

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY042621\
 Data File : VY004625.D
 Acq On : 26 Apr 2021 13:29
 Operator : SY/MD
 Sample : M2160-01
 Misc : 6.07G/5ML/MSVOA_Y/SOIL
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 OK-03-042321

Integration Parameters: RTEINT.P

Integrator: RTE

Smoother: 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_Y\methods\82Y041221S.M

Title : SW846 8260

Signal : TIC: VY004625.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.960	339	351	369	rBV	162328	449172	10.63%	5.464%
2	4.735	464	478	496	rBV4	11961	45324	1.07%	0.551%
3	7.728	960	969	975	rBV	95773	232146	5.49%	2.824%
4	7.801	975	981	992	rVB	159815	366055	8.66%	4.453%
5	8.155	1030	1039	1048	rBV	105276	234152	5.54%	2.849%
6	8.697	1120	1128	1139	rVB	259338	503157	11.91%	6.121%
7	10.185	1365	1372	1380	rBV	389552	664707	15.73%	8.087%
8	10.581	1430	1437	1444	rBV	198506	366412	8.67%	4.458%
9	10.715	1452	1459	1468	rVB	65074	107731	2.55%	1.311%
10	11.045	1507	1513	1519	rBV	26919	43975	1.04%	0.535%
11	11.276	1545	1551	1557	rBV	55107	84231	1.99%	1.025%
12	11.496	1579	1587	1595	rBV	320150	518106	12.26%	6.303%
13	12.496	1741	1751	1759	rBV	2693857	4226334	100.00%	51.416%
14	13.428	1899	1904	1911	rVB	205509	312231	7.39%	3.799%
15	13.971	1987	1993	1999	rVB2	40680	66088	1.56%	0.804%

