

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052924\
 Data File : VN082371.D
 Acq On : 29 May 2024 15:28
 Operator : JC\MD
 Sample : P2609-07
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 522

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % 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\82N051524W.M
 Title : SW846 8260

Signal : TIC: VN082371.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.083	17	22	33	rVB2	11640	24408	1.95%	0.314%
2	2.665	116	121	127	rVB2	6945	12997	1.04%	0.167%
3	4.289	386	397	412	rBV2	34205	104579	8.37%	1.343%
4	4.430	414	421	435	rVB2	12360	39102	3.13%	0.502%
5	7.224	885	896	912	rBV4	33157	90589	7.25%	1.164%
6	8.165	1044	1056	1061	rBV	167067	395192	31.62%	5.076%
7	8.224	1061	1066	1078	rVB	291122	640739	51.27%	8.230%
8	8.577	1112	1126	1140	rBV	186484	445619	35.66%	5.724%
9	9.100	1205	1215	1228	rBV	433004	886951	70.98%	11.393%
10	9.271	1237	1244	1256	rBV	13442	32063	2.57%	0.412%
11	9.659	1300	1310	1316	rBV5	5117	13614	1.09%	0.175%
12	10.318	1415	1422	1435	rBV6	7179	27016	2.16%	0.347%
13	10.571	1456	1465	1473	rBV	673210	1249651	100.00%	16.051%
14	11.865	1672	1685	1696	rBV	628132	1134828	90.81%	14.577%
15	12.070	1714	1720	1727	rVB2	15692	29882	2.39%	0.384%
16	12.400	1768	1776	1784	rBV5	11577	28914	2.31%	0.371%
17	12.847	1843	1852	1863	rBV	477340	849894	68.01%	10.917%
18	12.941	1863	1868	1876	rVB3	9264	15525	1.24%	0.199%
19	13.341	1929	1936	1949	rVB	384117	595421	47.65%	7.648%
20	13.688	1990	1995	2001	rVB3	29054	47772	3.82%	0.614%
21	13.794	2005	2013	2022	rBV	581991	979702	78.40%	12.584%
22	13.876	2022	2027	2035	rVB	23651	41793	3.34%	0.537%
23	15.053	2217	2227	2232	rBV4	10878	24223	1.94%	0.311%
24	15.211	2248	2254	2262	rVB4	7712	13817	1.11%	0.177%
25	15.394	2281	2285	2291	rVB2	15354	24297	1.94%	0.312%
26	16.170	2412	2417	2423	rVB4	10737	20089	1.61%	0.258%
27	16.500	2467	2473	2480	rVB6	7799	16622	1.33%	0.214%

