

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX020320\
 Data File : VX014796.D
 Acq On : 03 Feb 2020 15:34
 Operator : JC/SP
 Sample : L1329-19DL 4X
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COMP-5DL

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.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	1.070	26	30	43	rBV	944989	1145214	5.02%	1.910%
2	1.479	93	97	110	rBV	18972841	22814026	100.00%	38.043%
3	2.100	193	199	209	rBV	676697	1025933	4.50%	1.711%
4	2.338	232	238	248	rBV	6325837	10048788	44.05%	16.756%
5	2.430	248	253	266	rVB	625355	1039878	4.56%	1.734%
6	3.960	489	504	517	rBV	2955136	8486781	37.20%	14.152%
7	4.320	554	563	579	rBV	283480	768459	3.37%	1.281%
8	5.484	744	754	766	rBV	253635	710029	3.11%	1.184%
9	5.649	770	781	794	rVV	424840	1199935	5.26%	2.001%
10	6.045	837	846	857	rBV	275763	735284	3.22%	1.226%
11	6.843	966	977	988	rBV	676769	1597396	7.00%	2.664%
12	6.953	988	995	1006	rVB2	168370	398827	1.75%	0.665%
13	8.709	1276	1283	1289	rBV	1421228	2194867	9.62%	3.660%
14	8.776	1289	1294	1300	rVB	266462	399964	1.75%	0.667%
15	9.050	1331	1339	1350	rBV	587815	839483	3.68%	1.400%
16	10.105	1505	1512	1522	rBV	1467903	1977201	8.67%	3.297%
17	11.129	1675	1680	1687	rBV	1182003	1518133	6.65%	2.531%
18	12.074	1830	1835	1843	rVB	1472834	1873475	8.21%	3.124%
19	12.263	1861	1866	1874	rBV	295830	400842	1.76%	0.668%
20	13.434	2055	2058	2061	rBV	300904	335478	1.47%	0.559%
21	13.891	2129	2133	2139	rVV	340936	459826	2.02%	0.767%

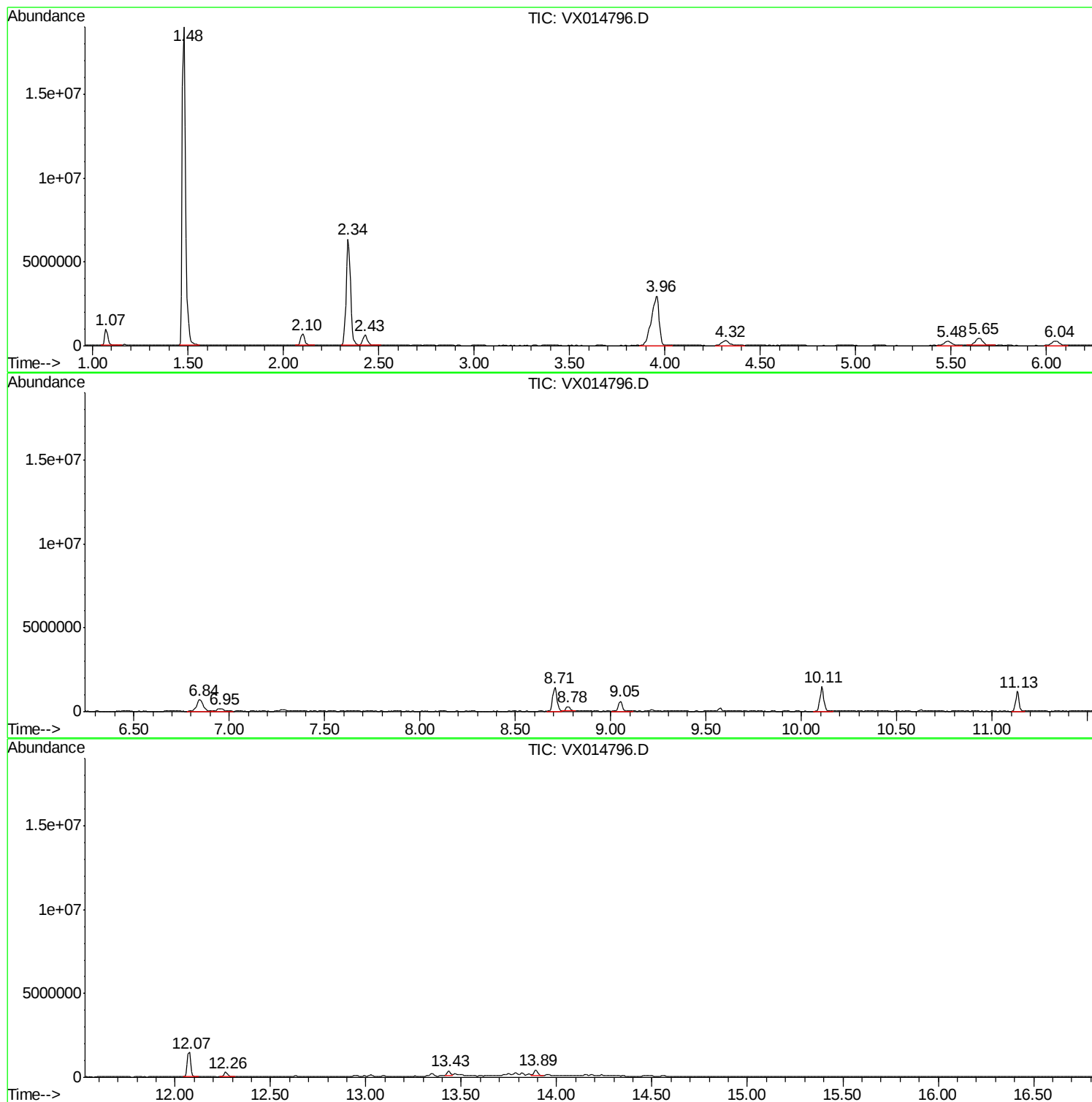
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.M
Quant Title : SW846 8260