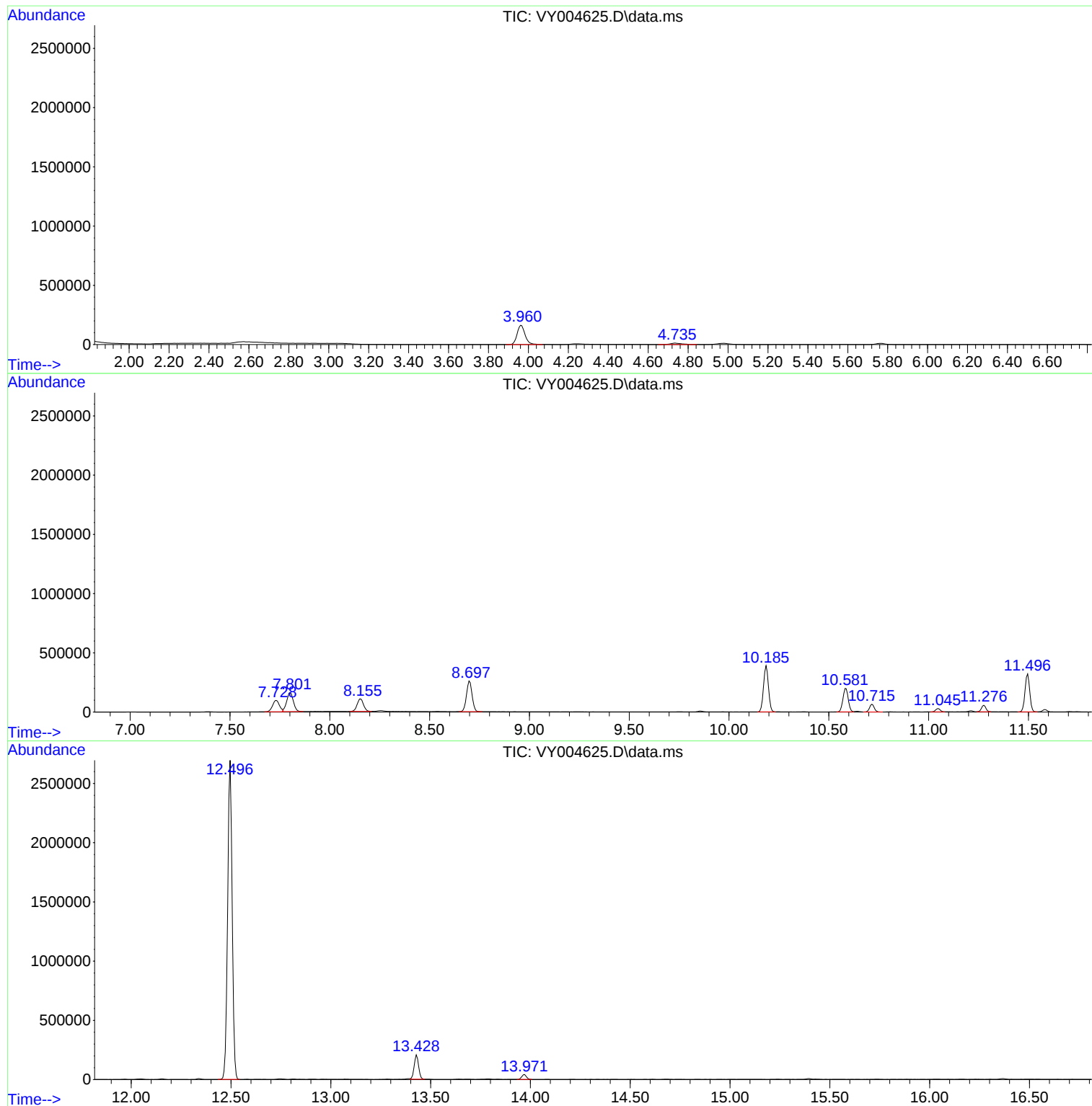
Sum of corrected areas: 8219821

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y041221S.M
Quant Title : SW846 8260

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



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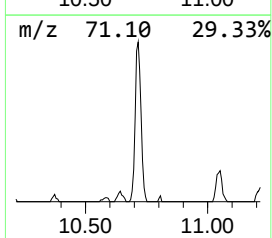
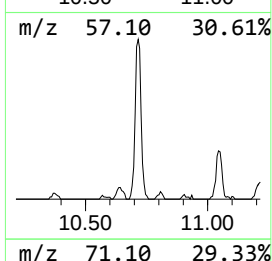