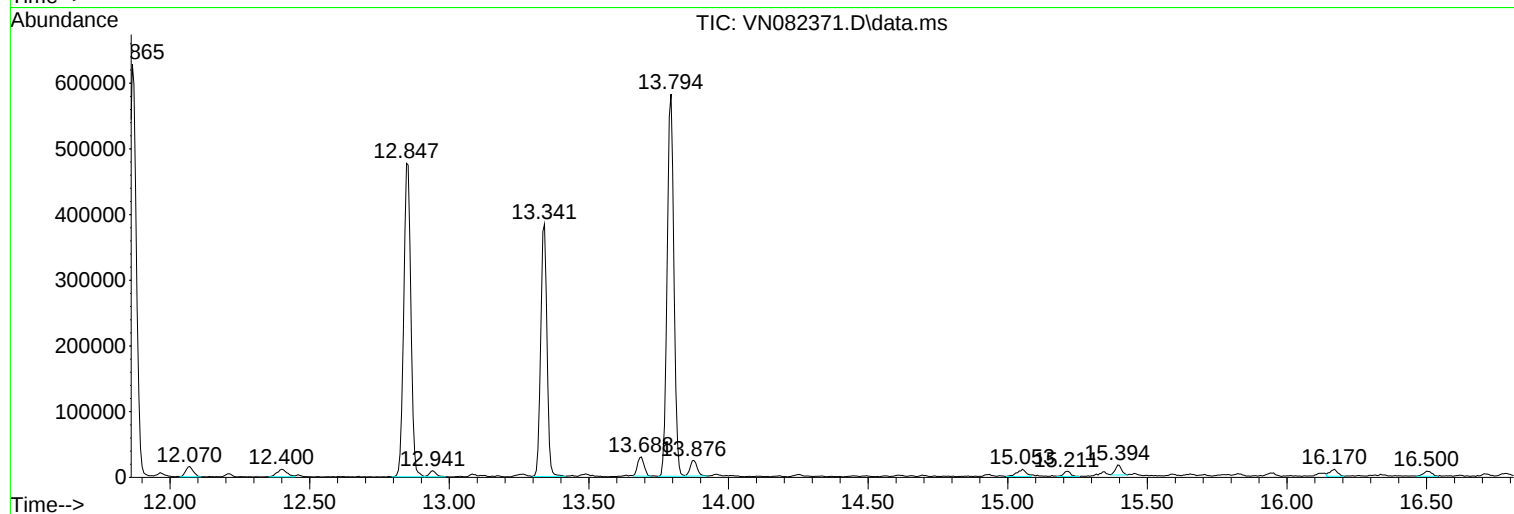
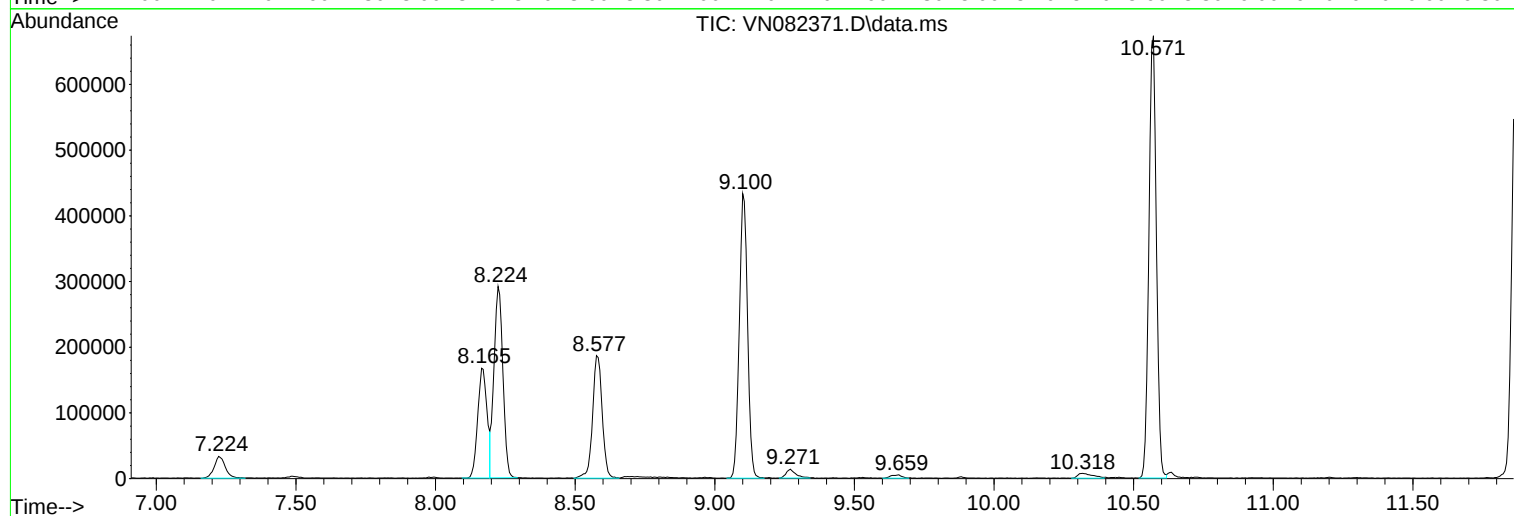
