

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091722\
 Data File : VN074558.D
 Acq On : 17 Sep 2022 16:04
 Operator : JC\MD
 Sample : N4549-24
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TB090822

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\82N091522W.M

Title : SW846 8260

Signal : TIC: VN074558.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	48	53	58	rBV	199463	349540	19.83%	3.351%
2	2.299	61	70	74	rVV4	30206	114313	6.48%	1.096%
3	2.687	131	136	140	rBV2	51474	112286	6.37%	1.076%
4	3.181	218	220	229	rVB3	29464	54768	3.11%	0.525%
5	4.499	438	444	445	rBV2	14953	23670	1.34%	0.227%
6	7.234	900	909	921	rBV3	23807	72844	4.13%	0.698%
7	7.951	1021	1031	1036	rBV	259795	597377	33.89%	5.727%
8	8.016	1036	1042	1053	rVB	381863	841600	47.74%	8.068%
9	8.375	1094	1103	1114	rBV2	273830	641394	36.38%	6.149%
10	8.904	1184	1193	1206	rBV	623650	1258932	71.42%	12.069%
11	10.381	1435	1444	1457	rBV	972086	1762818	100.00%	16.900%
12	11.686	1657	1666	1679	rBV	1007740	1729131	98.09%	16.577%
13	12.674	1826	1834	1849	rVB	777056	1321847	74.98%	12.672%
14	13.616	1987	1994	2006	rBV	957247	1550528	87.96%	14.865%

