

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012521\
 Data File : VN065590.D
 Acq On : 25 Jan 2021 20:37
 Operator : JC/MD
 Sample : M1188-03
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TP-230

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: VN065590.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.785	623	636	652	rBV	14616	36475	1.59%	0.300%
2	4.505	844	860	879	rVB3	9794	30004	1.31%	0.247%
3	5.695	1215	1230	1246	rBV4	7421	23773	1.03%	0.196%
4	7.550	1788	1807	1818	rBV	128258	320577	13.95%	2.638%
5	7.624	1818	1830	1849	rVB	250571	593601	25.83%	4.884%
6	7.987	1927	1943	1965	rBV	153242	361134	15.72%	2.971%
7	8.129	1977	1987	2002	rVB3	15822	34656	1.51%	0.285%
8	8.550	2103	2118	2138	rBV	387729	807163	35.12%	6.641%
9	9.151	2294	2305	2317	rBV2	16972	35551	1.55%	0.293%
10	9.235	2317	2331	2365	rBV	919863	1707179	74.29%	14.046%
11	9.871	2515	2529	2545	rBV	172697	302120	13.15%	2.486%
12	10.058	2573	2587	2614	rBV	617774	1131438	49.24%	9.309%
13	10.251	2637	2647	2662	rVB	17164	30271	1.32%	0.249%
14	10.515	2717	2729	2742	rVB	50723	85306	3.71%	0.702%
15	10.608	2743	2758	2773	rBV	98569	167598	7.29%	1.379%
16	10.733	2785	2797	2815	rVV	1398987	2298013	100.00%	18.907%
17	10.823	2815	2825	2849	rVB	144460	249558	10.86%	2.053%
18	11.138	2910	2923	2945	rBV	995049	1602212	69.72%	13.183%
19	11.376	2981	2997	3025	rVB	529912	926772	40.33%	7.625%
20	11.849	3133	3144	3157	rBV	25107	41886	1.82%	0.345%
21	12.373	3294	3307	3331	rBV	371744	652189	28.38%	5.366%
22	13.315	3585	3600	3624	rBV	418690	716500	31.18%	5.895%