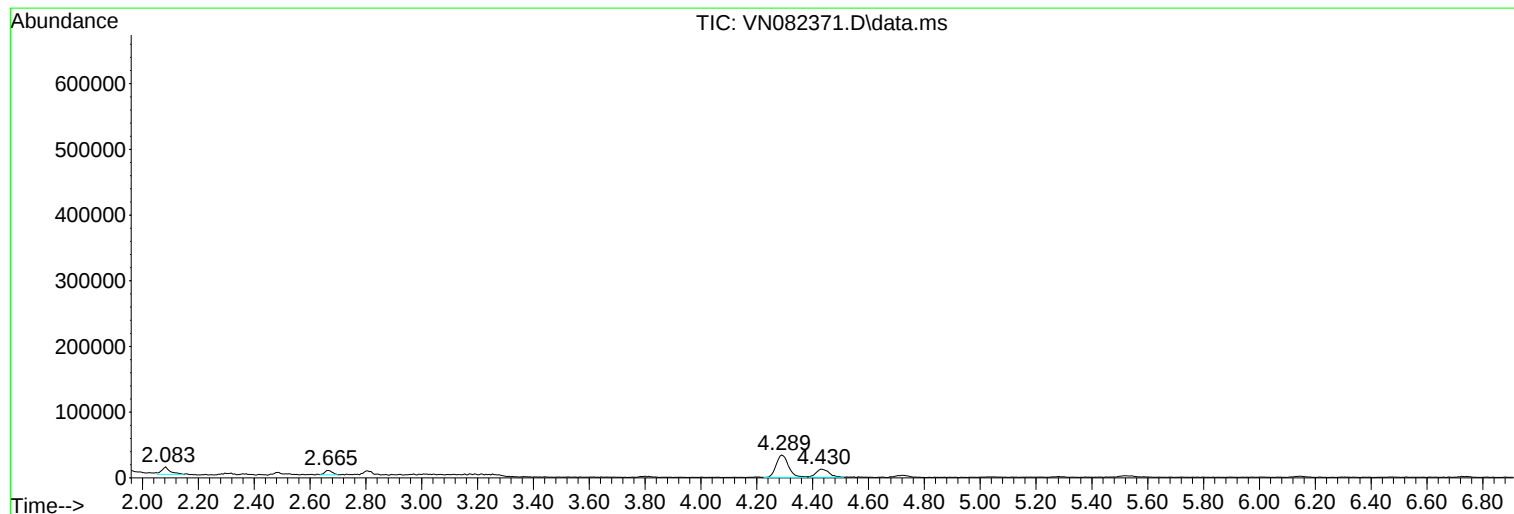
Sum of corrected areas: 7785299

