

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041523\
 Data File : VX035089.D
 Acq On : 14 Apr 2023 17:30
 Operator : JC/MD
 Sample : 02345-02 10X
 Misc : 1.62g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 1611

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_X\Method\82X032923W.M
 Title : SW846 8260

Signal : TIC: VX035089.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.386	205	213	228	rBV	330904	578469	15.69%	4.519%
2	5.385	692	705	714	rBV2	144563	427890	11.61%	3.343%
3	5.550	714	732	742	rVV3	258963	1027191	27.86%	8.025%
4	5.824	765	777	789	rBV2	123057	353400	9.58%	2.761%
5	5.958	789	799	819	rVB	171596	455819	12.36%	3.561%
6	6.610	894	906	919	rBV2	103607	253578	6.88%	1.981%
7	6.763	922	931	949	rVV	423741	1010816	27.42%	7.897%
8	7.379	1021	1032	1041	rBV	71753	165350	4.48%	1.292%
9	8.653	1234	1241	1246	rBV	861614	1365133	37.02%	10.665%
10	8.720	1246	1252	1267	rVB	2434356	3687067	100.00%	28.806%
11	10.055	1466	1471	1487	rVB	859276	1165504	31.61%	9.106%
12	11.085	1634	1640	1653	rBV	668332	911057	24.71%	7.118%
13	12.024	1788	1794	1801	rBV	864347	1087247	29.49%	8.494%
14	14.036	2121	2124	2128	rBV	34517	39914	1.08%	0.312%
15	14.639	2216	2223	2226	rBV	76004	114333	3.10%	0.893%
16	14.780	2244	2246	2253	rVB	40060	51940	1.41%	0.406%
17	15.560	2369	2374	2379	rBV	65902	104907	2.85%	0.820%

