

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012621\
 Data File : VN065609.D
 Acq On : 26 Jan 2021 17:16
 Operator : JC/MD
 Sample : M1188-06
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TP-SWITCH-GEAR

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 1 % 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_N\methods\82N012521W.M

Title : SW846 8260

Signal : TIC: VN065609.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.782	624	635	649	rVB	16787	40449	1.57%	0.315%
2	4.502	843	859	877	rVB2	10539	30321	1.18%	0.236%
3	7.550	1789	1807	1818	rBV	130243	322575	12.54%	2.511%
4	7.624	1818	1830	1851	rVB	255507	605420	23.53%	4.713%
5	7.988	1923	1943	1962	rBV	160472	371349	14.43%	2.891%
6	8.129	1973	1987	2005	rVB2	15855	36120	1.40%	0.281%
7	8.547	2102	2117	2149	rVB	394410	838108	32.57%	6.525%
8	9.151	2294	2305	2317	rBV3	18500	39249	1.53%	0.306%
9	9.235	2317	2331	2365	rVV	988098	1815030	70.54%	14.131%
10	9.872	2516	2529	2543	rBV	183491	320291	12.45%	2.494%
11	10.058	2573	2587	2605	rBV	618760	1141169	44.35%	8.884%
12	10.251	2638	2647	2657	rBV	17719	29765	1.16%	0.232%
13	10.512	2719	2728	2740	rVB	52071	87424	3.40%	0.681%
14	10.608	2747	2758	2773	rBV	106437	178177	6.92%	1.387%
15	10.733	2785	2797	2814	rVV	1601390	2573120	100.00%	20.033%
16	10.823	2815	2825	2839	rVB	158576	261965	10.18%	2.039%
17	11.139	2910	2923	2941	rBV	1115107	1766366	68.65%	13.752%
18	11.376	2985	2997	3018	rBV	525955	924229	35.92%	7.195%
19	11.849	3137	3144	3158	rVB	31114	47621	1.85%	0.371%
20	12.373	3295	3307	3327	rBV	384117	686038	26.66%	5.341%
21	13.312	3589	3599	3614	rBV	427719	729799	28.36%	5.682%

