LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN032419\
Data File : VN054646.D
Acq On : 24 Mar 2019 14:22
Operator : JC/SP
Sample : K2047-08
Misc : 6.55g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : WP022SB445-190320-FD-(17-19)

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\82N032019W.M
Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.519	206	232	233	rBV	41579	114251	3.84%	0.361%
2	5.551	1161	1175	1191	rBV5	11732	35934	1.21%	0.114%
3	7.590	1789	1809	1819	rBV	352764	912445	30.65%	2.886%
4	7.661	1820	1831	1848	rVB	603059	1458290	48.98%	4.613%
5	7.867	1883	1895	1913	rVB2	53095	128700	4.32%	0.407%
6	8.027	1923	1945	1965	rVB	399043	950365	31.92%	3.006%
7	8.201	1988	1999	2017	rVV	112611	292920	9.84%	0.927%
8	8.297	2021	2029	2044	rVB4	20936	43757	1.47%	0.138%
9	8.432	2056	2071	2092	rBV3	45227	106408	3.57%	0.337%
10	8.584	2103	2118	2158	rVB	936052	2072861	69.62%	6.557%
11	9.079	2247	2272	2283	rBV2	127536	312587	10.50%	0.989%
12	9.137	2284	2290	2302	rVB4	34569	67715	2.27%	0.214%
13	9.516	2389	2408	2421	rBV4	84344	179664	6.03%	0.568%
14	9.651	2434	2450	2462	rBV2	95210	219340	7.37%	0.694%
15	9.725	2463	2473	2495	rVV3	106459	279186	9.38%	0.883%
16	9.866	2499	2517	2537	rVV2	96177	245548	8.25%	0.777%
17	10.021	2551	2565	2573	rBV	65854	120808	4.06%	0.382%
18	10.088	2573	2586	2620	rVV	1444132	2977367	100.00%	9.418%
19	10.262	2632	2640	2661	rVB10	29816	87958	2.95%	0.278%
20	10.429	2686	2692	2704	rVB2	43933	74569	2.50%	0.236%
21	10.532	2713	2724	2734	rBV6	29171	74525	2.50%	0.236%
22	10.625	2745	2753	2764	rVB3	27567	50467	1.70%	0.160%
23	10.715	2764	2781	2795	rBV3	63163	118170	3.97%	0.374%
24	10.818	2803	2813	2826	rBV2	53422	105638	3.55%	0.334%
25	10.882	2827	2833	2841	rBV7	17136	29994	1.01%	0.095%
26	10.950	2846	2854	2862	rVB	63481	98192	3.30%	0.311%
27	11.005	2862	2871	2881	rVB2	71906	125035	4.20%	0.396%
28	11.124	2897	2908	2914	rBV2	59400	101393	3.41%	0.321%
29	11.194	2916	2930	2951	rVB5	158034	419386	14.09%	1.327%
30	11.297	2951	2962	2982	rBV	205782	374038	12.56%	1.183%
31	11.413	2982	2998	2999	rBV	1368579	1990221	66.85%	6.296%
32	11.593	3046	3054	3063	rBV6	39457	72445	2.43%	0.229%
33	11.654	3063	3073	3081	rBV4	129911	236504	7.94%	0.748%
34	11.853	3126	3135	3143	rBV3	101045	161515	5.42%	0.511%

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Instrument : MSVOA_N
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Title : SW846 8260