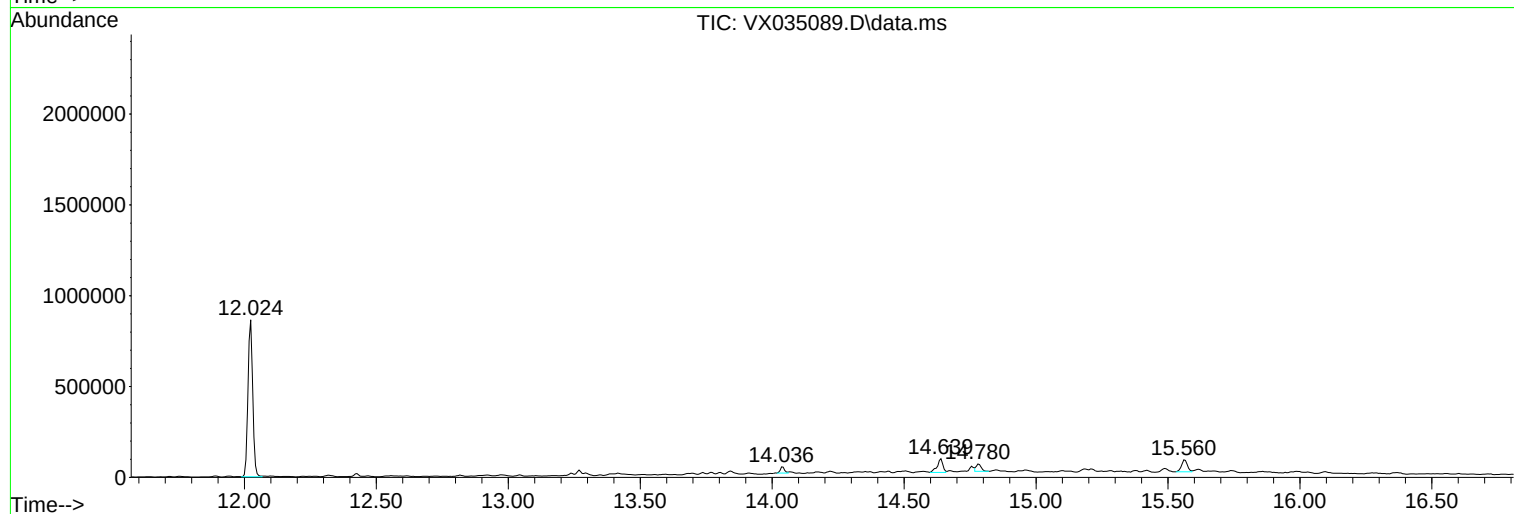
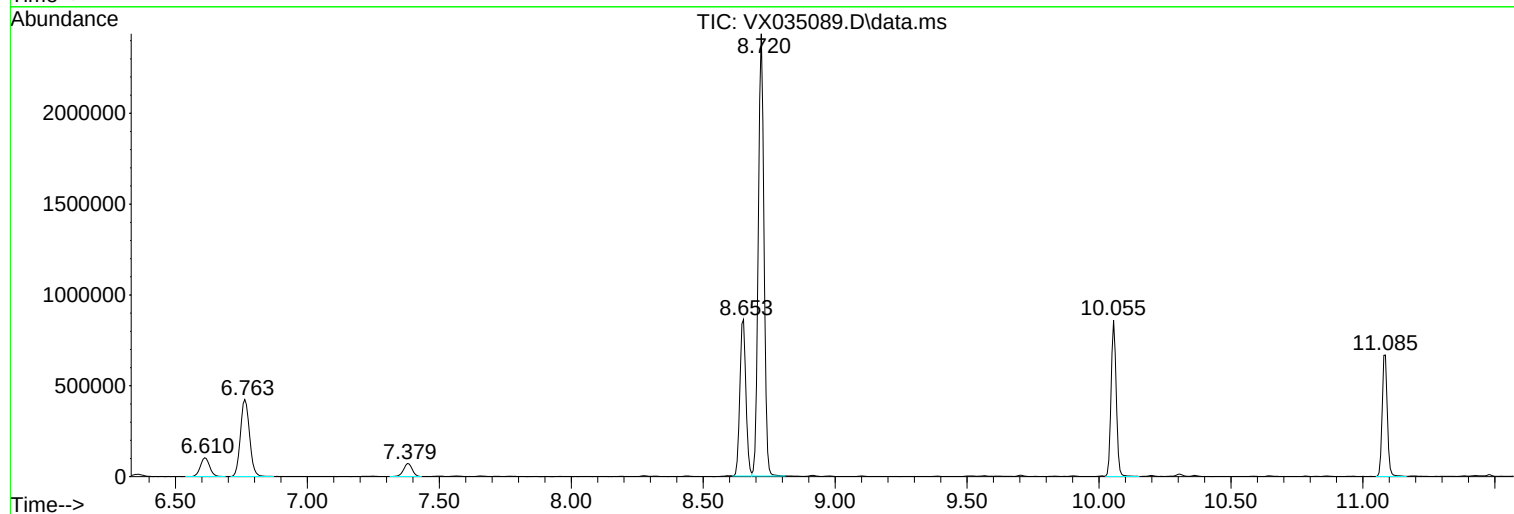
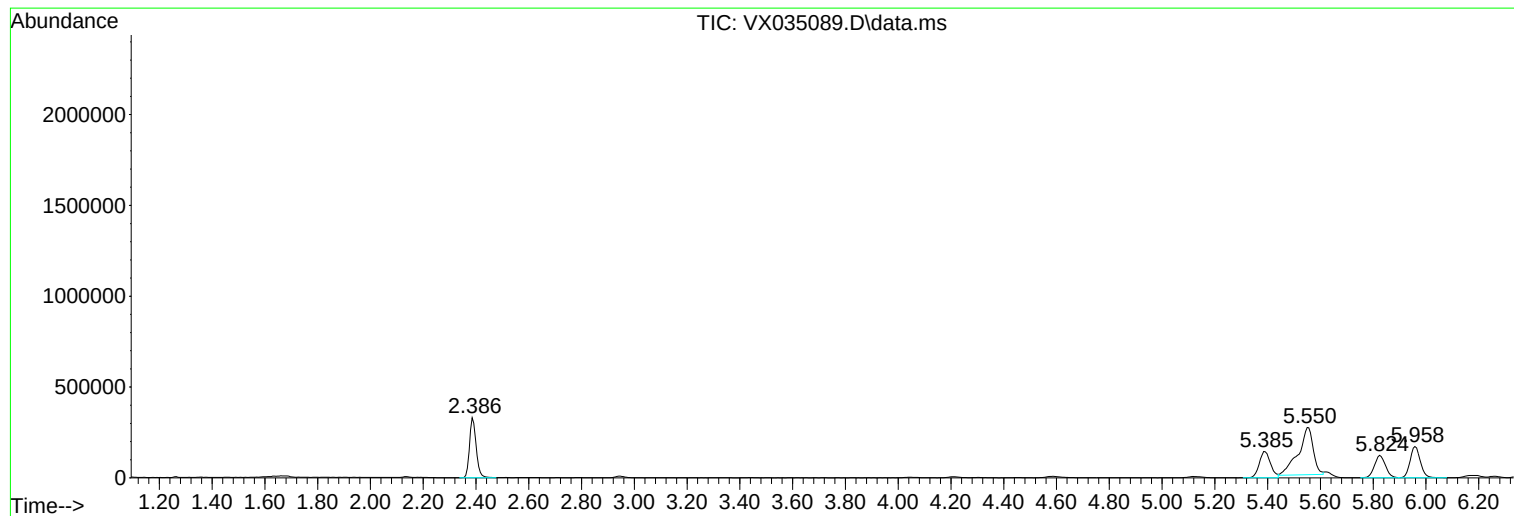
Sum of corrected areas: 12799615