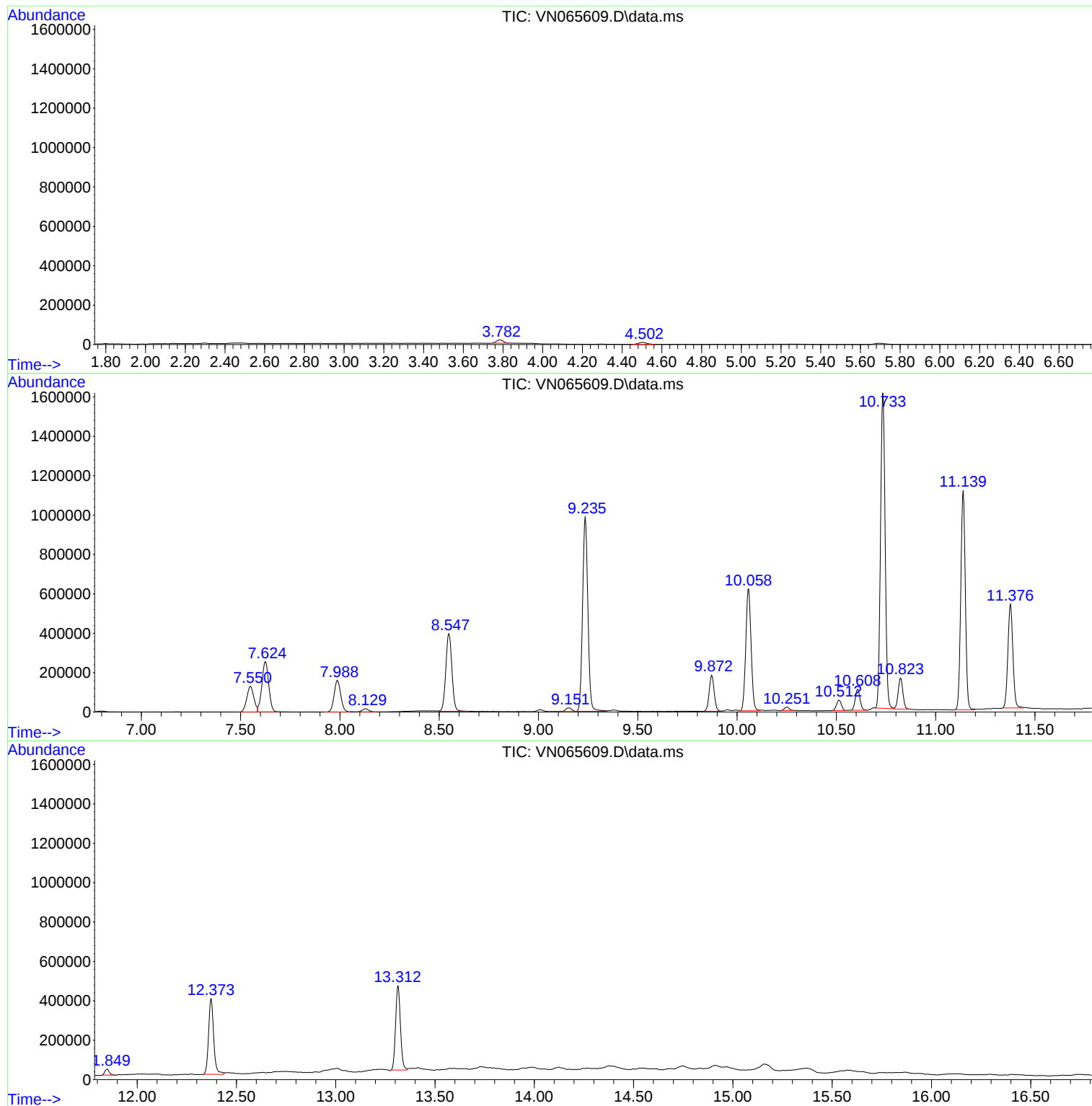
Sum of corrected areas: 12844585

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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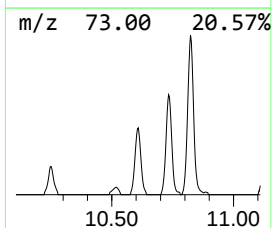
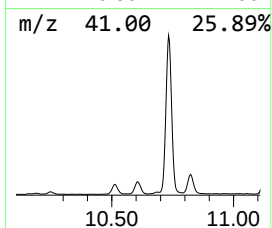
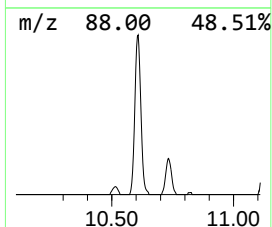
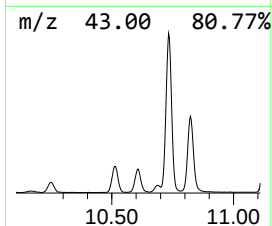
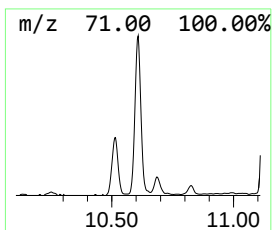
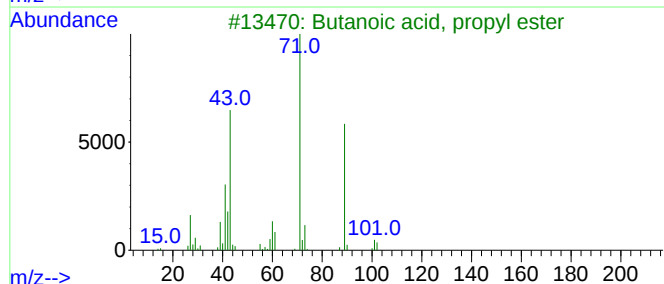
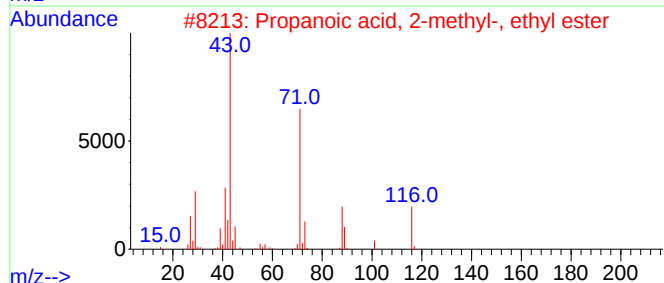
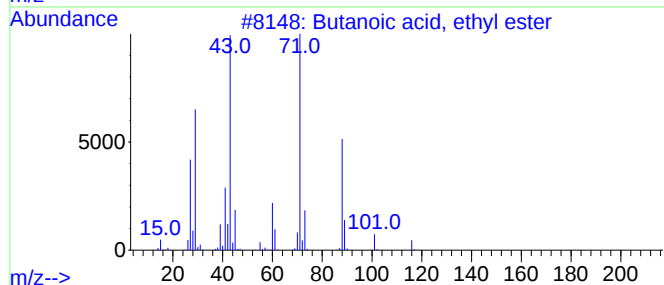
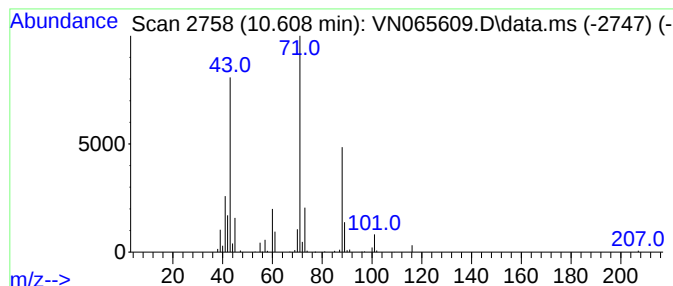
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butanoic acid, ethyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.608	9.64 ug/l	178177	Chlorobenzene-d5	11.376