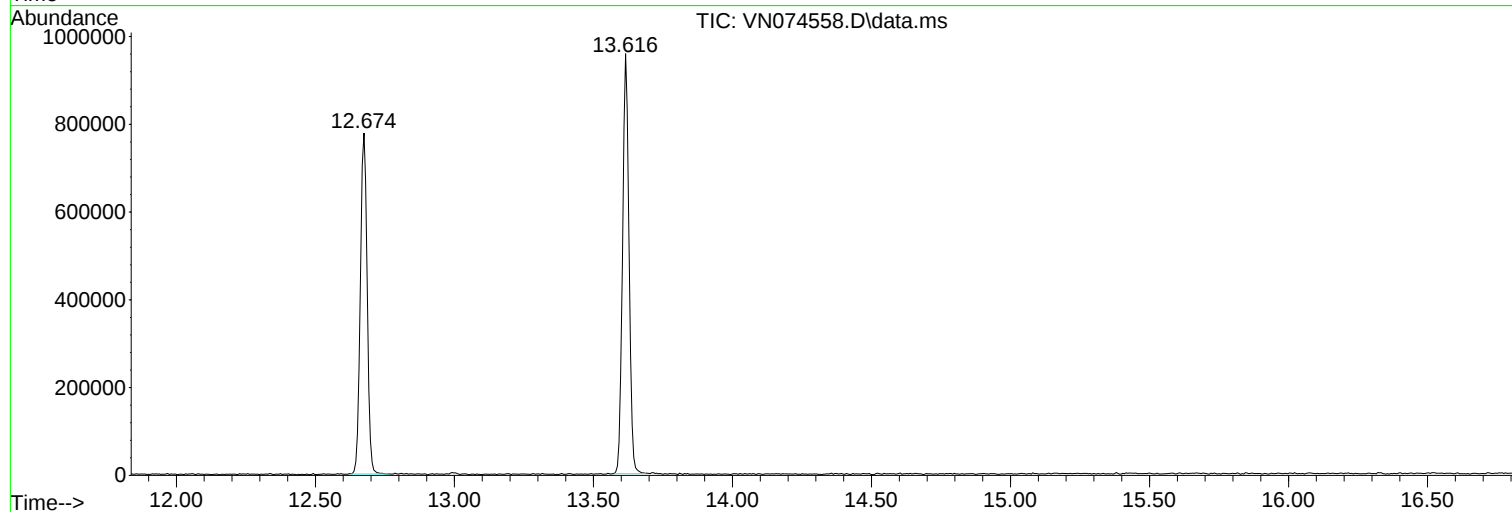
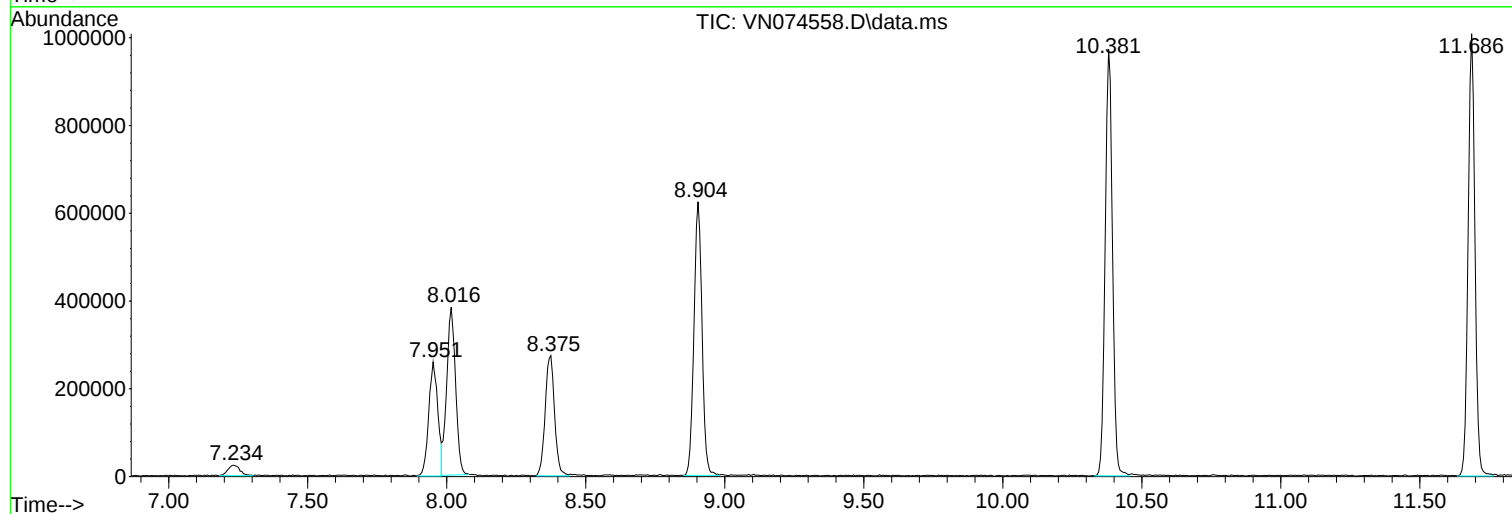
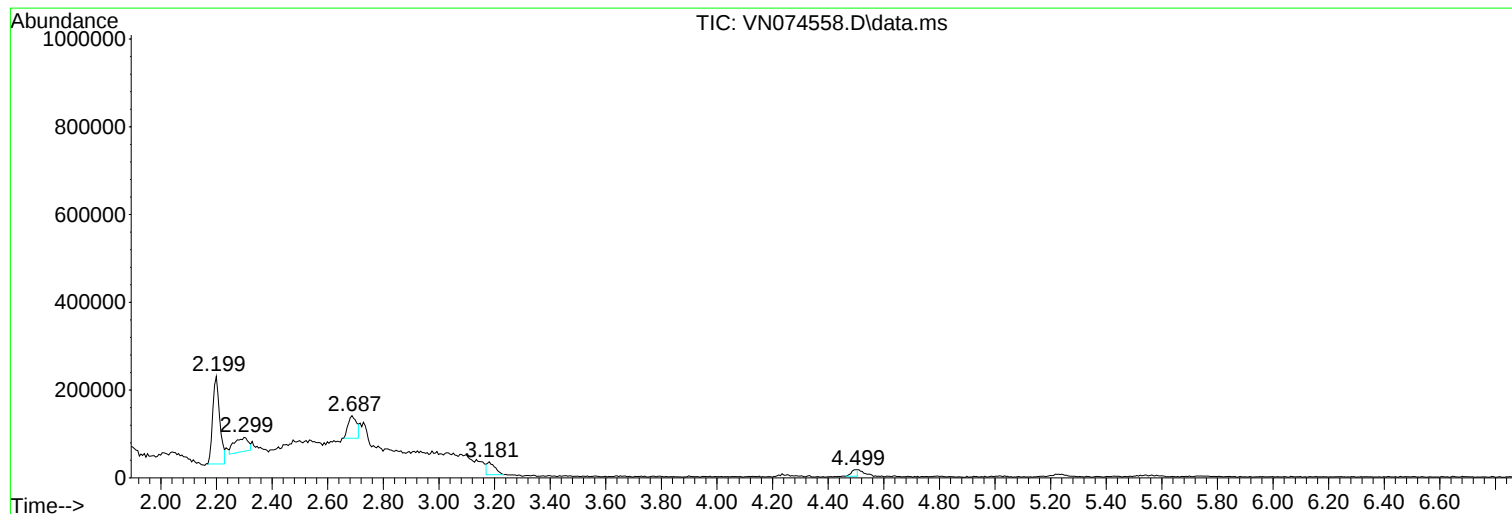
Sum of corrected areas: 10431048