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

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



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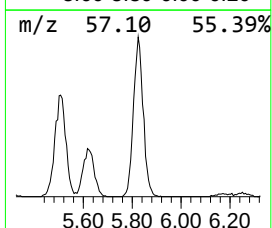
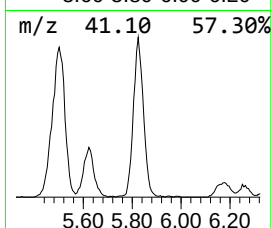
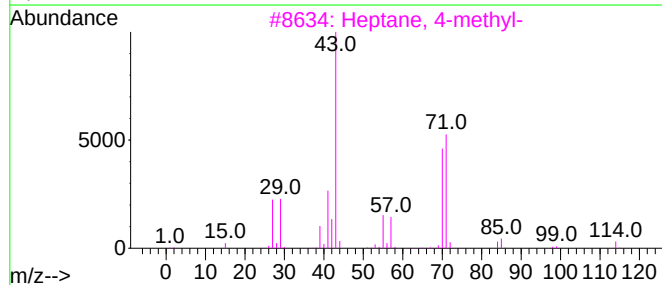
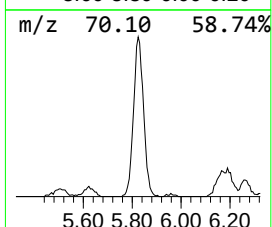
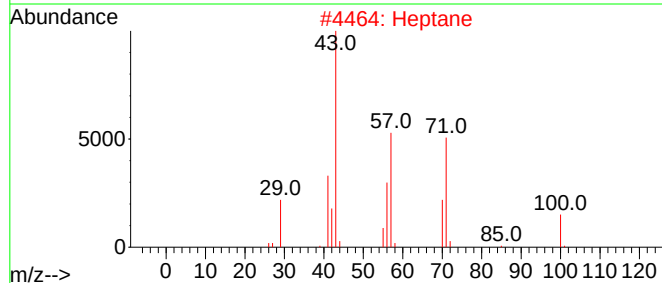
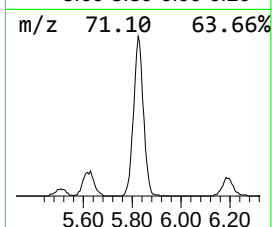
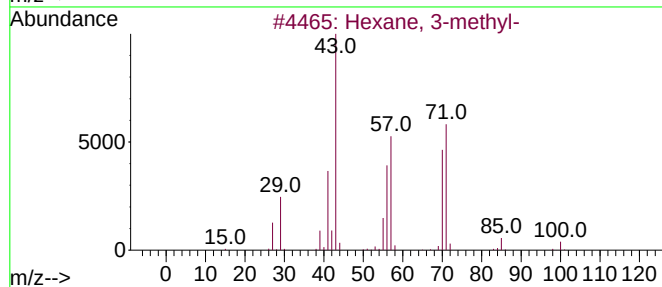
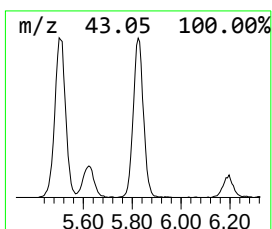
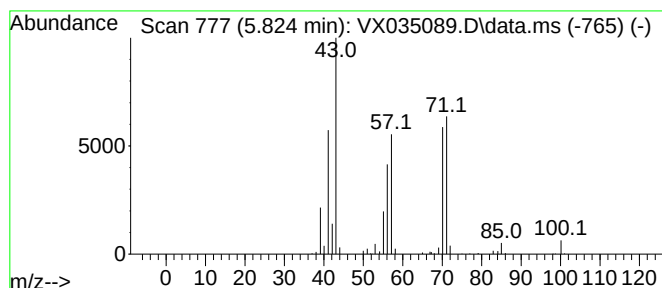
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

