

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042121\
 Data File : VX021806.D
 Acq On : 21 Apr 2021 20:23
 Operator : JC/MD
 Sample : M2125-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 PB-2021-WW-000-07

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_X\Method\82X042021W.M
 Title : SW846 8260

Signal : TIC: VX021806.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.422	214	219	229	rVB	14358	25001	3.04%	0.491%
2	2.867	287	292	299	rVB2	11112	23205	2.82%	0.456%
3	3.166	328	341	356	rVB3	49948	140576	17.11%	2.761%
4	3.495	386	395	407	rBV	80378	184183	22.41%	3.617%
5	3.916	456	464	476	rBV2	17577	46141	5.62%	0.906%
6	4.373	529	539	550	rVB2	44405	129474	15.76%	2.543%
7	4.647	576	584	593	rBV3	3906	12095	1.47%	0.238%
8	5.464	707	718	733	rBV	97599	279763	34.05%	5.494%
9	5.629	734	745	762	rVB	163196	452064	55.01%	8.878%
10	6.031	800	811	822	rBV	97834	253803	30.89%	4.984%
11	6.830	932	942	954	rBV	248324	586660	71.39%	11.521%
12	7.190	992	1001	1010	rBV2	12615	26888	3.27%	0.528%
13	8.695	1241	1248	1255	rBV	525939	821721	100.00%	16.138%
14	8.763	1255	1259	1267	rVB	9466	17728	2.16%	0.348%
15	9.317	1344	1350	1360	rVB	49213	71401	8.69%	1.402%
16	9.561	1383	1390	1401	rBV2	5790	9450	1.15%	0.186%
17	10.092	1471	1477	1494	rVB	488632	692298	84.25%	13.596%
18	11.122	1640	1646	1654	rBV	430478	547321	66.61%	10.749%
19	12.061	1794	1800	1807	rVB	573044	701710	85.40%	13.781%
20	12.256	1827	1832	1843	rBV	28365	45663	5.56%	0.897%
21	13.627	2052	2057	2064	rVB2	18763	24732	3.01%	0.486%

