

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121222\
 Data File : VN075723.D
 Acq On : 12 Dec 2022 19:17
 Operator : JC\MD
 Sample : N5978-06
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TOLL-MW-07

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\82N120922W.M
 Title : SW846 8260

Signal : TIC: VN075723.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.301	35	42	46	rBV	21450	52934	4.77%	0.796%
2	2.336	46	48	57	rVB2	14829	27954	2.52%	0.421%
3	2.830	126	132	138	rVB4	8475	18961	1.71%	0.285%
4	5.806	628	638	652	rBV3	15080	48960	4.41%	0.737%
5	7.500	918	926	934	rBB4	5551	13429	1.21%	0.202%
6	8.177	1030	1041	1045	rBV	154944	374159	33.71%	5.630%
7	8.230	1045	1050	1060	rVV	309559	672348	60.57%	10.116%
8	8.336	1060	1068	1076	rVB3	20514	47521	4.28%	0.715%
9	8.588	1100	1111	1120	rBV	153292	347100	31.27%	5.223%
10	8.765	1131	1141	1154	rBV	113191	270454	24.36%	4.069%
11	9.106	1190	1199	1213	rBV	410892	825725	74.38%	12.424%
12	9.735	1298	1306	1312	rBB2	8769	16897	1.52%	0.254%
13	10.018	1345	1354	1363	rBV	74899	144587	13.02%	2.176%
14	10.153	1367	1377	1384	rBV	100359	204646	18.44%	3.079%
15	10.494	1430	1435	1440	rBV3	9013	14350	1.29%	0.216%
16	10.571	1440	1448	1462	rVB	613513	1110084	100.00%	16.703%
17	11.871	1660	1669	1683	rBV	521220	944067	85.04%	14.205%
18	12.853	1826	1836	1847	rBB	414027	687222	61.91%	10.340%
19	13.794	1989	1996	2009	rVB	498736	824711	74.29%	12.409%