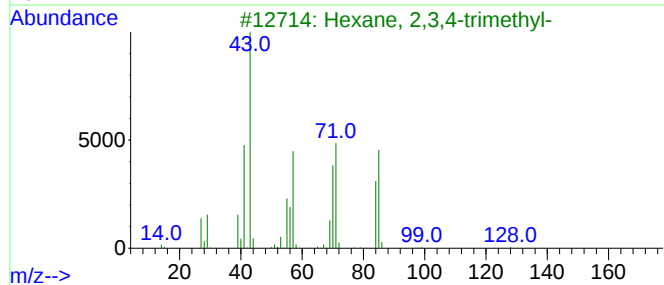
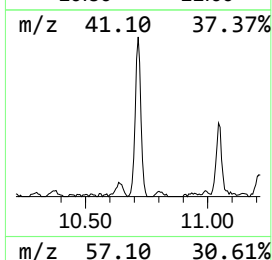
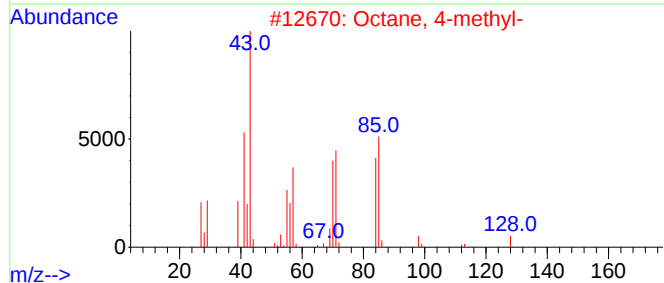
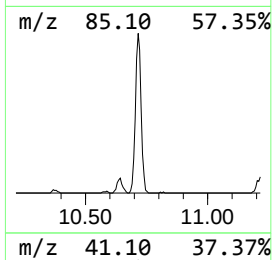
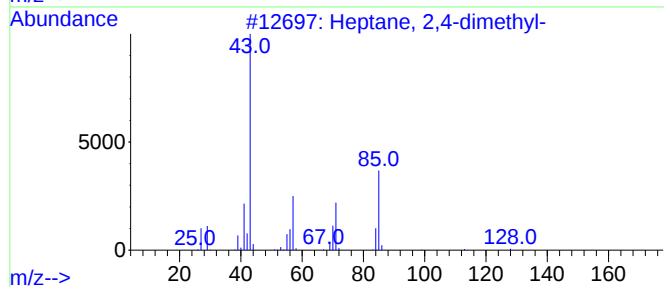
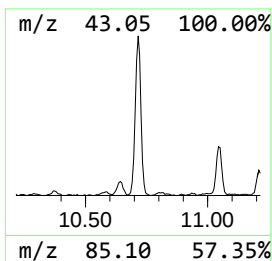
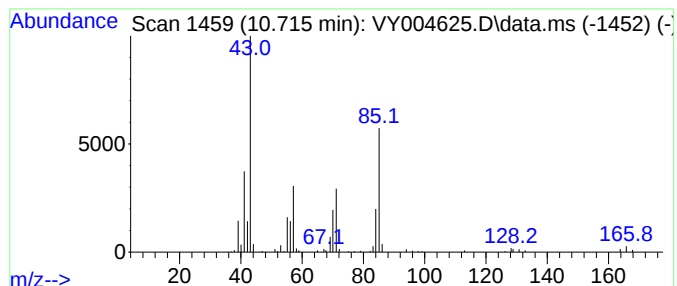
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y041221S.M
Quant Title : SW846 8260