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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



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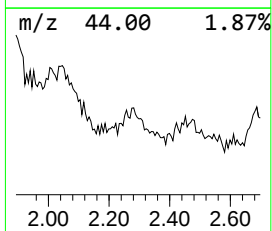
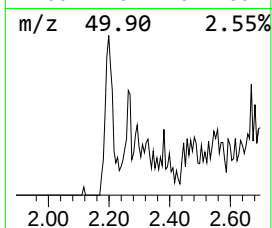
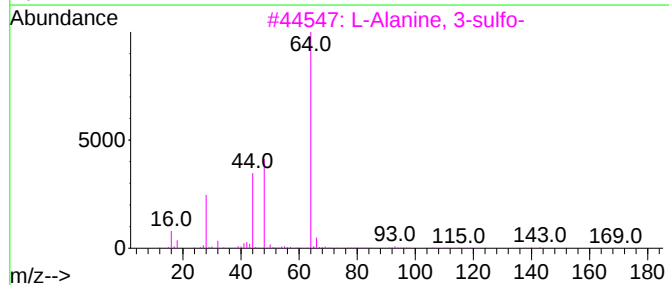
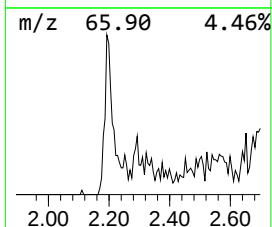
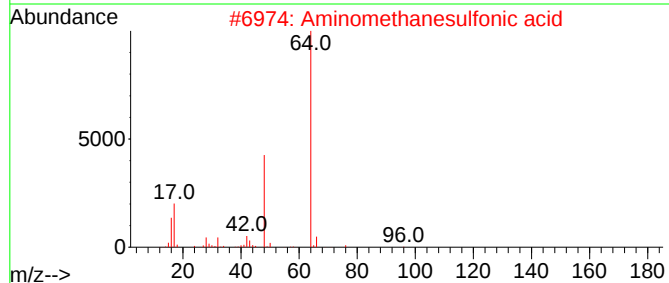
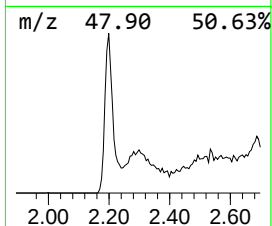
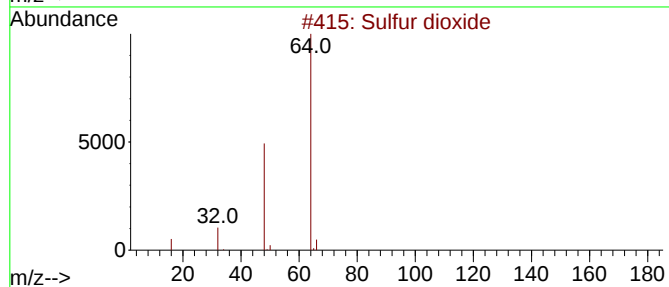
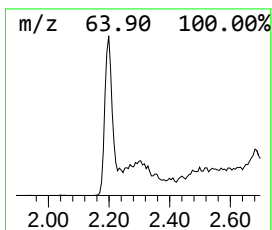
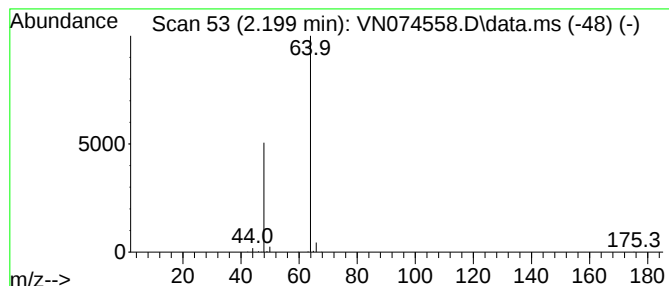
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.199	20.77 ug/l	349540	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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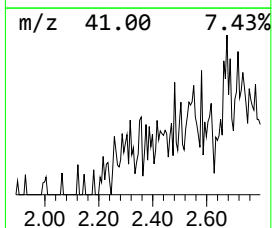
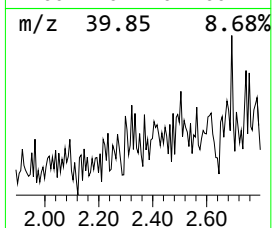