35	11.924	3144	3157	3168	rBV6	226882	506744	17.02%	1.603%
36	11.976	3169	3173	3179	rVV3	35921	43607	1.46%	0.138%
37	12.043	3186	3194	3203	rVB	304767	434579	14.60%	1.375%
38	12.117	3208	3217	3222	rVV4	154111	266234	8.94%	0.842%
39	12.159	3223	3230	3241	rVB3	268330	509752	17.12%	1.613%
40	12.294	3260	3272	3278	rBV8	217478	505587	16.98%	1.599%
41	12.336	3279	3285	3294	rVB	371958	539528	18.12%	1.707%
42	12.403	3296	3306	3315	rVV	906335	1522206	51.13%	4.815%
43	12.561	3348	3355	3370	rVB6	205201	426348	14.32%	1.349%
44	12.644	3370	3381	3392	rBV8	101444	280718	9.43%	0.888%
45	12.728	3394	3407	3416	rVV7	319000	824616	27.70%	2.609%
46	12.779	3418	3423	3434	rVB4	183178	299143	10.05%	0.946%
47	12.873	3444	3452	3459	rBV6	173988	327350	10.99%	1.036%
48	12.924	3464	3468	3472	rVV2	234592	315883	10.61%	0.999%
49	12.963	3473	3480	3491	rVV	727158	1202364	40.38%	3.803%
50	13.024	3493	3499	3511	rVB4	153271	268317	9.01%	0.849%
51	13.088	3512	3519	3528	rBV	240053	375747	12.62%	1.189%
52	13.143	3529	3536	3550	rVB5	196412	453498	15.23%	1.435%
53	13.239	3551	3566	3573	rBV2	501141	1006234	33.80%	3.183%
54	13.281	3573	3579	3586	rVV3	382768	633556	21.28%	2.004%
55	13.342	3587	3598	3618	rVB	1132408	2352363	79.01%	7.441%
56	13.660	3687	3697	3706	rBV6	515259	987216	33.16%	3.123%
57	13.712	3708	3713	3719	rVB2	128489	166260	5.58%	0.526%
58	13.834	3744	3751	3762	rBV8	174530	379226	12.74%	1.200%
59	13.992	3793	3800	3809	rBV6	148109	228969	7.69%	0.724%
60	14.178	3847	3858	3885	rVB9	478556	1372549	46.10%	4.342%
61	14.297	3888	3895	3900	rVV4	151590	234716	7.88%	0.742%
62	14.329	3901	3905	3914	rVB3	186242	255226	8.57%	0.807%
63	14.641	3997	4002	4013	rVB5	118397	181613	6.10%	0.574%
64	14.847	4062	4066	4075	rVB7	57491	74123	2.49%	0.234%