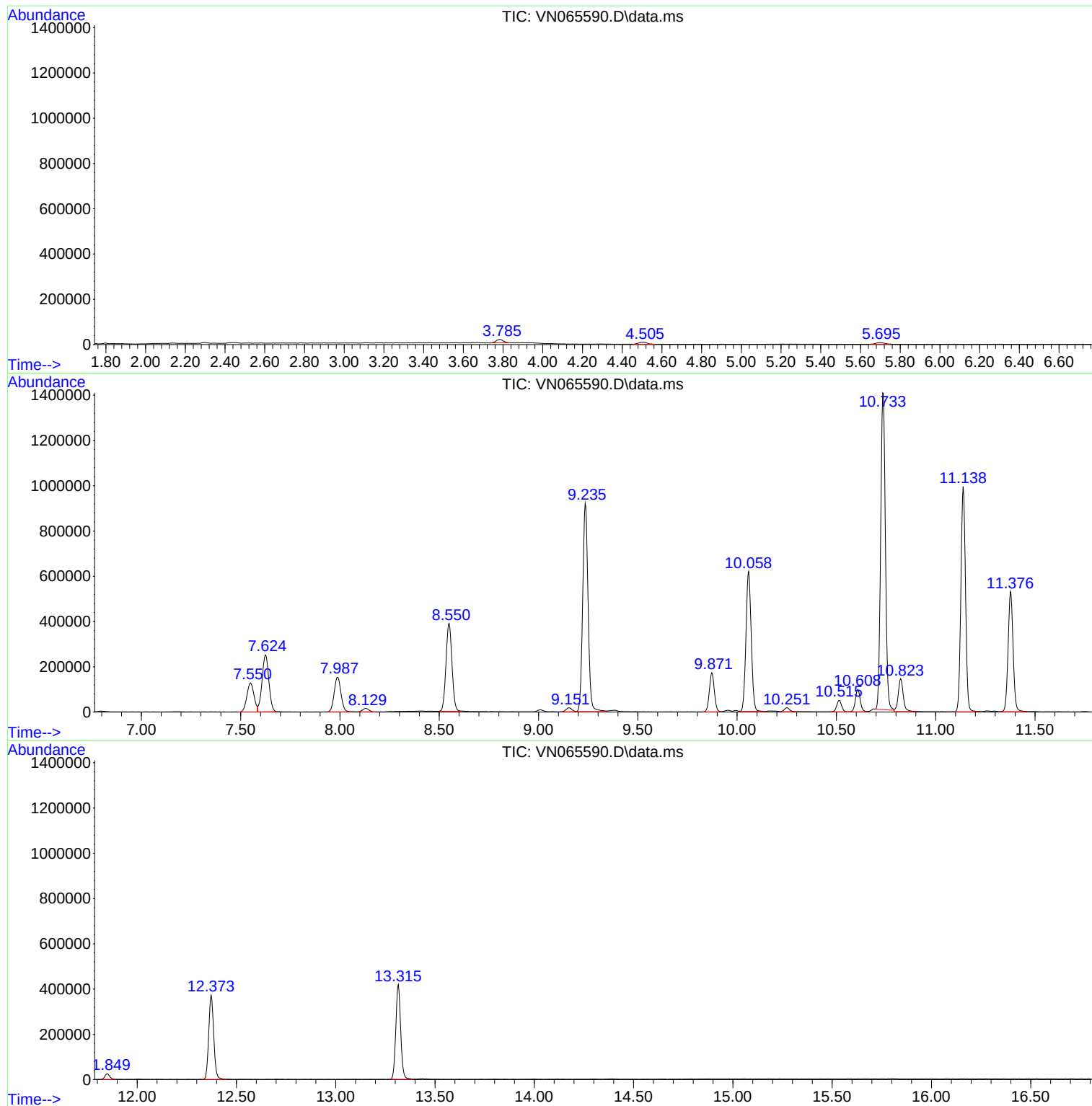
Sum of corrected areas: 12153976

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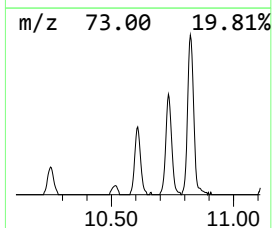
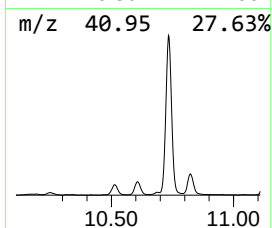
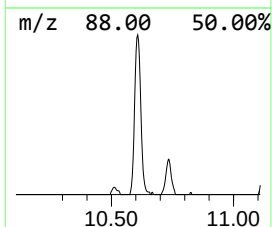
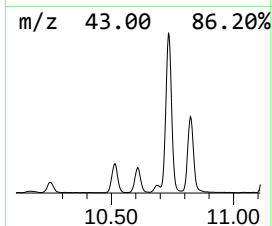
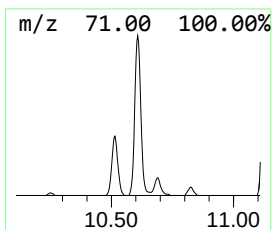
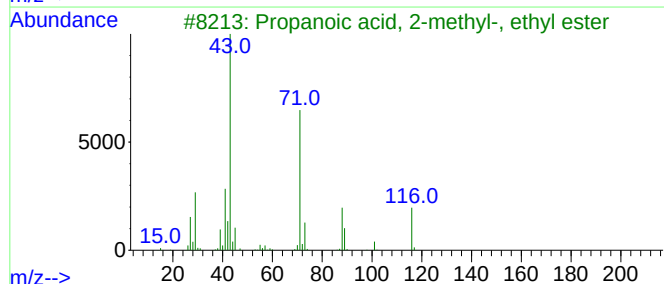
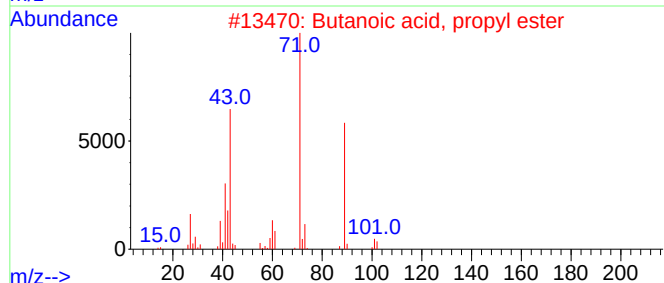
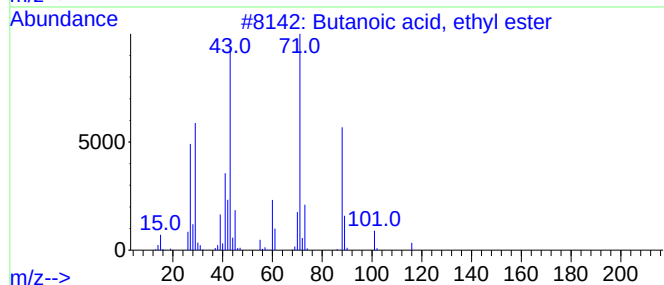
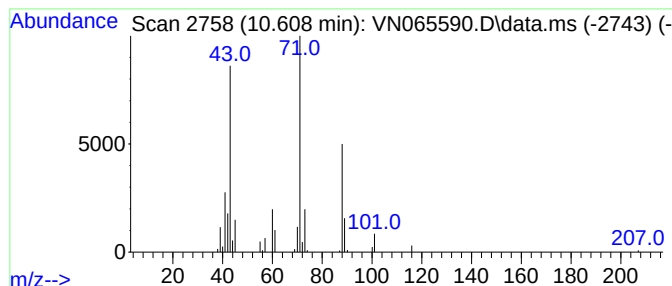
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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	9.04 ug/l	167598	Chlorobenzene-d5	11.376