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Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

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



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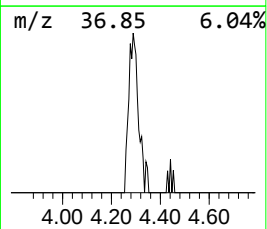
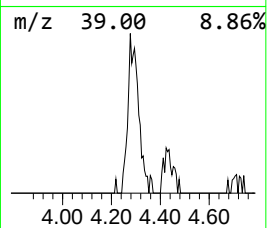
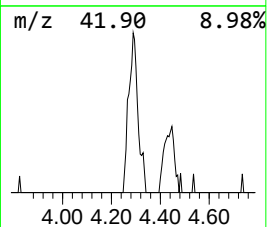
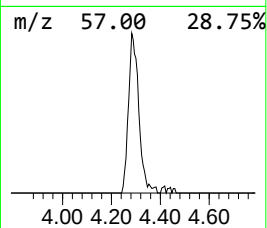
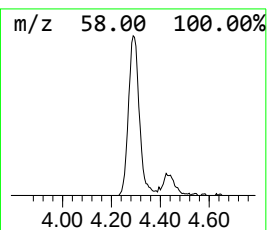
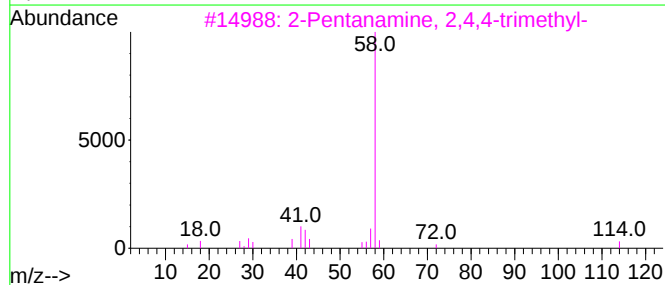
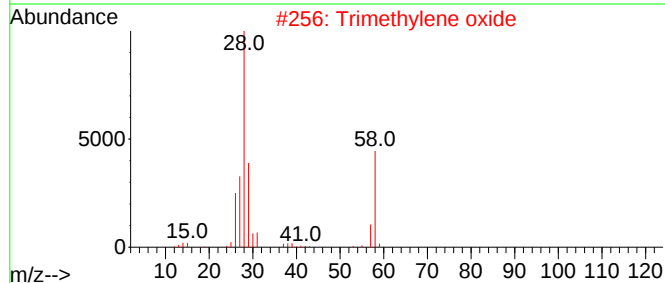
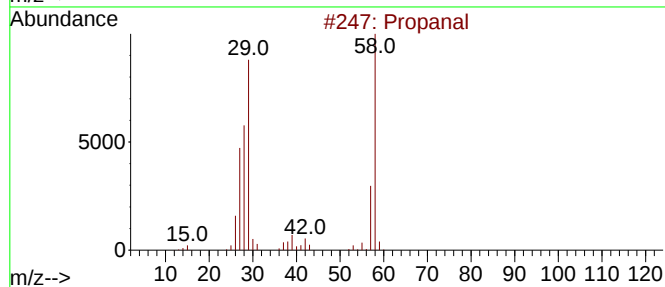
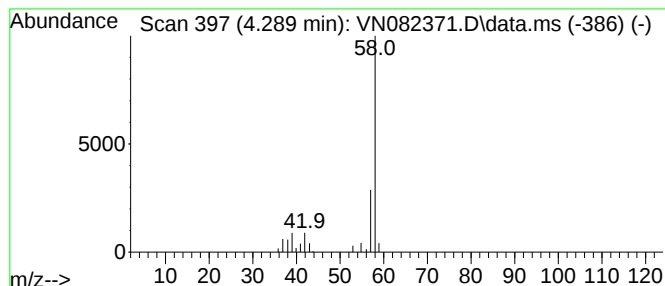
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

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

Peak Number 1 Propanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.289	8.16 ug/l	104579	Pentafluorobenzene	8.224

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanal	58	C3H6O	000123-38-6	78
2			Trimethylene oxide	58	C3H6O	000503-30-0	9
3			2-Pentanamine, 2,4,4-trimethyl-	129	C8H19N	000107-45-9	9
4			Docosylamine, N,N-dimethyl-	353	C24H51N	1000406-30-6	9
5			2-(Aminomethyl)-4-methylpentanoi...	187	C10H21NO2	1891211-54-3	9