Sum of corrected areas: 31612468

LSC Report - Integrated Chromatogram

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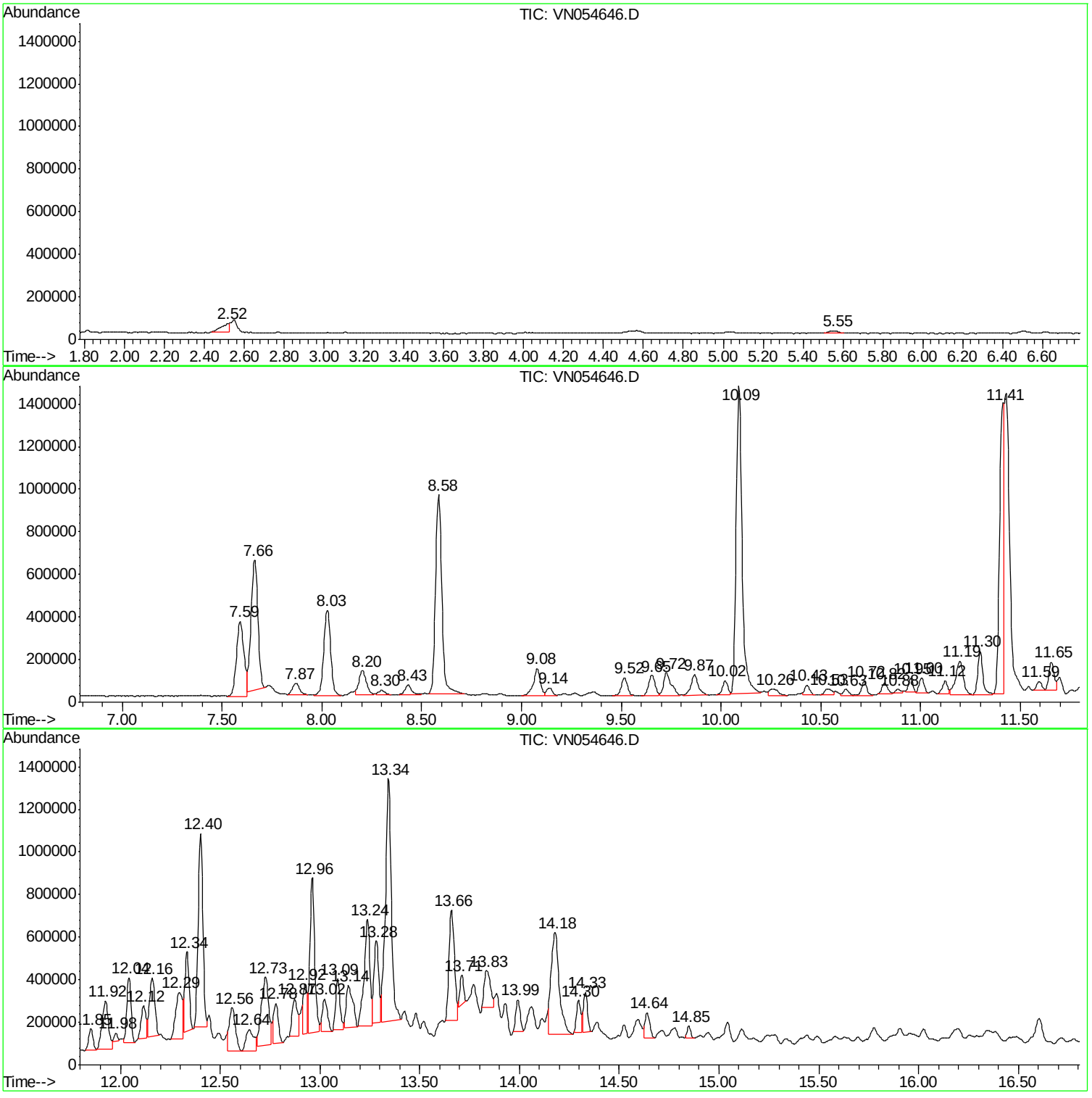
ClientSampleId :
WP022SB445-190320-FD-(17-19)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.M
Quant Title : SW846 8260

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



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TIC Integration Parameters: LSCINT.P

****

Peak Number 1 Octane, 4-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.19	10.54 ug/l	419386	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 4-methyl-	128	C9H20	002216-34-4	90
2	Hexane, 3-ethyl-	114	C8H18	000619-99-8	72
3	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	72
4	Hexane, 2,3,5-trimethyl-	128	C9H20	001069-53-0	58
5	1-Pentanol, 2-methyl-	102	C6H14O	000105-30-6	53

****

Peak Number 2 Octane, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.30	9.40 ug/l	374038	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 3-methyl-	128	C9H20	002216-33-3	91
2	Heptane, 4-propyl-	142	C10H22	003178-29-8	64
3	Heptane, 4-(1-methylethyl)-	142	C10H22	052896-87-4	64
4	Undecane, 6-methyl-	170	C12H26	017302-33-9	59
5	Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	58

****

Peak Number 3 unknown11.92 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	12.73 ug/l	506744	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	49
2	Nonane, 4-methyl-	142	C10H22	017301-94-9	47
3	trans-1,2-Diethyl cyclopentane	126	C9H18	000932-40-1	46
4	Pentane, 2,2,3,3-tetramethyl-	128	C9H20	007154-79-2	43
5	Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	43

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Peak Number 4 Octane, 2,6-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.