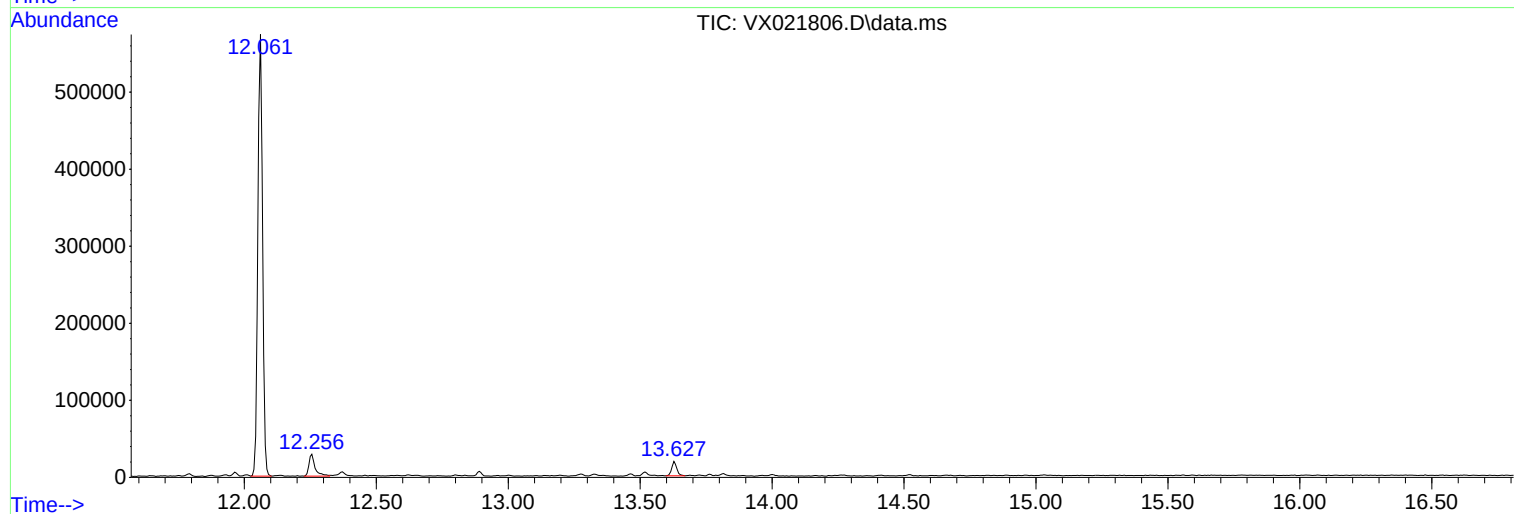
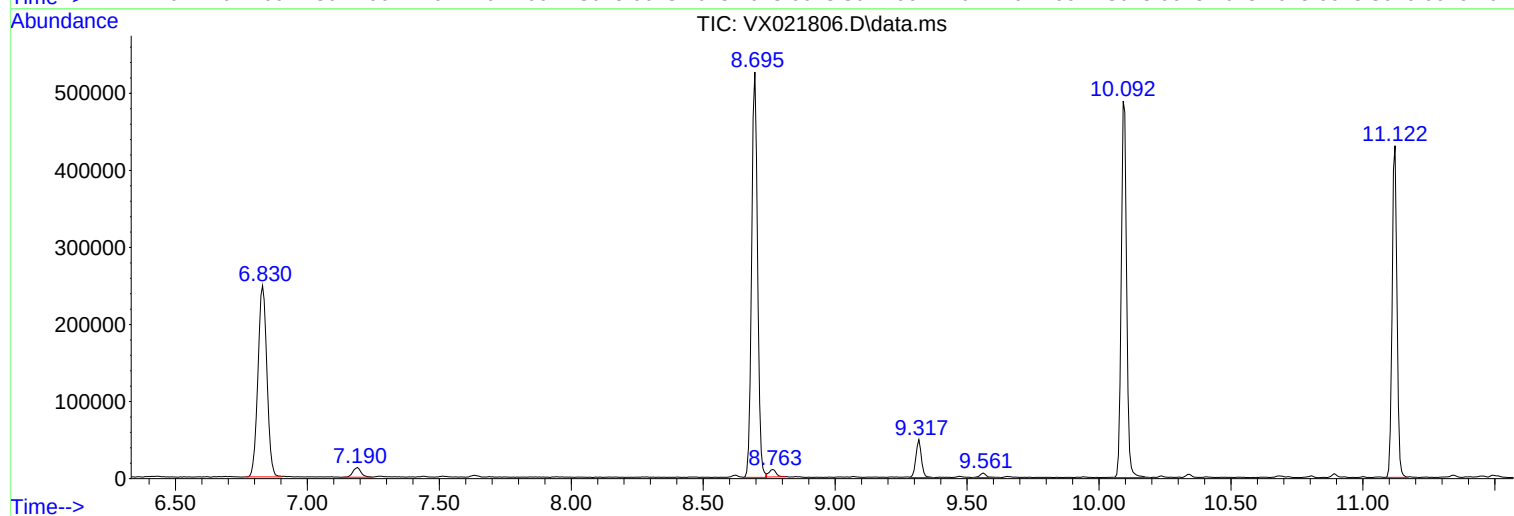
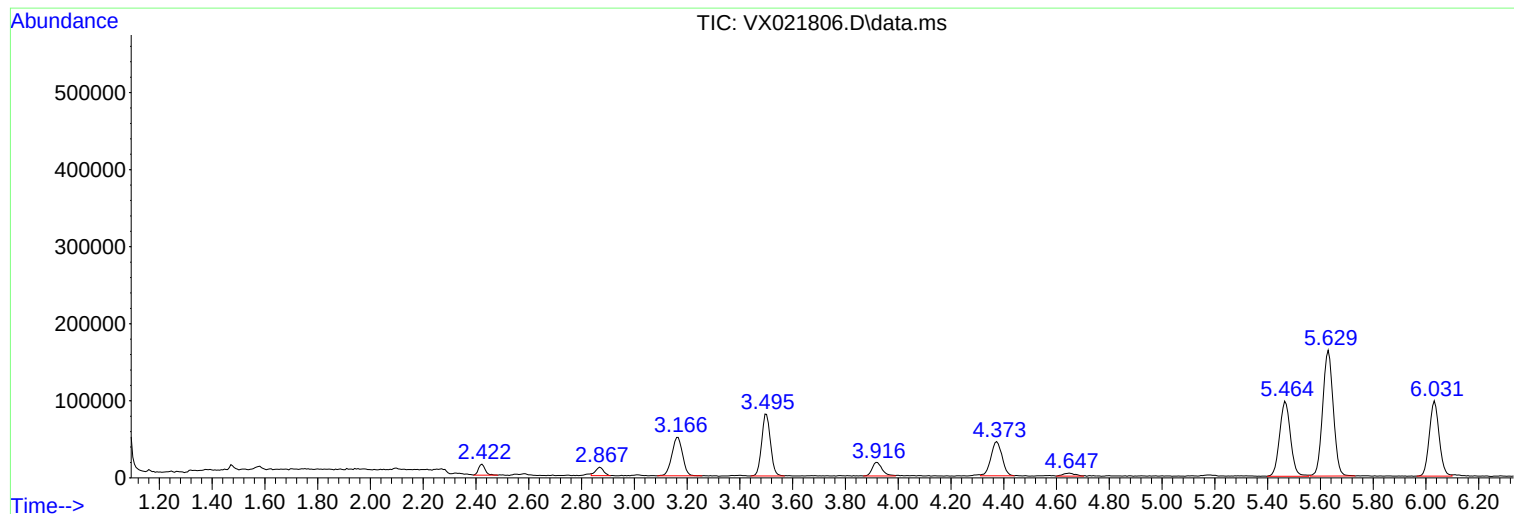
Sum of corrected areas: 5091877