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

Peak Number 1 Hexane, 3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.824	17.20 ug/l	353400	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 3-methyl-	100	C7H16	000589-34-4	94
2			Heptane	100	C7H16	000142-82-5	80
3			Heptane, 4-methyl-	114	C8H18	000589-53-7	59
4			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53
5			1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	53



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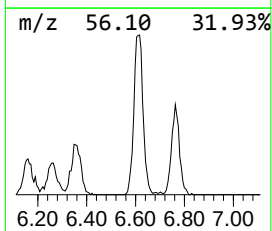
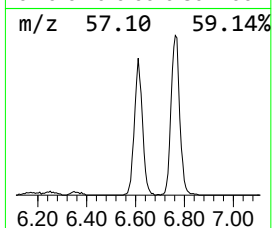
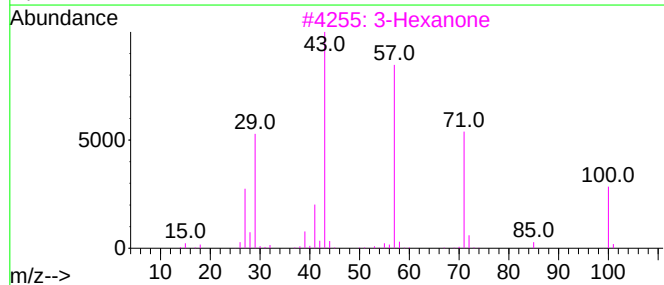
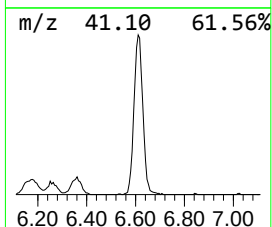
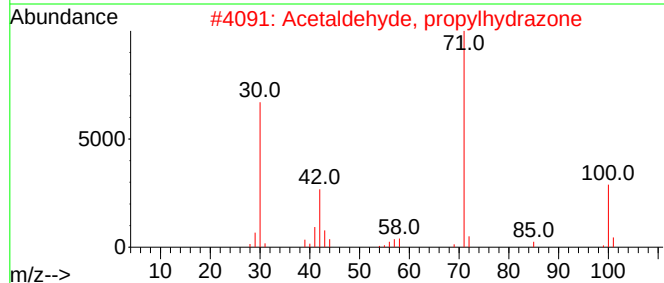
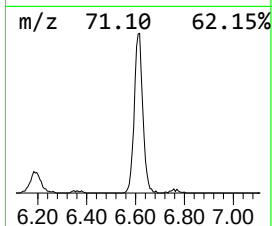
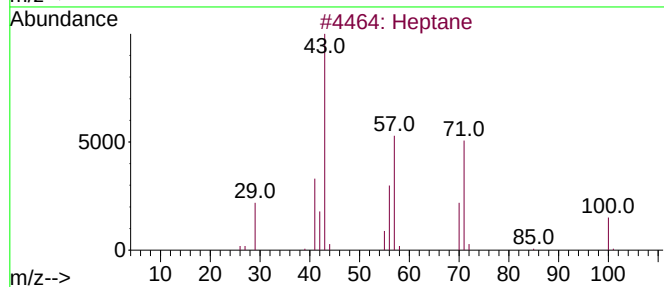
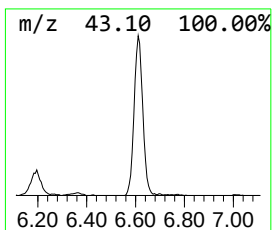
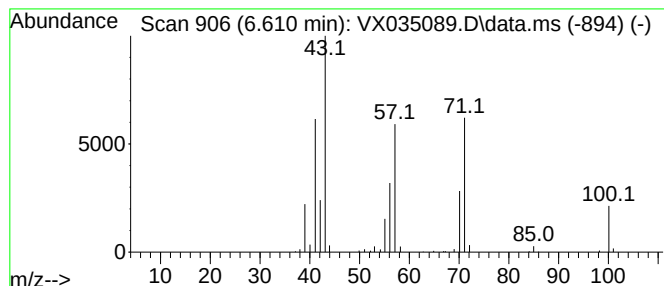
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Peak Number 2 Heptane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.610	12.54 ug/l	253578	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane	100	C7H16	000142-82-5	91
2			Acetaldehyde, propylhydrazone	100	C5H12N2	007422-88-0	49
3			3-Hexanone	100	C6H12O	000589-38-8	46
4			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	38
5			Hexane, 3-methyl-	100	C7H16	000589-34-4	38