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Misc : 6.55g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : WP022SB445-190320-FD-(17-19)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.M
Quant Title : SW846 8260

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.04	10.92 ug/l	434579	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	91
2	Nonane, 3-methyl-	142	C10H22	005911-04-6	91
3	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	86
4	Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	64
5	Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	64

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Peak Number 5 Cyclohexane, propyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.16	12.81 ug/l	509752	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, propyl-	126	C9H18	001678-92-8	68
2	Cyclohexane, methyl-	98	C7H14	000108-87-2	58
3	1-Butene, 2,3,3-trimethyl-	98	C7H14	000594-56-9	49
4	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	46
5	3-Hexen-2-one	98	C6H10O	000763-93-9	46

****

Peak Number 6 Undecane, 5,6-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.29	12.70 ug/l	505587	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 5,6-dimethyl-	184	C13H28	017615-91-7	72
2	Heptane, 4-ethyl-	128	C9H20	002216-32-2	50
3	Decane, 5-methyl-	156	C11H24	013151-35-4	50
4	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	49
5	Octane, 4-ethyl-	142	C10H22	015869-86-0	47

****

Peak Number 7 Nonane, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.34	13.55 ug/l	539528	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual

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Instrument : MSVOA_N
ClientSampleId : WP022SB445-190320-FD-(17-19)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.M
Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

1	Nonane, 4-methyl-	142 C10H22	017301-94-9	72
2	Heptane, 2,3,4-trimethyl-	142 C10H22	052896-95-4	45
3	Octane, 3,5-dimethyl-	142 C10H22	015869-93-9	43
4	Octane, 2,5-dimethyl-	142 C10H22	015869-89-3	42
5	Decane, 2,5,9-trimethyl-	184 C13H28	062108-22-9	38

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Peak Number 8 Cyclohexane, 1-methyl-2-pro... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	17.53 ug/l	824616	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-methyl-2-propyl-	140	C10H20	004291-79-6	72
2	Cyclohexane, 1-methyl-3-propyl-	140	C10H20	004291-80-9	64
3	Cyclohexane, 1,1-dimethyl-	112	C8H16	000590-66-9	58
4	1-Methyl-4-(1-methylethyl)-cyclo...	140	C10H20	000099-82-1	52
5	Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	001678-82-6	52

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Peak Number 9 unknown13.83 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	8.06 ug/l	379226	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6-Dimethyldecane	170	C12H26	013150-81-7	46
2	Cyclopentane, 1-ethyl-2-methyl-,...	112	C8H16	000930-89-2	46
3	Nonane, 4,5-dimethyl-	156	C11H24	017302-23-7	38
4	Cyclohexane, (2-methylpropyl)-	140	C10H20	001678-98-4	35
5	Decane, 3,6-dimethyl-	170	C12H26	017312-53-7	35

****

Peak Number 10 Cyclohexane, pentyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.18	29.17 ug/l	1372550	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, pentyl-	154	C11H22	004292-92-6	60
2	Cyclohexane, 1,1'-(1,5-pentanedi...	236	C17H32	054833-31-7	50
3	Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	47

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Quant Title : SW846 8260

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

4	Cyclohexane, undecyl-	238	C17H34	054105-66-7	43
5	n-Nonylcyclohexane	210	C15H30	002883-02-5	43

Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Octane, 4-methyl-	11.19	10.5	ug/l	419386	3	11.41	1990220	50.0
Octane, 3-methyl-	11.30	9.4	ug/l	374038	3	11.41	1990220	50.0
unknown11.92	11.92	12.7	ug/l	506744	3	11.41	1990220	50.0
Octane, 2,6-dimet...	12.04	10.9	ug/l	434579	3	11.41	1990220	50.0
Cyclohexane, propyl-	12.16	12.8	ug/l	509752	3	11.41	1990220	50.0
Undecane, 5,6-dim...	12.29	12.7	ug/l	505587	3	11.41	1990220	50.0
Nonane, 4-methyl-	12.34	13.6	ug/l	539528	3	11.41	1990220	50.0
Cyclohexane, 1-me...	12.73	17.5	ug/l	824616	4	13.34	2352360	50.0
unknown13.83	13.83	8.1	ug/l	379226	4	13.34	2352360	50.0
Cyclohexane, pentyl-	14.18	29.2	ug/l	1372550	4	13.34	2352360	50.0