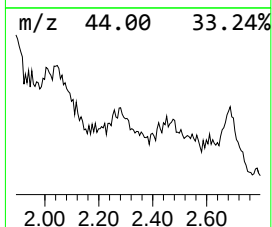
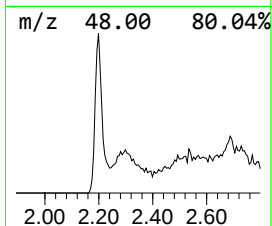
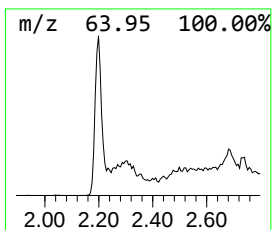
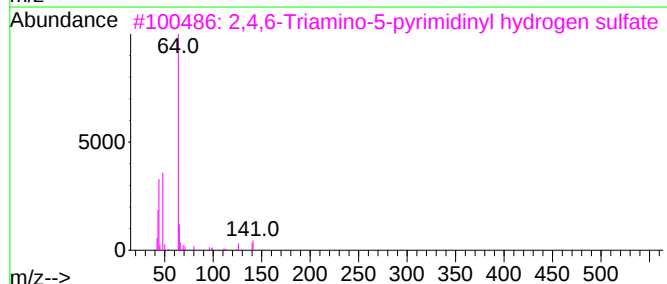
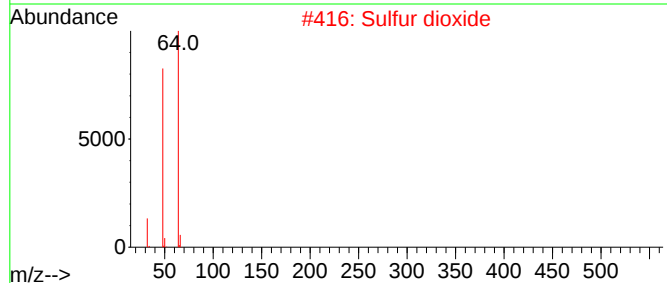
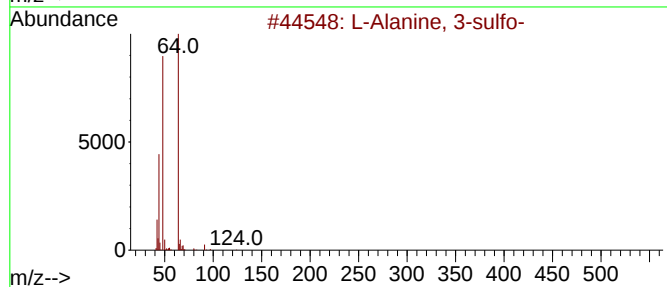
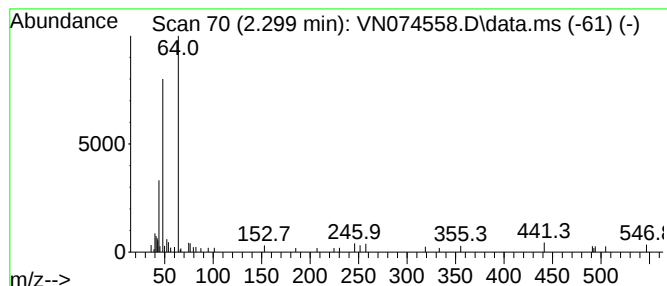
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Peak Number 2 L-Alanine, 3-sulfo- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.299	6.79 ug/l	114313	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	83
2			Sulfur dioxide	64	O2S	007446-09-5	9
3			2,4,6-Triamino-5-pyrimidinyl hyd...	221	C4H7N5O4S	071552-23-3	9
4			Thiosulfuric acid S-[2-[[5-[O-to...	347	C15H25NO4S2	038920-47-7	9
5			S,S'-3,8-Diazaundecamethylene bi...	382	C9H22N2O6S4	035871-62-6	9



