

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031224\
 Data File : VN081377.D
 Acq On : 12 Mar 2024 17:02
 Operator : JC\MD
 Sample : P1734-05 50X
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 1342

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\82N030524W.M

Title : SW846 8260

Signal : TIC: VN081377.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.665	113	121	138	rBV	1771640	3160404	100.00%	22.930%
2	2.806	140	145	152	rVB4	22176	52359	1.66%	0.380%
3	3.795	305	313	321	rBV	19455	49017	1.55%	0.356%
4	7.224	883	896	908	rBV3	89637	254753	8.06%	1.848%
5	8.171	1046	1057	1061	rBV	254618	611621	19.35%	4.437%
6	8.224	1061	1066	1079	rVB	468206	1056222	33.42%	7.663%
7	8.583	1111	1127	1140	rBV	296192	681503	21.56%	4.944%
8	9.106	1207	1216	1229	rBV	674525	1401870	44.36%	10.171%
9	10.571	1454	1465	1477	rBV	1021717	1862573	58.93%	13.513%
10	11.871	1673	1686	1696	rBV	887893	1574404	49.82%	11.423%
11	12.853	1845	1853	1865	rBV	635334	1088646	34.45%	7.898%
12	13.341	1929	1936	1947	rBV	259738	395860	12.53%	2.872%
13	13.688	1989	1995	2001	rBV3	69931	111440	3.53%	0.809%
14	13.794	2005	2013	2021	rBV	786335	1304193	41.27%	9.462%
15	13.876	2021	2027	2036	rBV	102906	178255	5.64%	1.293%