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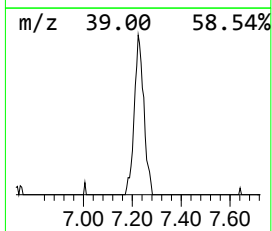
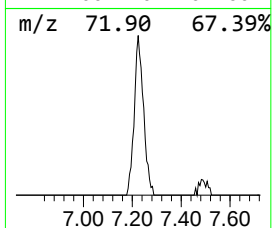
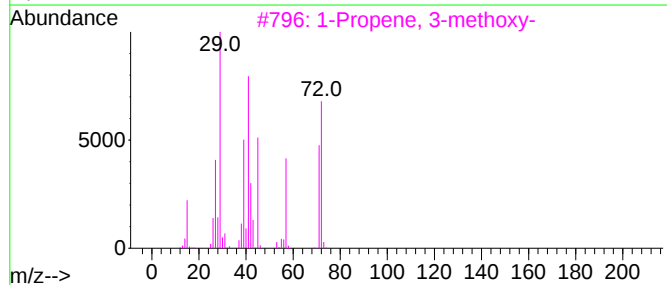
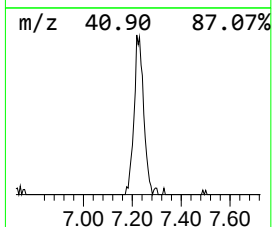
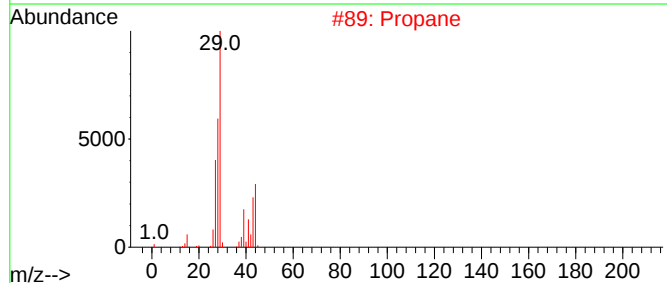
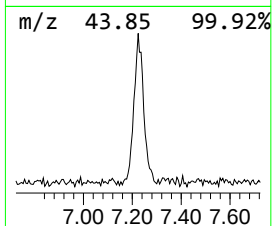
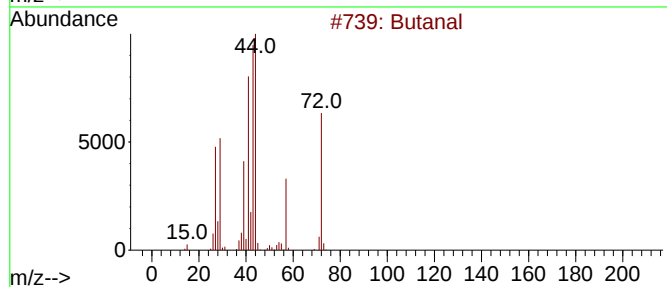
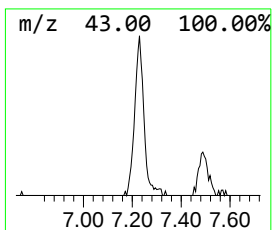
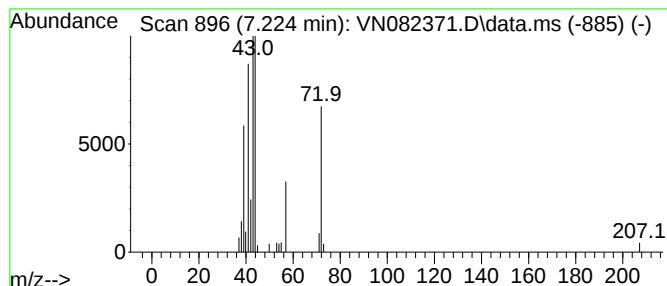
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Peak Number 2 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.224	7.07 ug/l	90589	Pentafluorobenzene	8.224

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	94
2			Propane	44	C3H8	000074-98-6	47
3			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	43
4			Ethene, ethoxy-	72	C4H8O	000109-92-2	38
5			Propanal, 2-methyl-	72	C4H8O	000078-84-2	35