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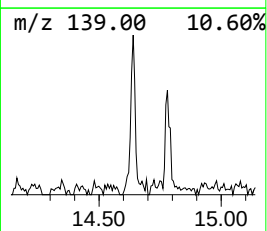
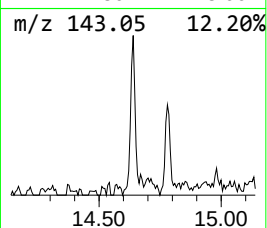
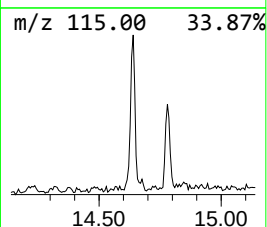
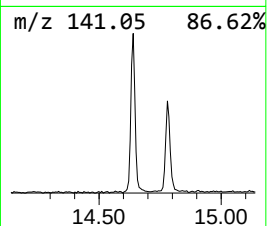
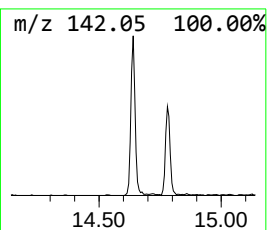
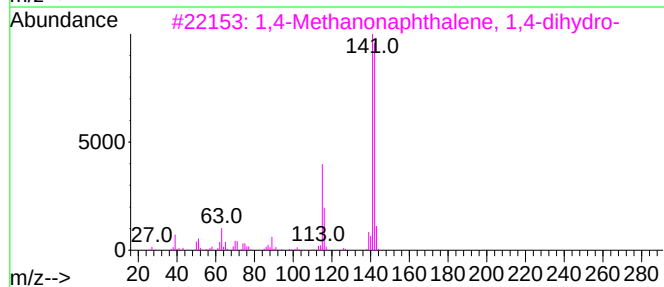
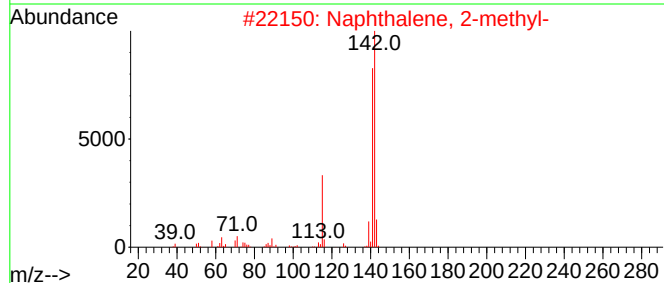
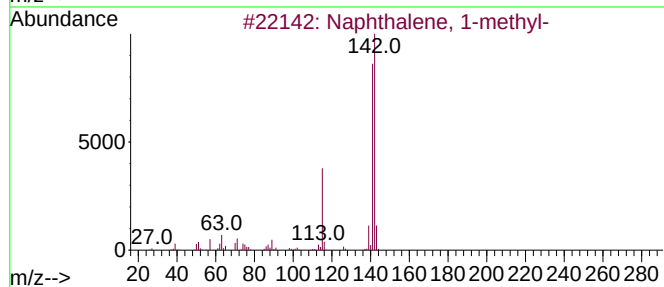
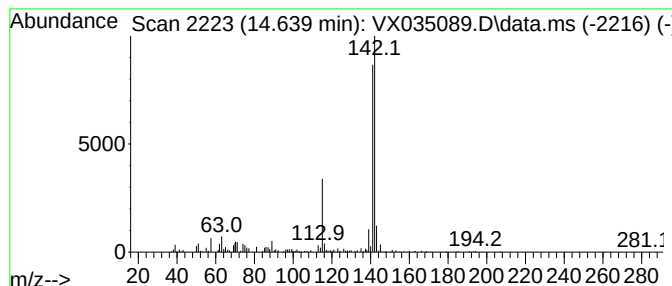
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Peak Number 3 Naphthalene, 1-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	5.26 ug/l	114333	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	93
4			Benzocycloheptatriene	142	C11H10	000264-09-5	90
5			1-Naphthaleneacetamide	185	C12H11NO	000086-86-2	53



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexane, 3-methyl-	5.824	17.2	ug/l	353400	1	5.556	1027190	50.0
Heptane	6.610	12.5	ug/l	253578	2	6.763	1010820	50.0
Naphthalene, 1-...	14.640	5.3	ug/l	114333	4	12.024	1087250	50.0