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042021W.M
Quant Title : SW846 8260

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



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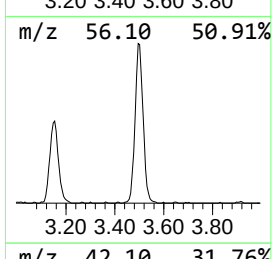
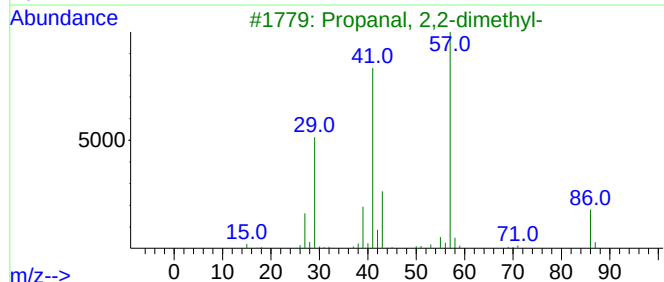
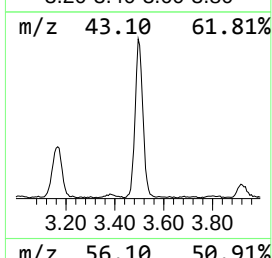
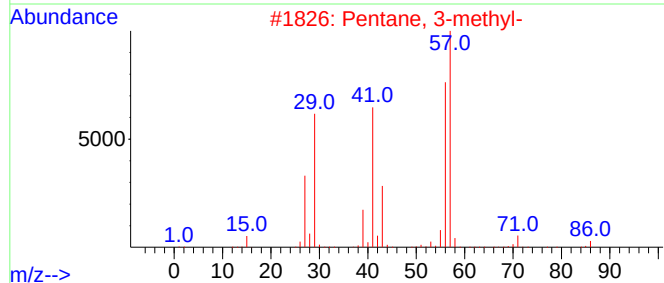
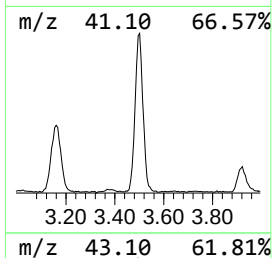
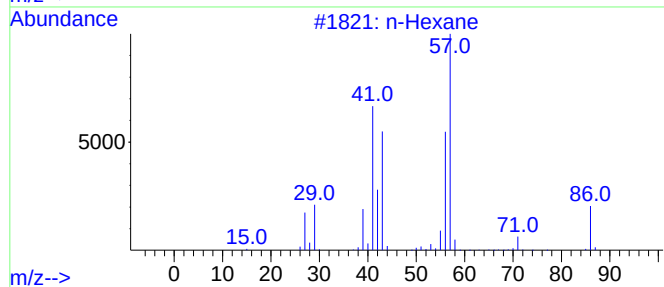
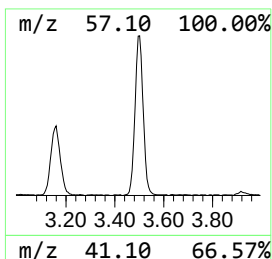
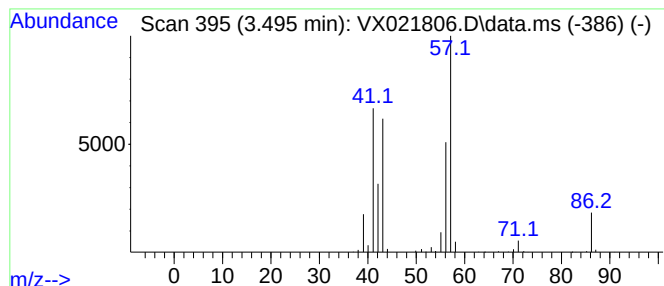
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Hexane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.495	20.37 ug/l	184183	Pentafluorobenzene	5.629