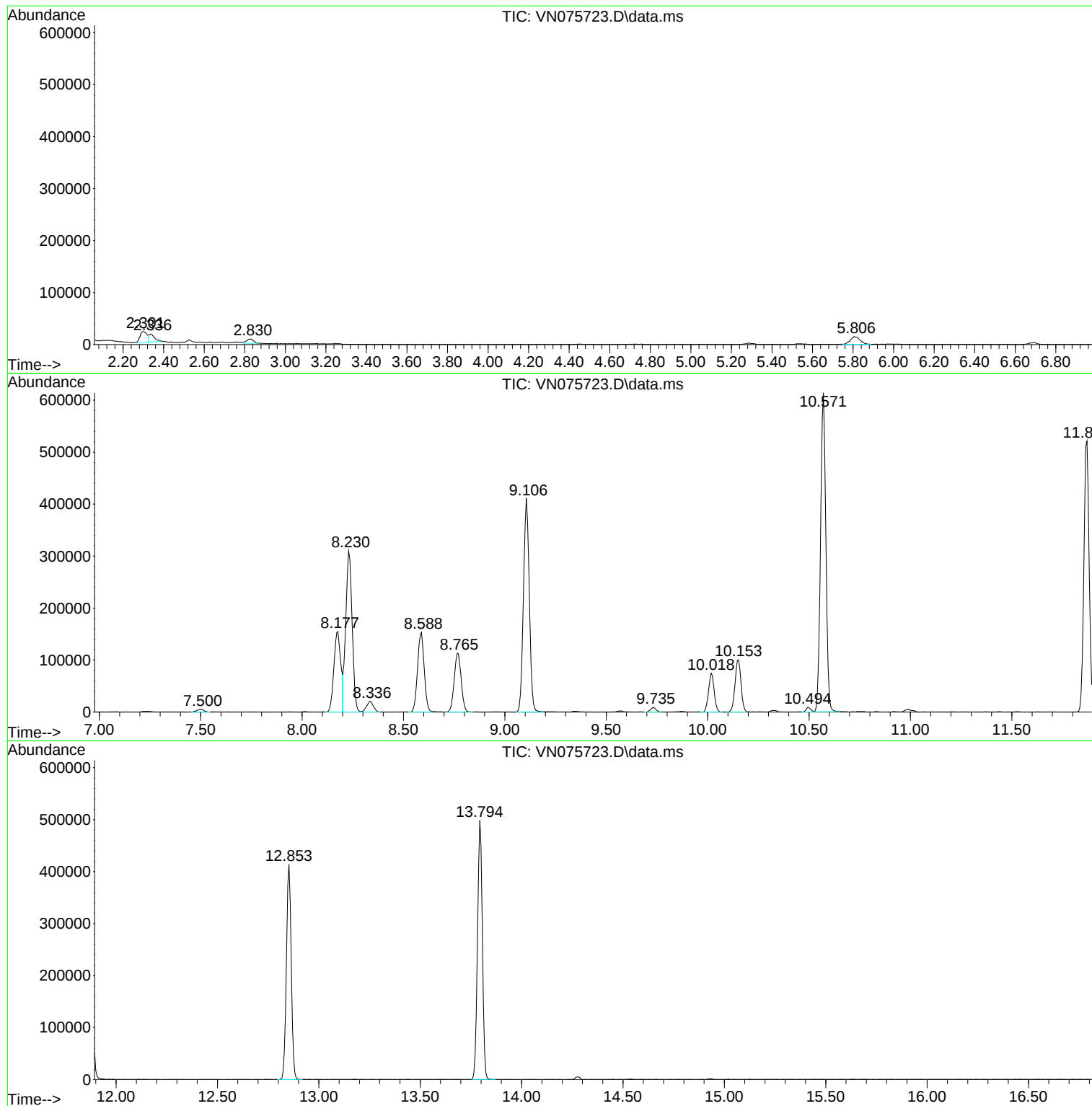
Sum of corrected areas: 6646109

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120922W.M
Quant Title : SW846 8260

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



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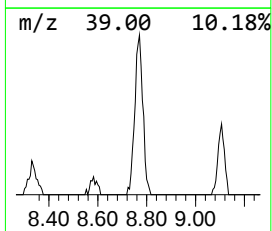
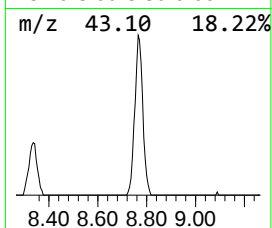
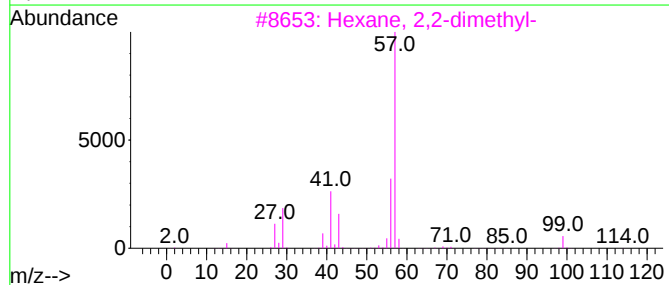
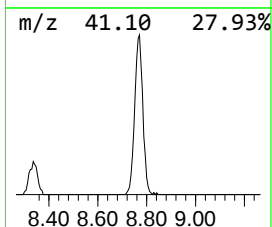
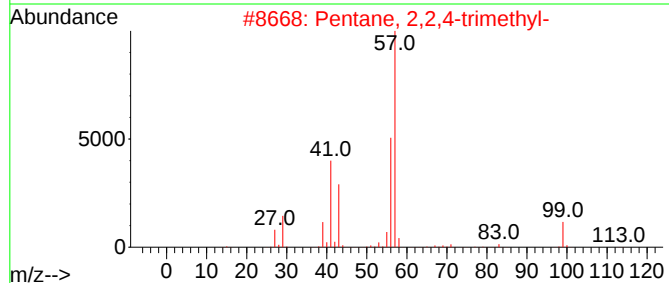
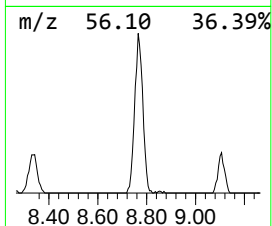
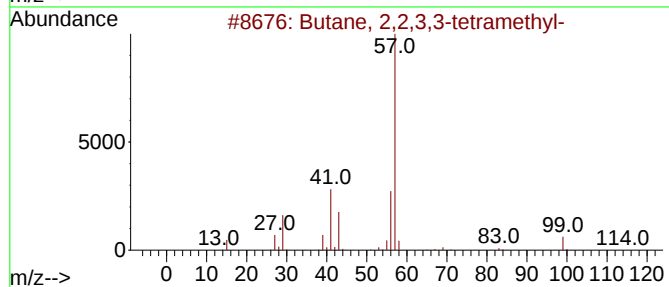
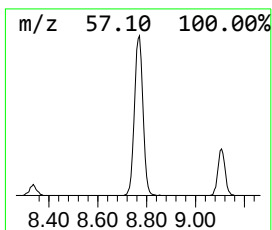
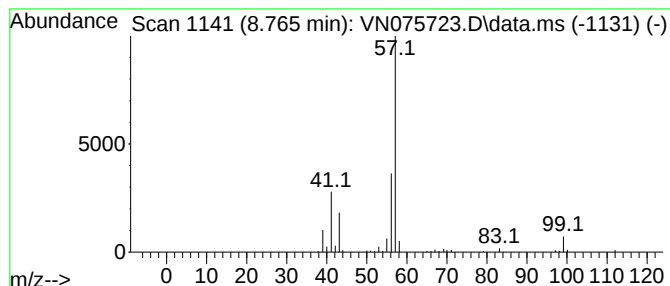
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120922W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane, 2,2,3,3-tetramethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.765	16.38 ug/l	270454	1,4-Difluorobenzene	9.106