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	94
2			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	47
3			Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	42
4			3-Mercaptohexyl butanoate	204	C10H20O2S	136954-21-7	42
5			Hexane-1,3,4-triol, 3,5-dimethyl-	162	C8H18O3	1000268-02-6	37



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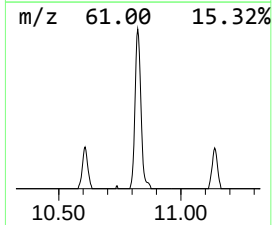
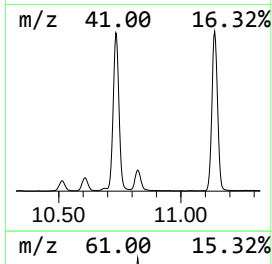
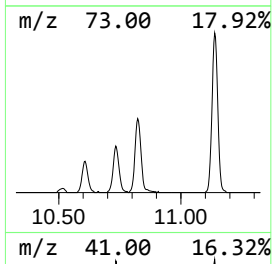
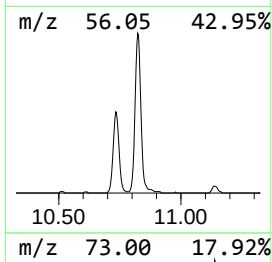
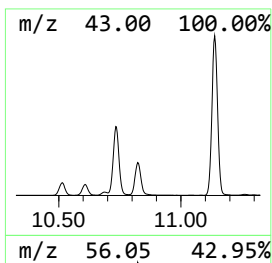
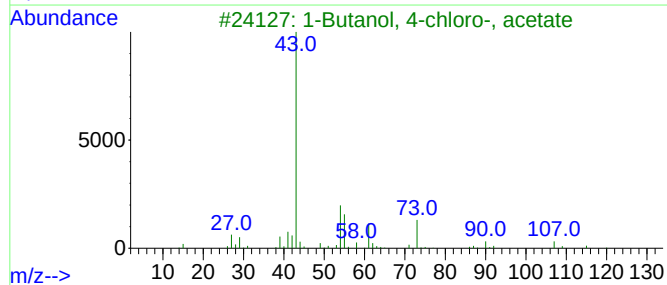
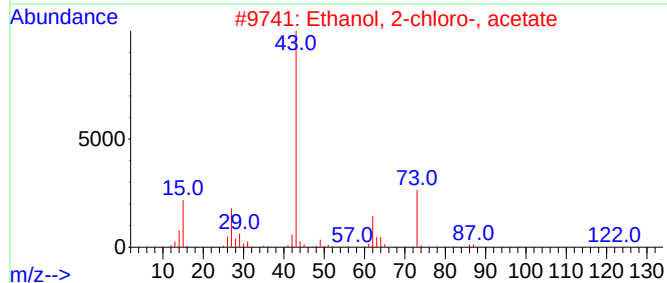
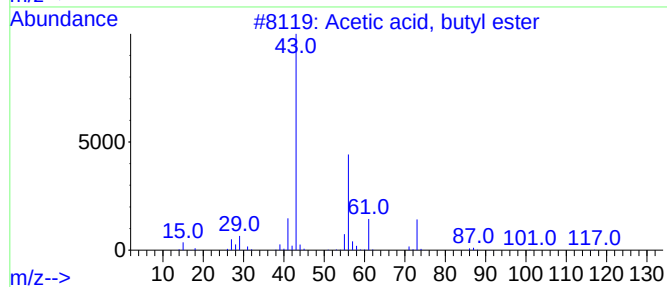
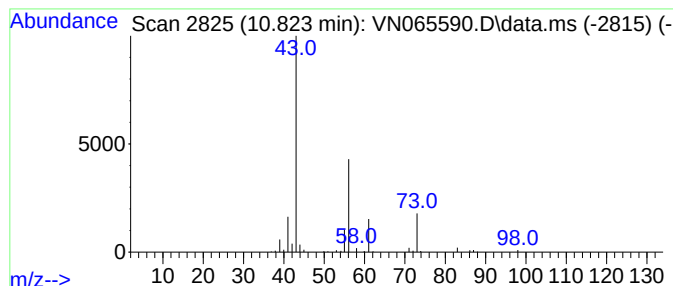
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TIC Integration Parameters: LSCINT.P

