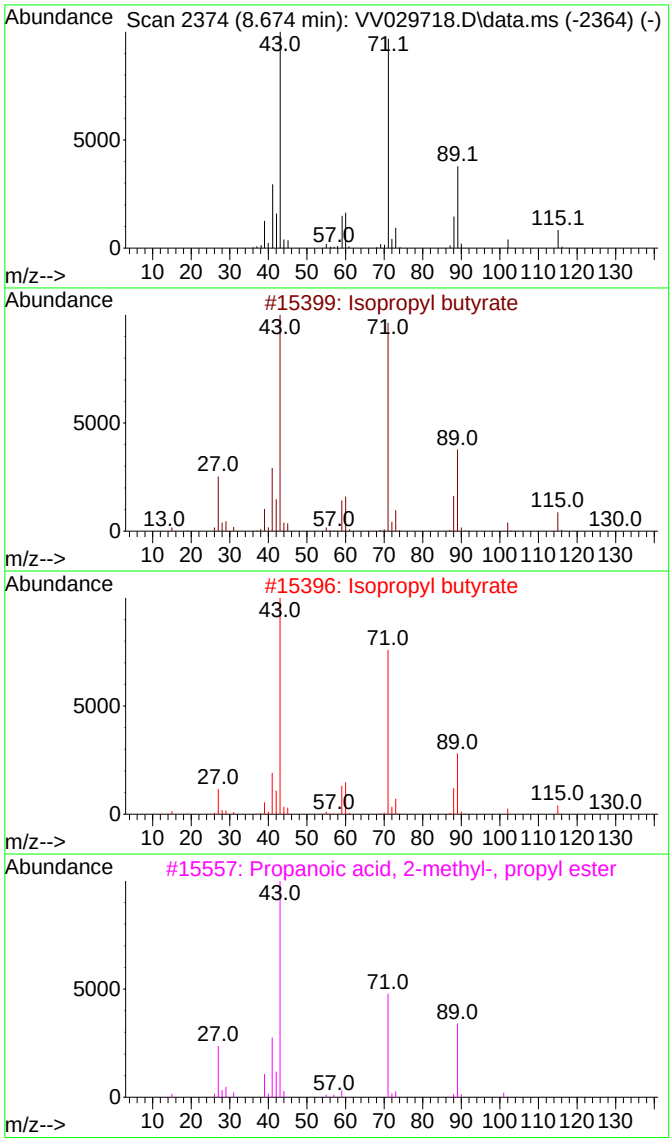
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

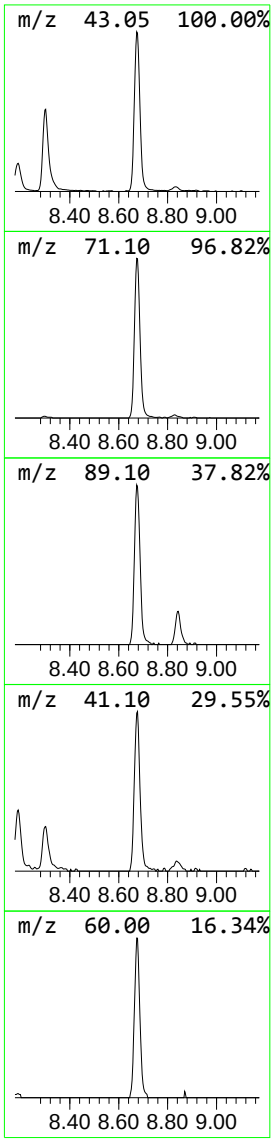
****

Peak Number 7 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.674	8.08 ug/L	200499	Chlorobenzene-d5	8.844

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	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
4	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121922\
Data File : VV029718.D
Acq On : 19 Dec 2022 13:52
Operator : SY/MD
Sample : N6075-08 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BGSM3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.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	6.461	12.6	ug/L	257191	1	5.609	1021090	50.0
Propanoic acid,...	7.182	2.7	ug/L	55549	1	5.609	1021090	50.0
Propanoic acid,...	7.918	2.9	ug/L	71505	2	8.844	1240220	50.0
Propanoic acid,...	8.188	4.6	ug/L	113066	2	8.844	1240220	50.0
Acetic acid, bu...	8.301	2.8	ug/L	68641	2	8.844	1240220	50.0
Isopropyl butyrate	8.674	8.1	ug/L	200499	2	8.844	1240220	50.0