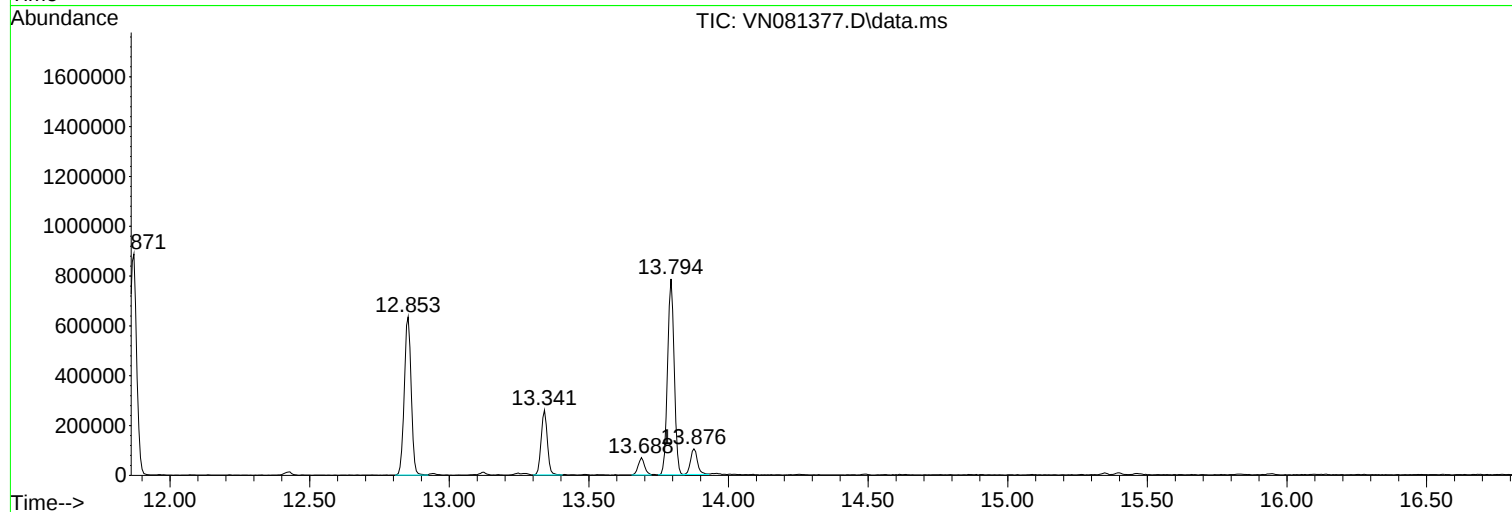
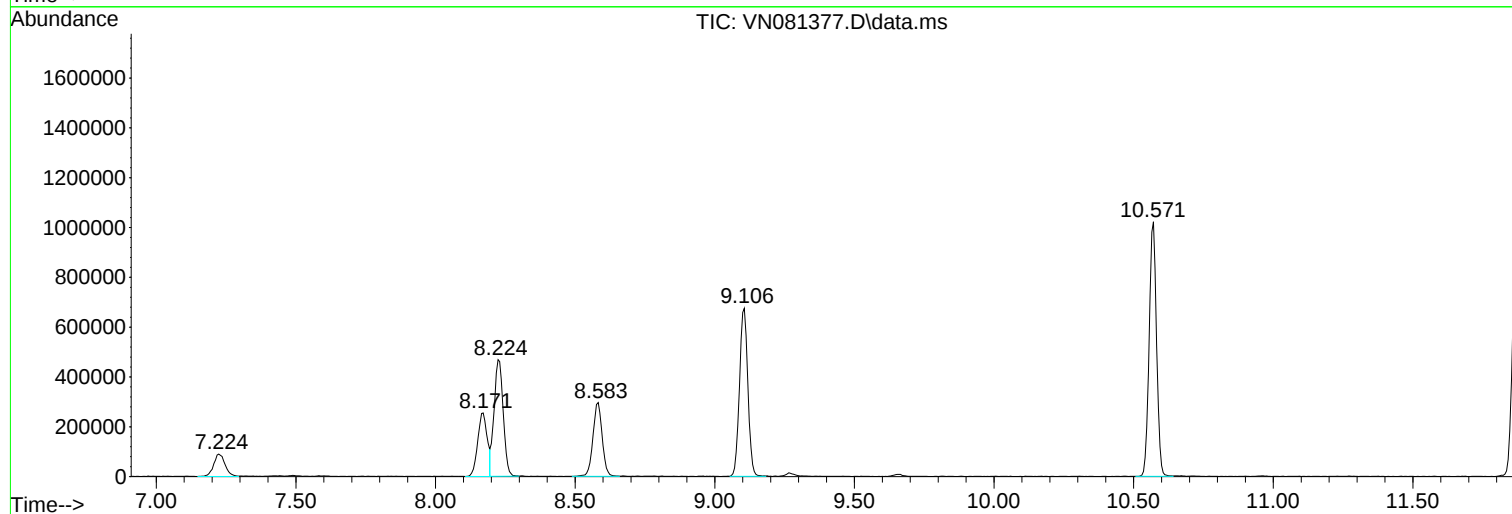
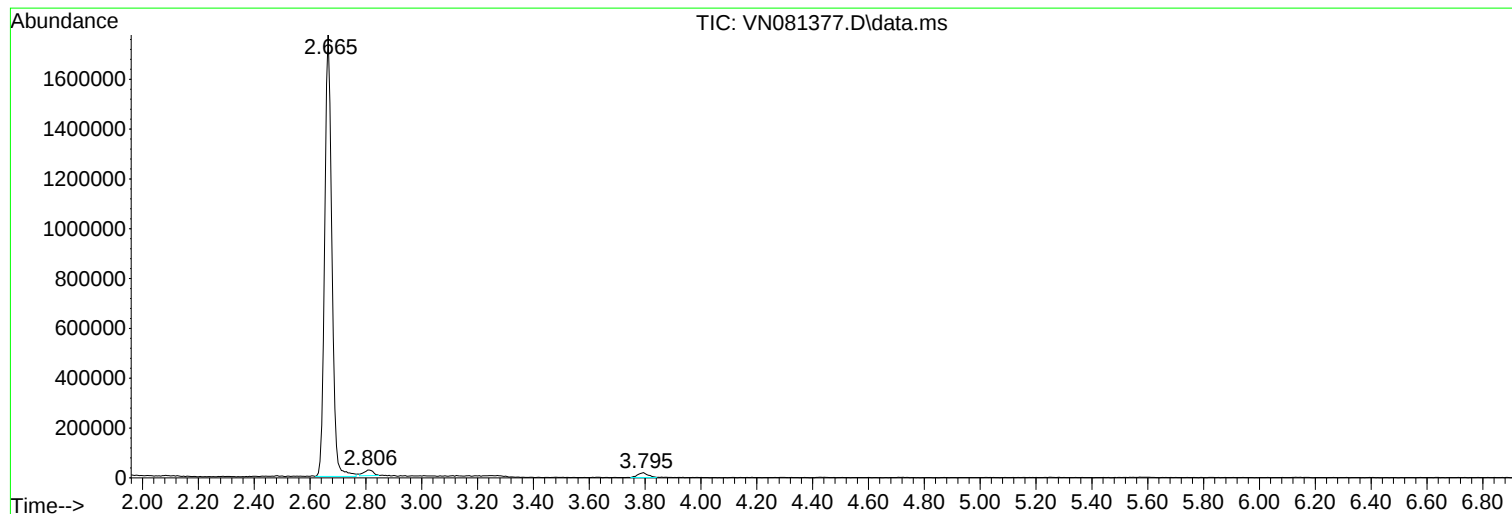
Sum of corrected areas: 13783120