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	72
2			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
3			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	64
4			Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	59
5			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	59



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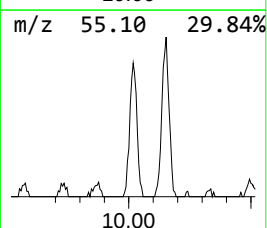
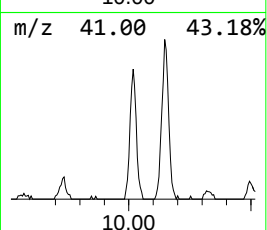
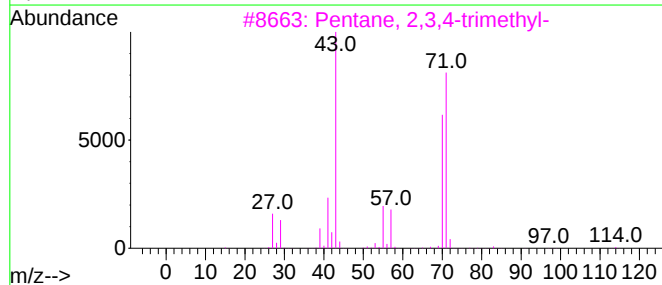
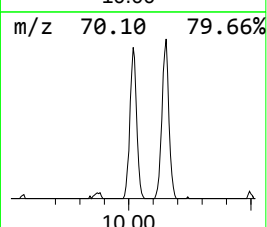
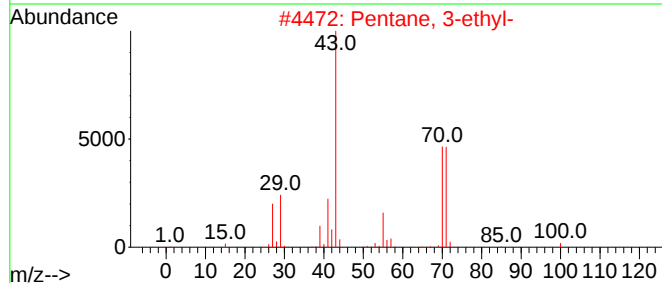
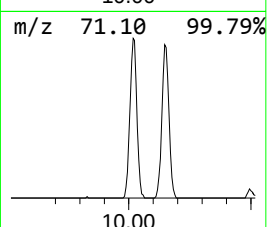
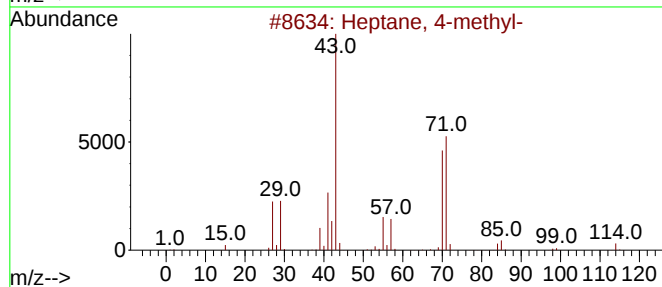
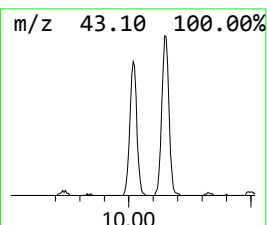
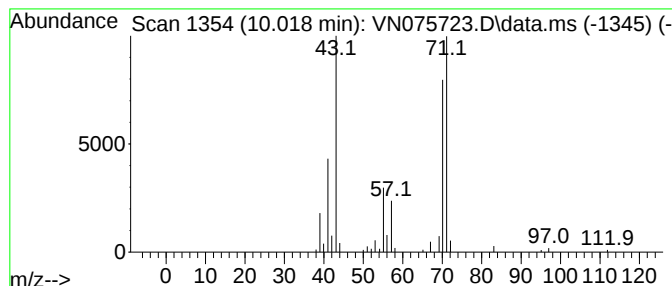
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Peak Number 2 Heptane, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.018	8.76 ug/l	144587	1,4-Difluorobenzene	9.106