Peak Number 2 Acetic acid, butyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.823	13.46 ug/l	249558	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			Ethanol, 2-chloro-, acetate	122	C4H7ClO2	000542-58-5	9
3			1-Butanol, 4-chloro-, acetate	150	C6H11ClO2	006962-92-1	9
4			2-Pentanone	86	C5H10O	000107-87-9	9
5			Isobutyl acetate	116	C6H12O2	000110-19-0	9



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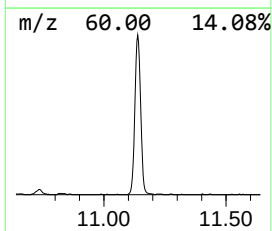
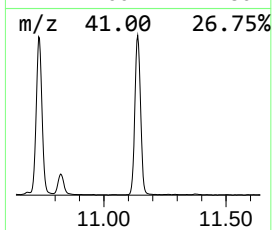
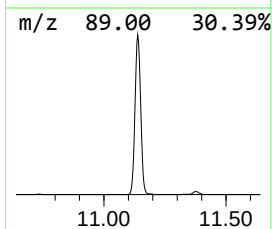
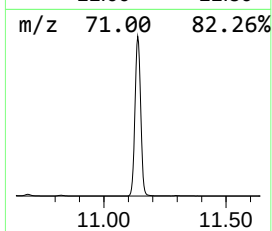
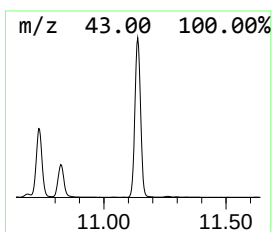
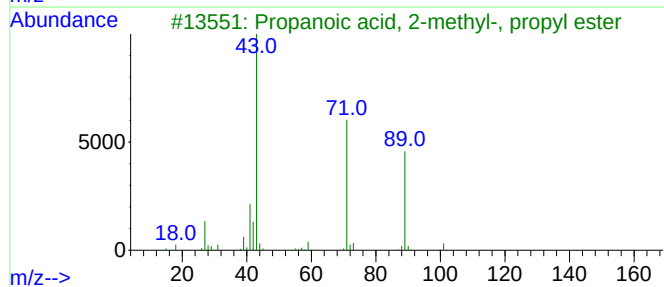
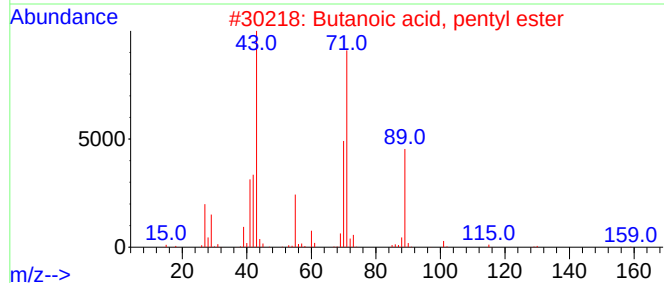
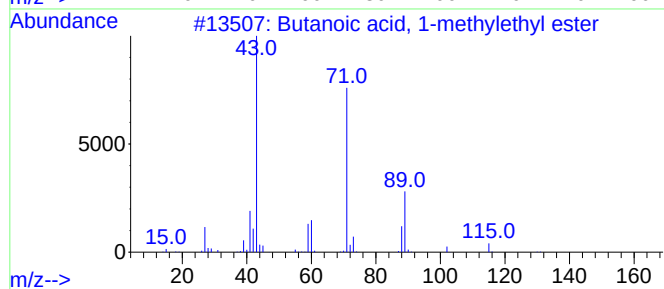
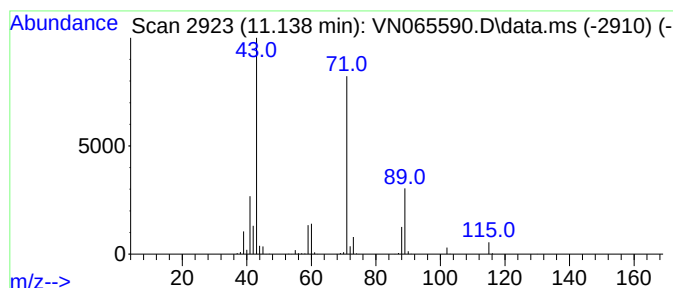
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Peak Number 3 Butanoic acid, 1-methylethy... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.138	86.44 ug/l	1602210	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			Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	42
5			Pentane, 3-bromo-	150	C5H11Br	001809-10-5	40



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butanoic acid, ...	10.608	9.0	ug/l	167598	3	11.376	926772	50.0
Acetic acid, bu...	10.823	13.5	ug/l	249558	3	11.376	926772	50.0
Butanoic acid, ...	11.138	86.4	ug/l	1602210	3	11.376	926772	50.0