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexane	86	C6H14	000110-54-3	94
2			Pentane, 3-methyl-	86	C6H14	000096-14-0	42
3			Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	38
4			Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	33
5			Methane, isocyanato-	57	C2H3NO	000624-83-9	32



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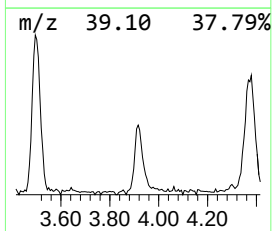
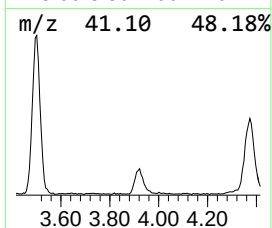
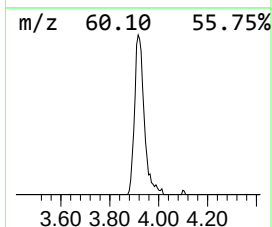
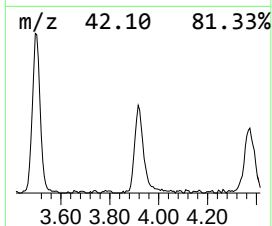
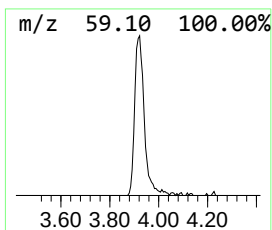
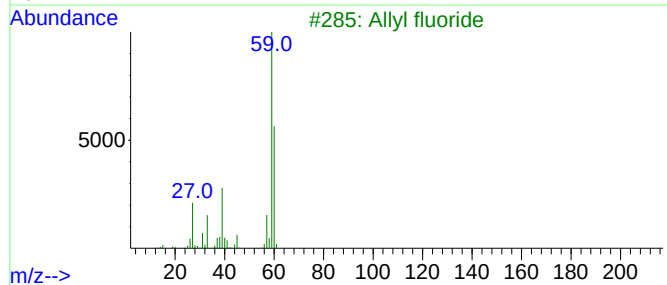
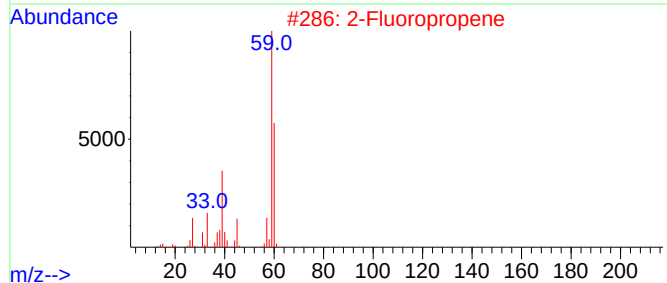
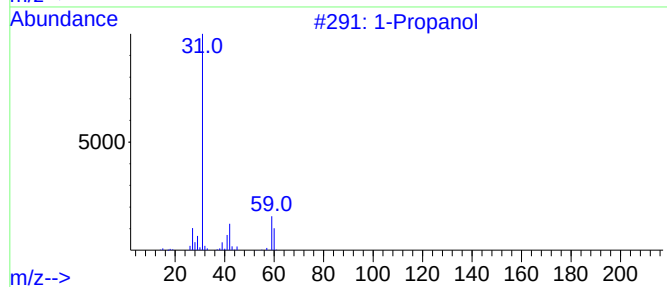
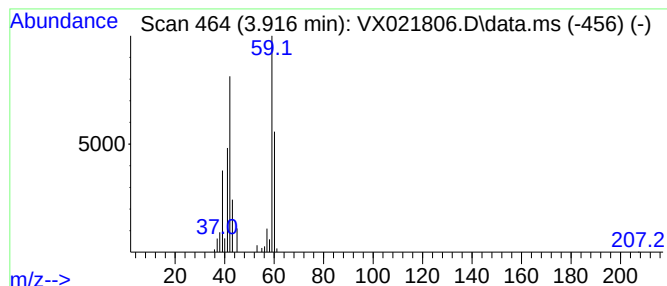
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Peak Number 2 1-Propanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.916	5.10 ug/l	46141	Pentafluorobenzene	5.629

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Propanol	60	C3H8O	000071-23-8	78
2		2-Fluoropropene	60	C3H5F	001184-60-7	49
3		Allyl fluoride	60	C3H5F	000818-92-8	47
4		Cyclopropane	42	C3H6	000075-19-4	16
5		Acetaldoxime	59	C2H5NO	000107-29-9	7