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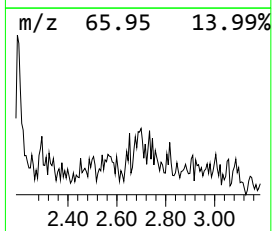
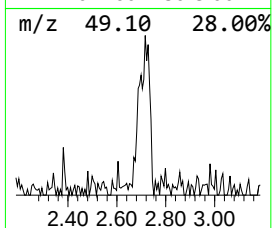
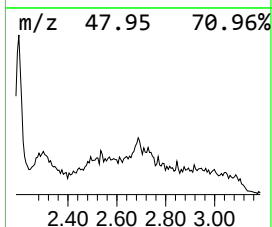
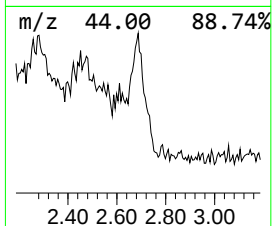
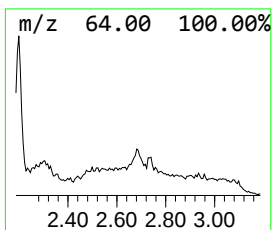
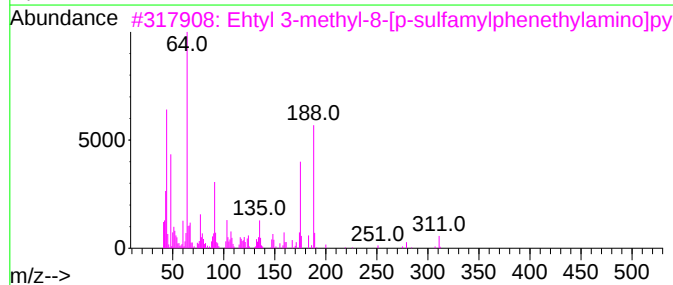
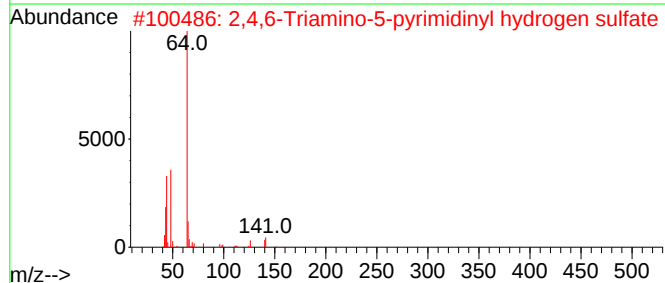
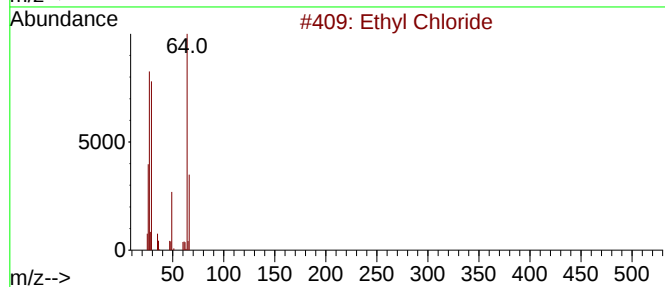
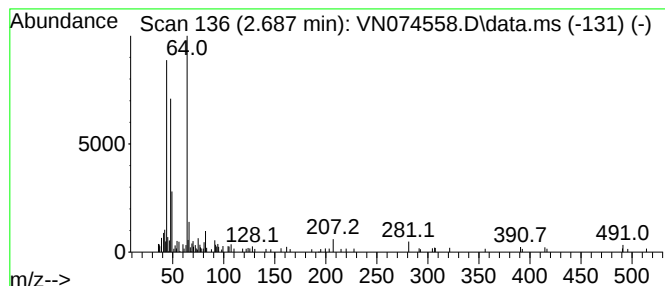
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Peak Number 3 Ethyl Chloride Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.687	6.67 ug/l	112286	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyl Chloride	64	C2H5Cl	000075-00-3	59
2			2,4,6-Triamino-5-pyrimidinyl hyd...	221	C4H7N5O4S	071552-23-3	50
3			Ehtyl 3-methyl-8-[p-sulfamylphen...	430	C19H22N6O4S	021271-93-2	39
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	36
5			Benzenesulfonic acid, 3-[2-pyrid...	354	C17H14N4O3S	052018-85-6	33



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Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.199	20.8	ug/l	349540	1	8.016	841600	50.0
L-Alanine, 3-su...	2.299	6.8	ug/l	114313	1	8.016	841600	50.0
Ethyl Chloride	2.687	6.7	ug/l	112286	1	8.016	841600	50.0