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

Peak Number 3 Heptane, 2,4-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.715	10.40 ug/l	107731	Chlorobenzene-d5	11.496

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	68
2			Octane, 4-methyl-	128	C9H20	002216-34-4	64
3			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	58
4			Hexane, 2,3,5-trimethyl-	128	C9H20	001069-53-0	52
5			Pentane, 3-ethyl-3-methyl-	114	C8H18	001067-08-9	47



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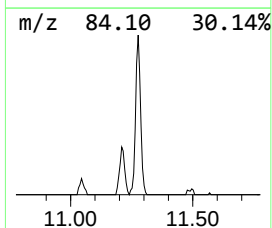
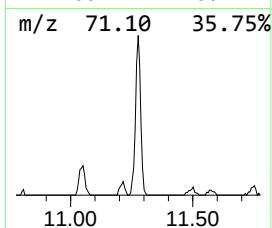
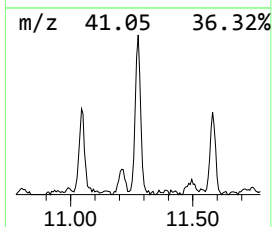
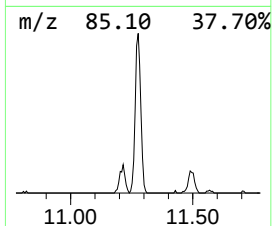
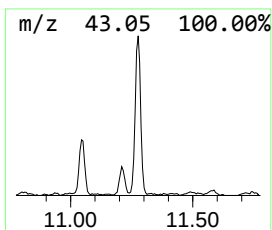
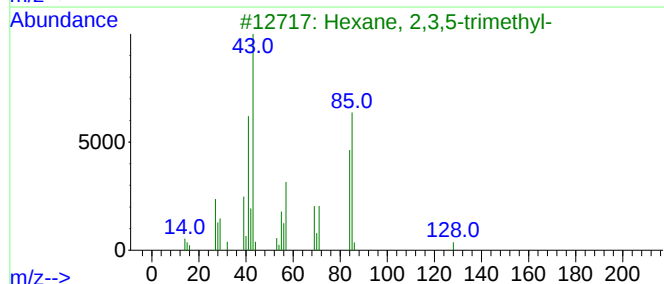
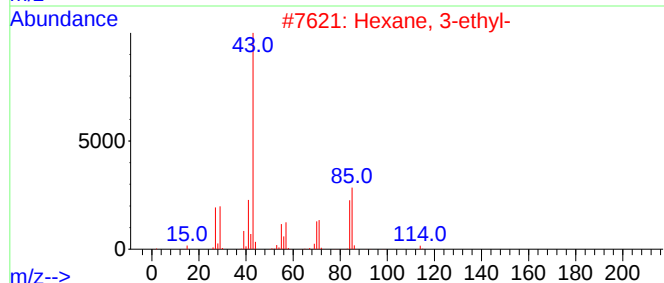
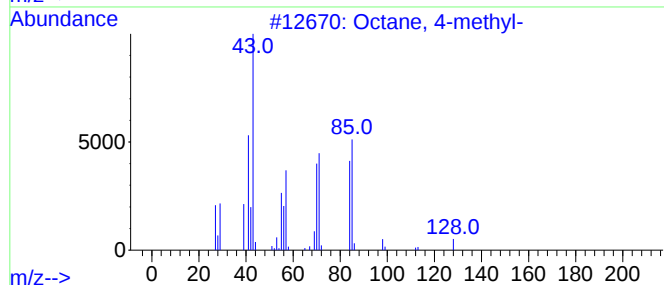
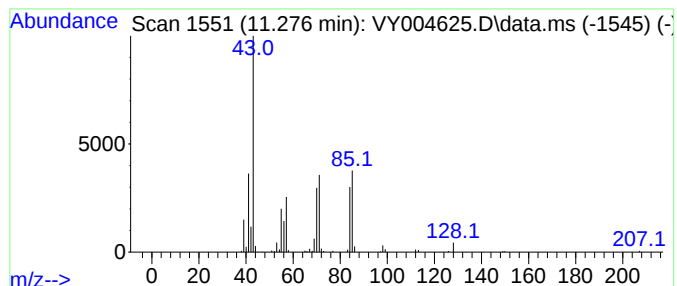
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Peak Number 4 Octane, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.276	8.13 ug/l	84231	Chlorobenzene-d5	11.496

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 4-methyl-	128	C9H20	002216-34-4	95
2			Hexane, 3-ethyl-	114	C8H18	000619-99-8	86
3			Hexane, 2,3,5-trimethyl-	128	C9H20	001069-53-0	70
4			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	53
5			Heptane, 2,3-dimethyl-	128	C9H20	003074-71-3	53