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Instrument :
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ClientSampleId :
1342

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030524W.M
Quant Title : SW846 8260

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



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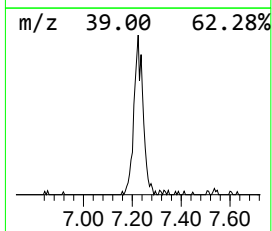
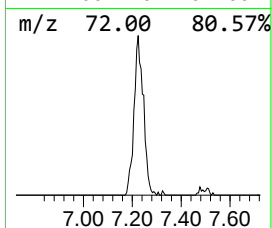
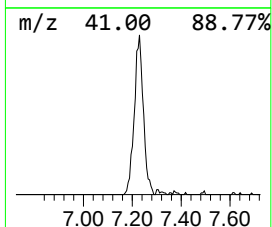
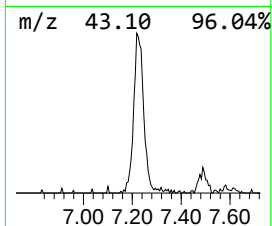
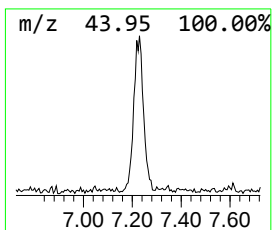
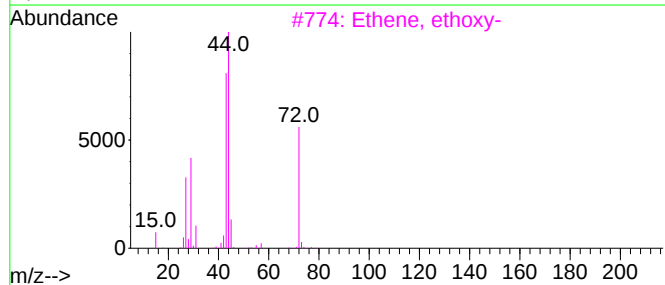
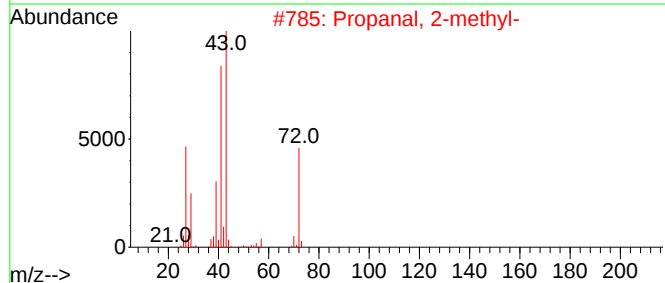
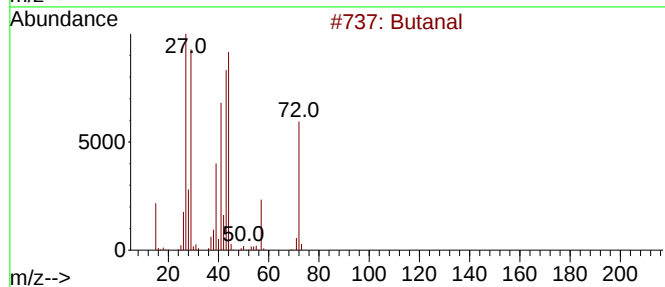
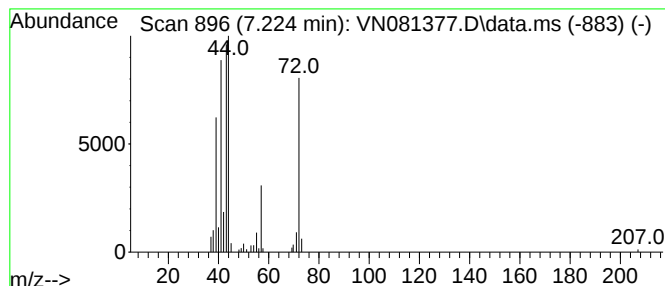
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030524W.M
Quant Title : SW846 8260

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

Peak Number 2 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.224	12.06 ug/l	254753	Pentafluorobenzene	8.224