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	97
2			Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	53
3			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	50
4			3-Mercaptohexyl butanoate	204	C10H20O2S	136954-21-7	42
5			Butanoic acid, 3-methylbutyl ester	158	C9H18O2	000106-27-4	38



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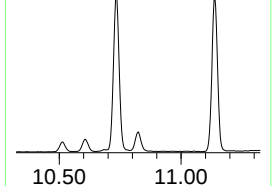
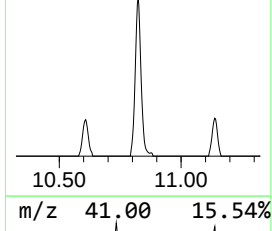
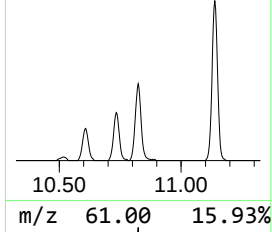
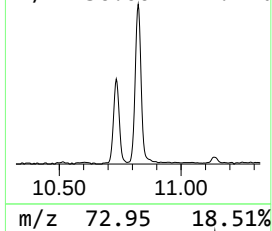
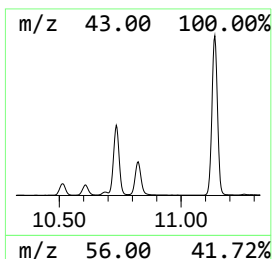
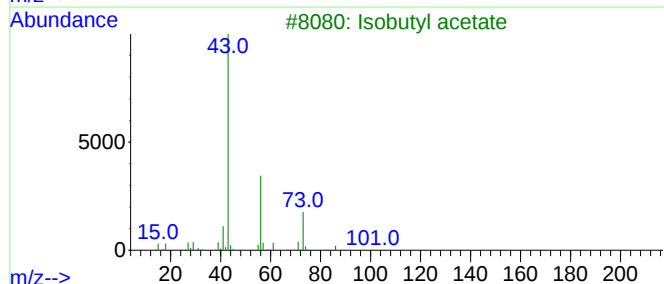
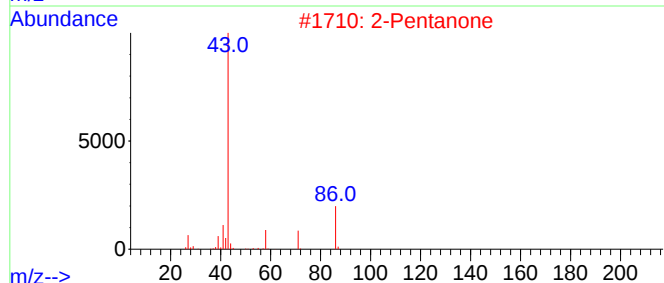
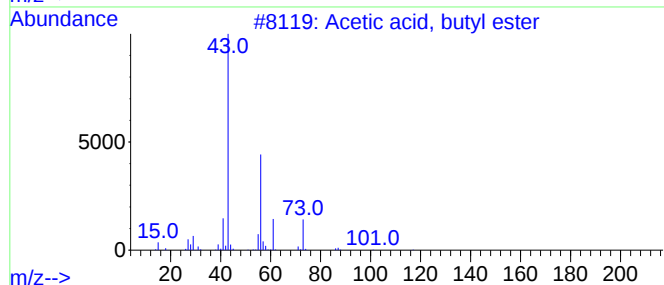
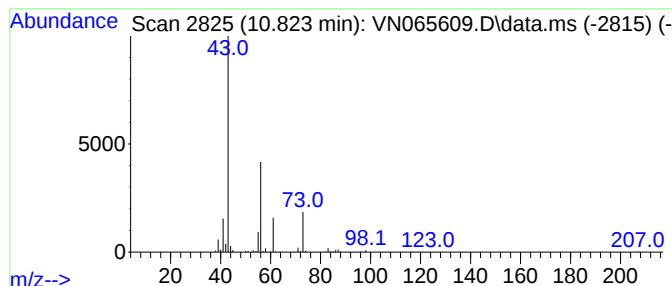
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Peak Number 2 Acetic acid, butyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.823	14.17 ug/l	261965	Chlorobenzene-d5	11.376