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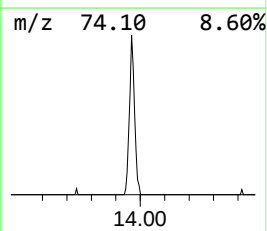
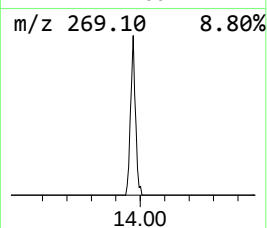
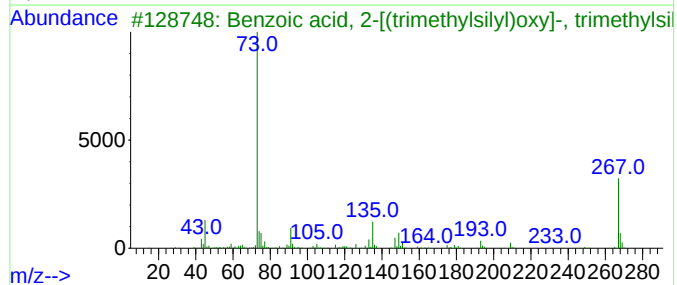
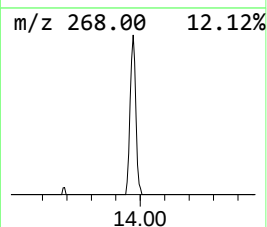
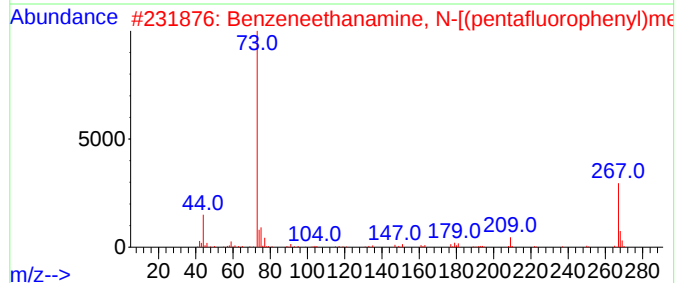
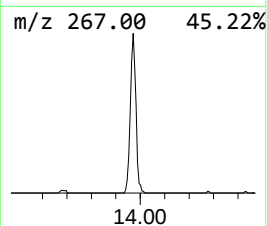
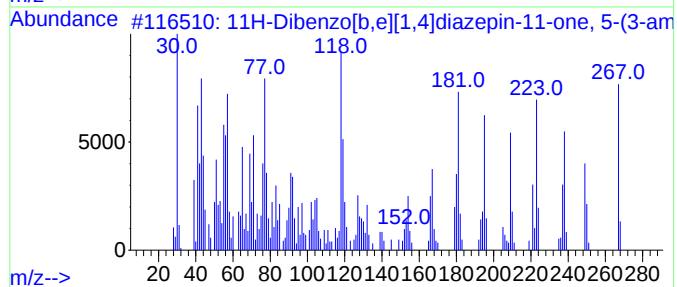
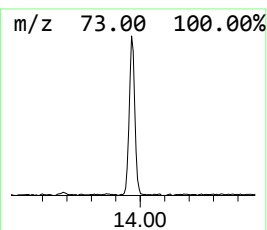
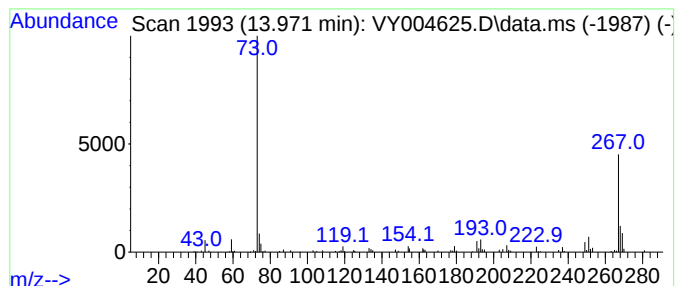
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Peak Number 5 unknown13.971 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.971	10.58 ug/l	66088	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11H-Dibenzo[b,e][1,4]diazepin-11...	267	C16H17N3O	013450-73-2	43
2			Benzeneethanamine, N-[(pentaflu...	475	C21H26F5NO2Si2	055429-85-1	43
3			Benzoic acid, 2-[(trimethylsilyl...	282	C13H22O3Si2	003789-85-3	38
4			4-Methylcatechol, bis(trimethyls...	268	C13H24O2Si2	1000332-79-9	22
5			3,5-Dimethoxyphenylacetic acid, ...	268	C13H20O4Si	1000071-82-4	10



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Heptane, 2,4-di...	10.715	10.4	ug/l	107731	3	11.496	518106	50.0
Octane, 4-methyl-	11.276	8.1	ug/l	84231	3	11.496	518106	50.0
unknown13.971	13.971	10.6	ug/l	66088	4	13.428	312231	50.0