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butanal	72	C4H8O	000123-72-8	91
2		Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
3		Ethene, ethoxy-	72	C4H8O	000109-92-2	42
4		Silacyclobutane	72	C3H8Si	1000434-34-1	40
5		2-Propen-1-ol, 2-methyl-, acetate	114	C6H10O2	000820-71-3	38



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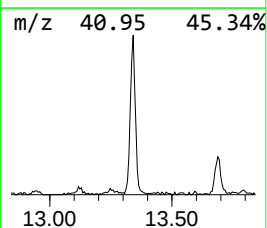
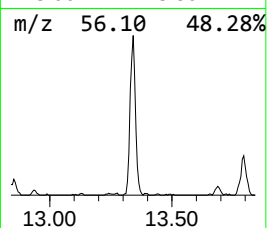
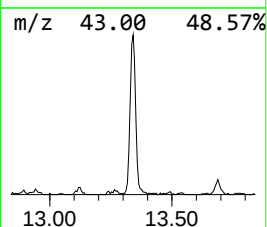
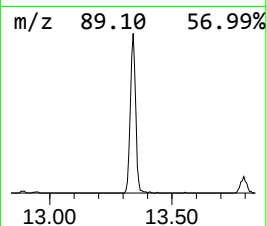
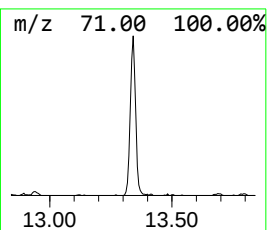
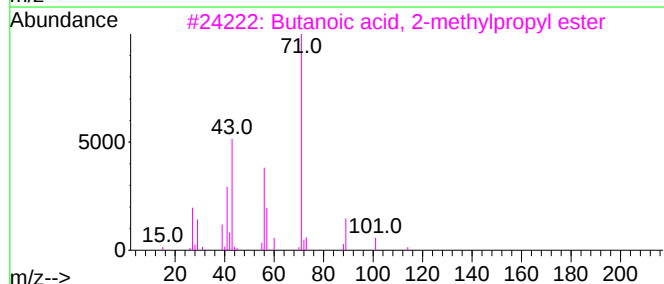
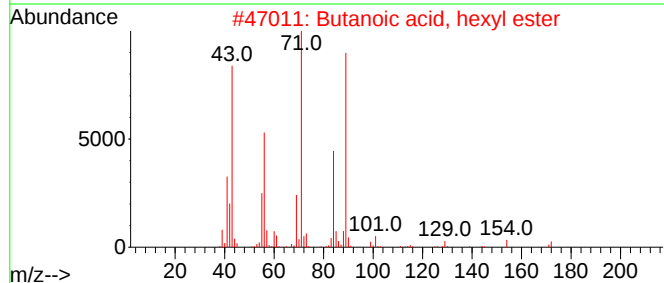
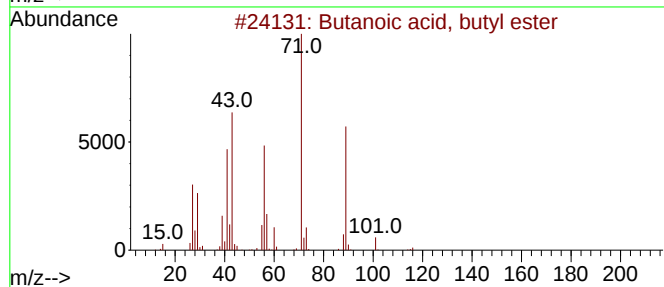
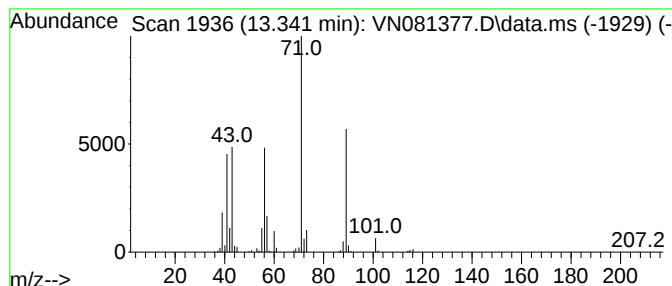
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Peak Number 3 Butanoic acid, butyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.341	15.18 ug/l	395860	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			Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	64
4			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59
5			Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	56