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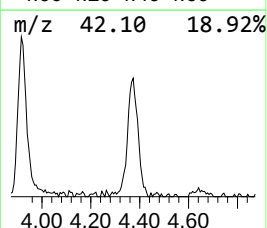
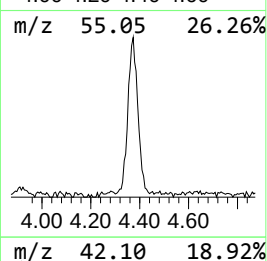
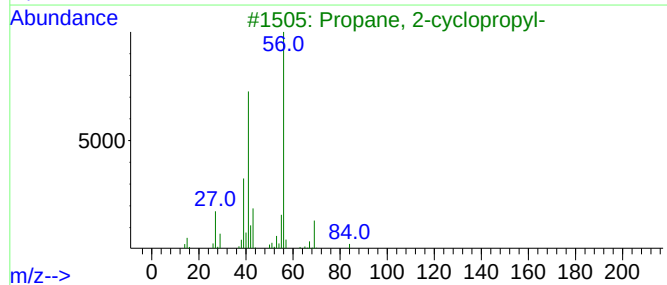
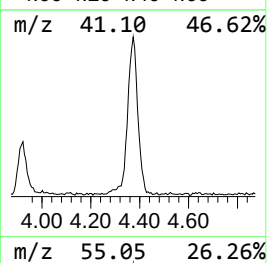
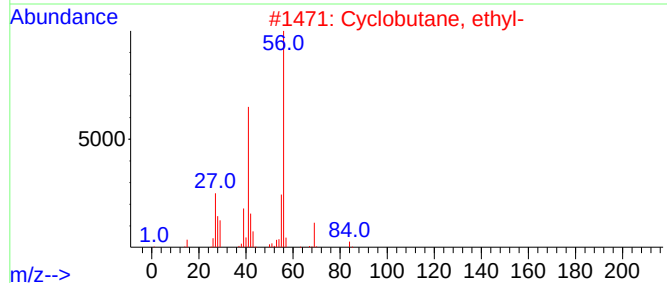
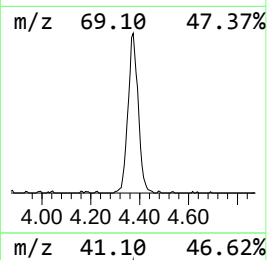
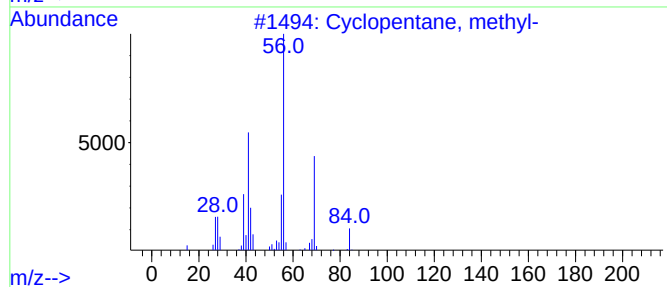
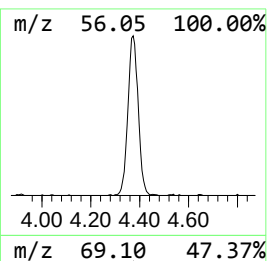
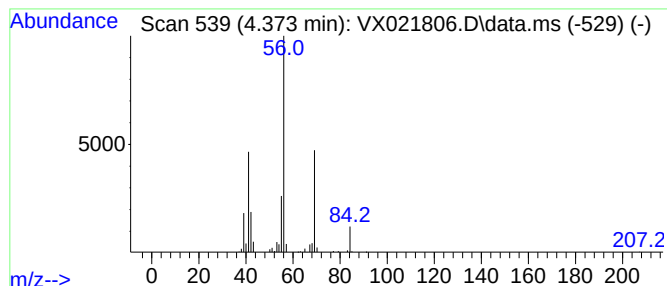
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Peak Number 3 Cyclopentane, methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.373	14.32 ug/l	129474	Pentafluorobenzene	5.629

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2			Cyclobutane, ethyl-	84	C6H12	004806-61-5	78
3			Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	72
4			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
5			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	52



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexane	3.495	20.4	ug/l	184183	1	5.629	452064	50.0
1-Propanol	3.916	5.1	ug/l	46141	1	5.629	452064	50.0
Cyclopentane, m...	4.373	14.3	ug/l	129474	1	5.629	452064	50.0