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptane, 4-methyl-	114	C8H18	000589-53-7	83
2		Pentane, 3-ethyl-	100	C7H16	000617-78-7	78
3		Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	78
4		Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	78
5		Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	74



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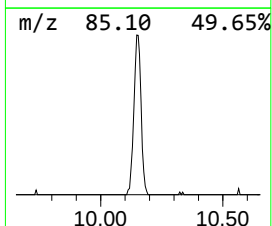
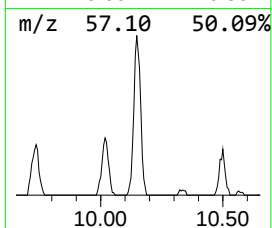
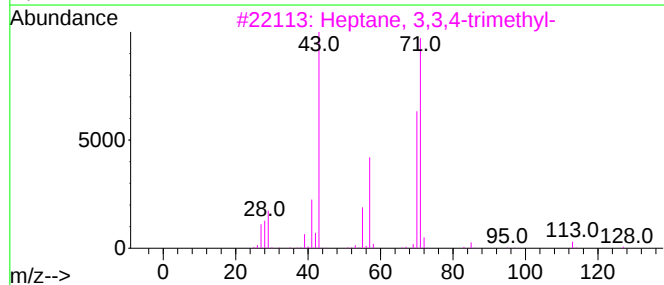
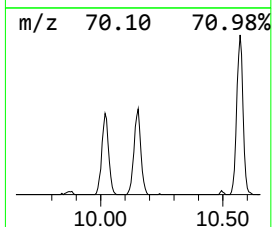
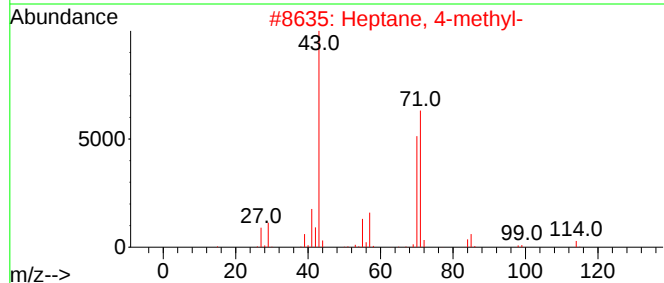
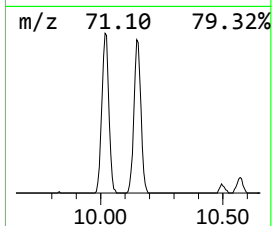
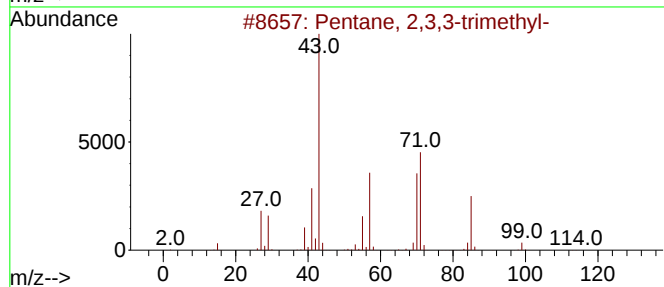
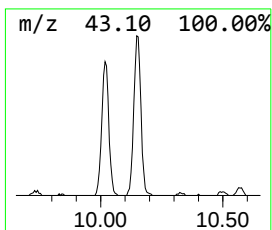
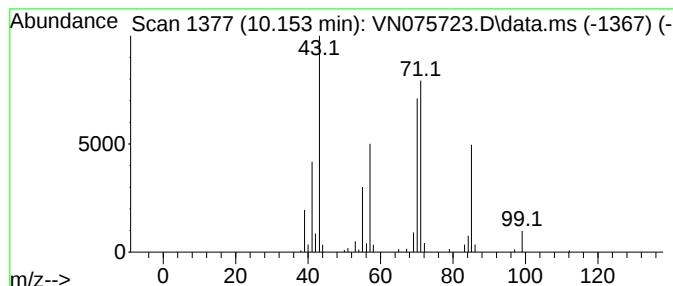
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Pentane, 2,3,3-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.153	12.39 ug/l	204646	1,4-Difluorobenzene	9.106

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2			Heptane, 4-methyl-	114	C8H18	000589-53-7	59
3			Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	53
4			Pentane, 3-ethyl-	100	C7H16	000617-78-7	50
5			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	50



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2,2,3,3...	8.765	16.4	ug/l	270454	2	9.106	825725	50.0
Heptane, 4-methyl-	10.018	8.8	ug/l	144587	2	9.106	825725	50.0
Pentane, 2,3,3-...	10.153	12.4	ug/l	204646	2	9.106	825725	50.0