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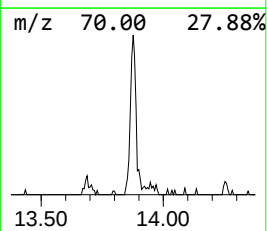
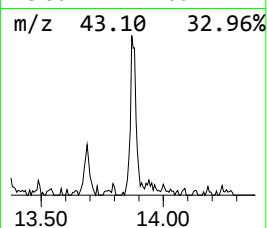
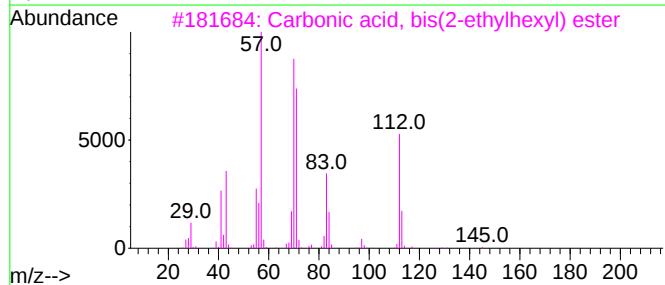
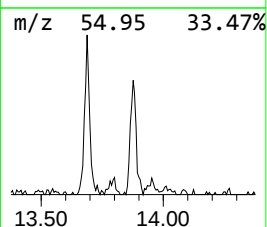
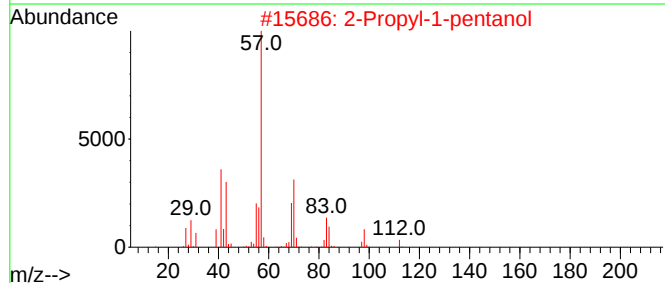
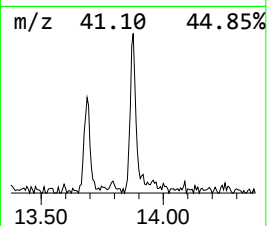
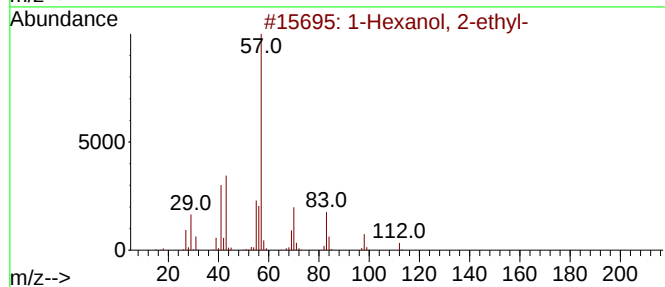
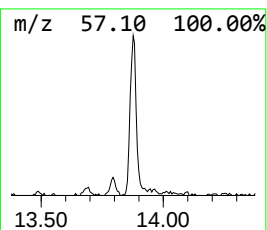
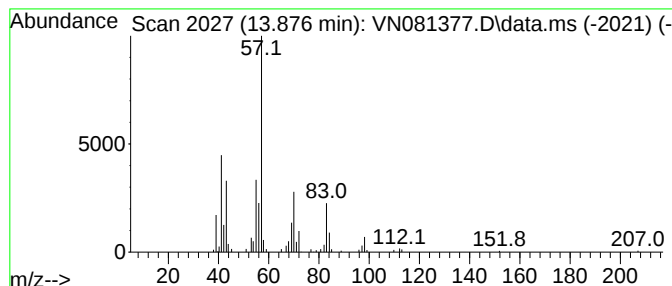
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Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	6.83 ug/l	178255	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-		130	C8H18O	000104-76-7	72	
2	2-Propyl-1-pentanol		130	C8H18O	058175-57-8	59	
3	Carbonic acid, bis(2-ethylhexyl)...		286	C17H34O3	014858-73-2	47	
4	Carbonic acid, butyl heptyl ester		216	C12H24O3	1000314-63-4	47	
5	2-Propyl-1-pentanol, pentafluoro...		276	C11H17F5O2	1000365-51-2	47	



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butanal	7.224	12.1	ug/l	254753	1	8.224	1056220	50.0
Butanoic acid, ...	13.341	15.2	ug/l	395860	4	13.794	1304190	50.0
1-Hexanol, 2-et...	13.876	6.8	ug/l	178255	4	13.794	1304190	50.0