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78
2			2-Pentanone	86	C5H10O	000107-87-9	9
3			Isobutyl acetate	116	C6H12O2	000110-19-0	9
4			1-Butanol, 4-chloro-, acetate	150	C6H11ClO2	006962-92-1	9
5			5-Oxohexanenitrile	111	C6H9NO	010412-98-3	9



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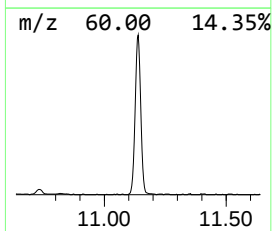
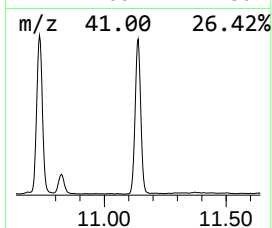
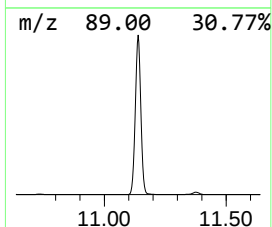
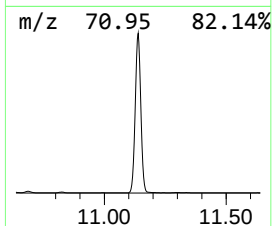
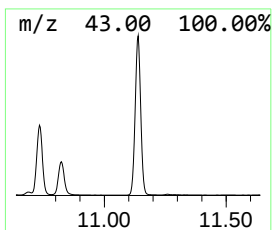
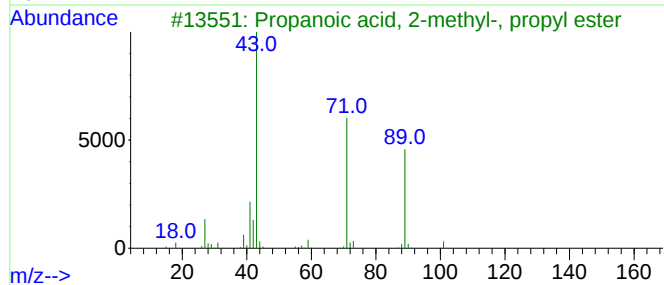
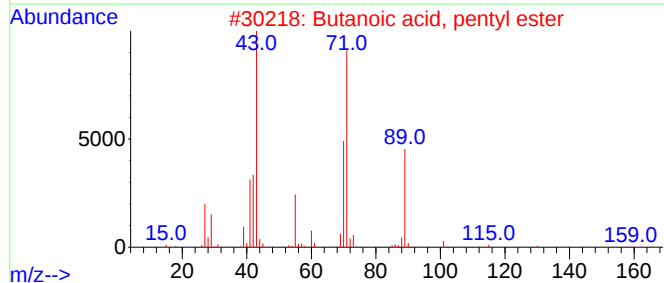
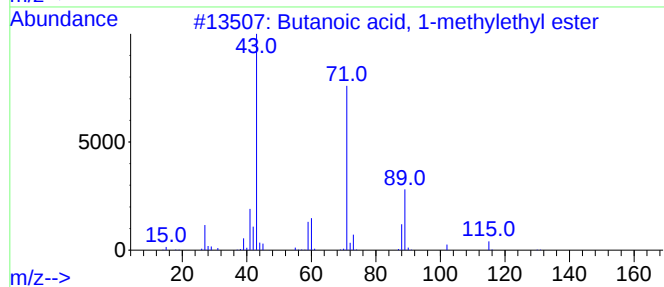
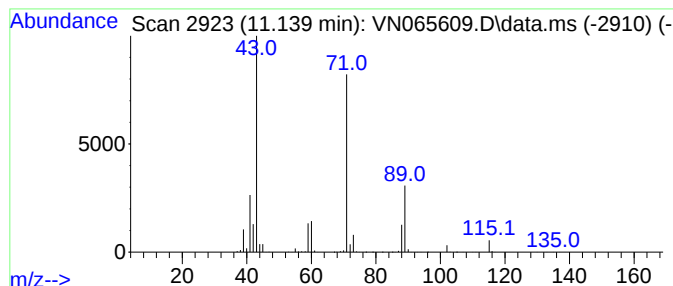
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Butanoic acid, 1-methylethy... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.139	95.56 ug/l	1766370	Chlorobenzene-d5	11.376

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	95
2			Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64
3			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	56
4			Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	47
5			Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	42



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butanoic acid, ...	10.608	9.6	ug/l	178177	3	11.376	924229	50.0
Acetic acid, bu...	10.823	14.2	ug/l	261965	3	11.376	924229	50.0
Butanoic acid, ...	11.139	95.6	ug/l	1766370	3	11.376	924229	50.0