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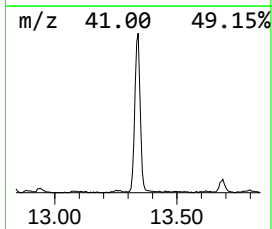
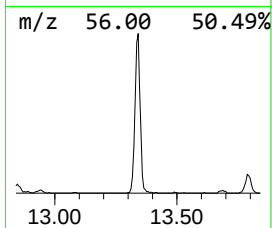
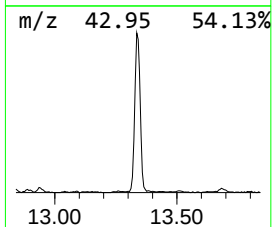
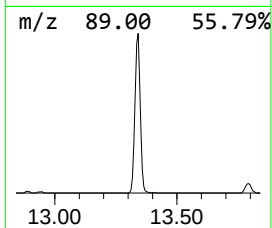
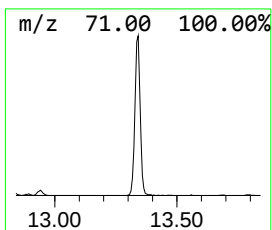
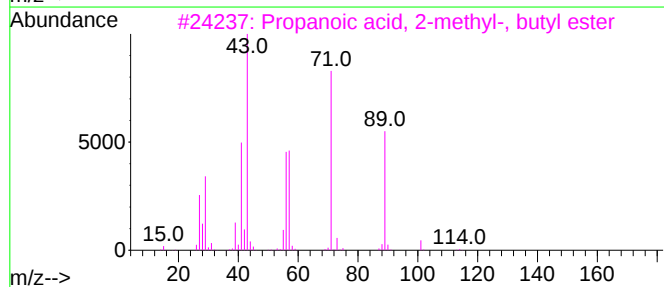
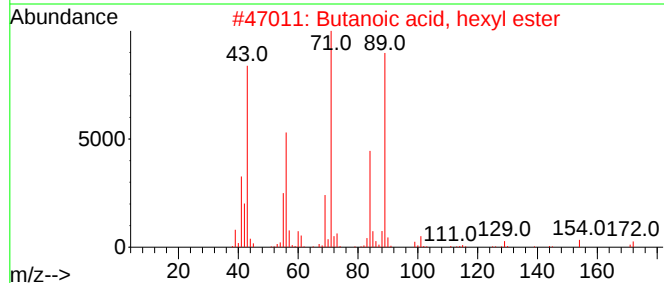
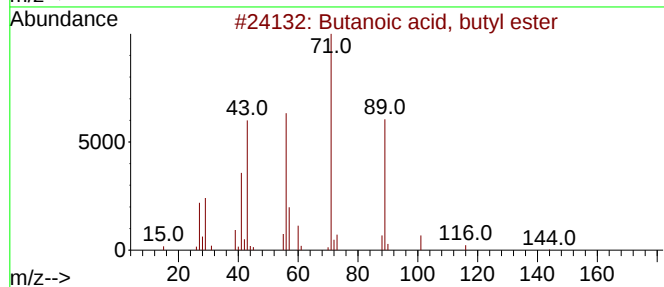
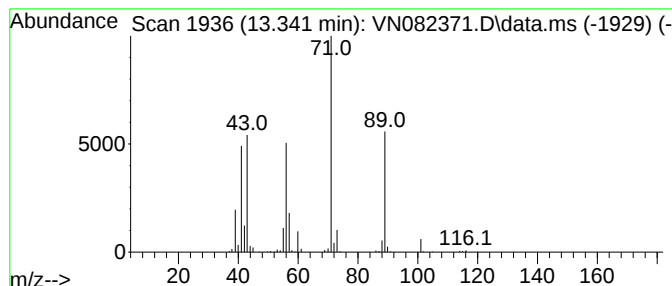
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Peak Number 3 Butanoic acid, butyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.341	30.39 ug/l	595421	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	90
2			Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	74
3			Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	72
4			Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	72
5			Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanal	4.289	8.2	ug/l	104579	1	8.224	640739	50.0
Butanal	7.224	7.1	ug/l	90589	1	8.224	640739	50.0
Butanoic acid, ...	13.341	30.4	ug/l	595421	4	13.794	979702	50.0