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



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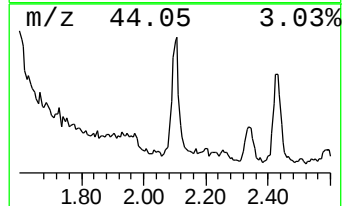
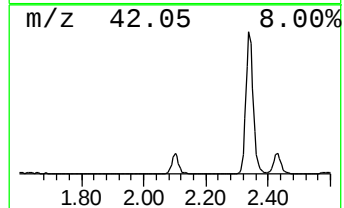
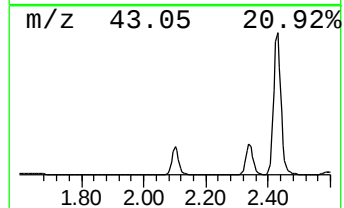
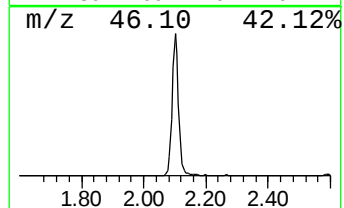
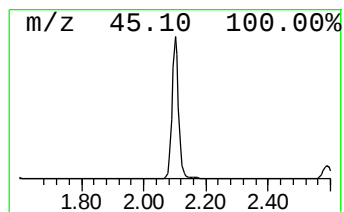
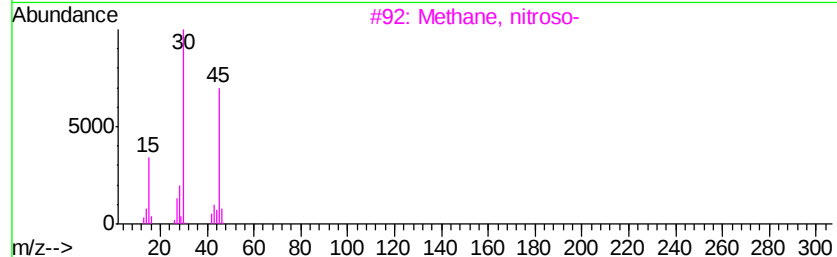
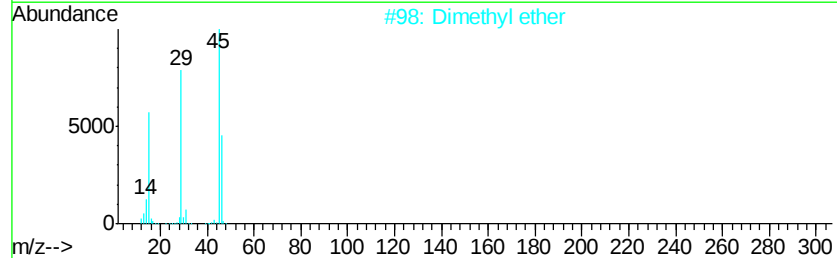
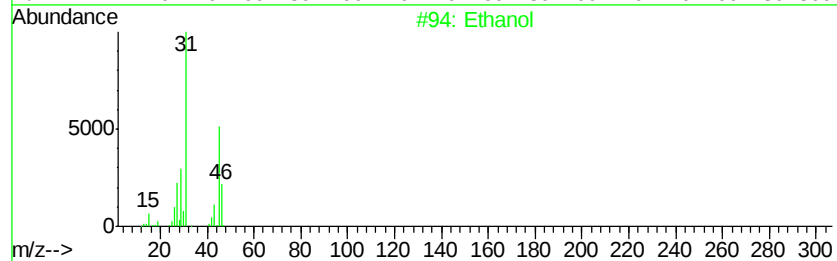
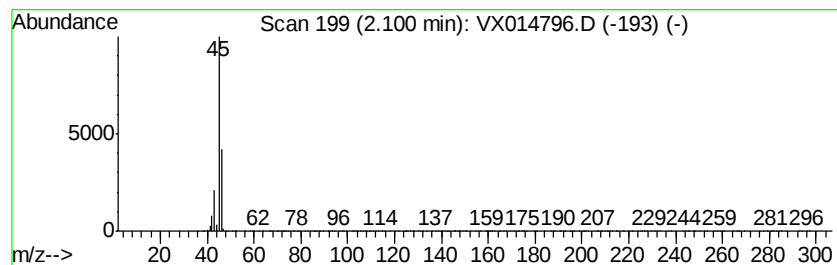
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.M
Quant Title : SW846 8260

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

Peak Number 3 Ethanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.10	42.75 ug/l	1025930	Pentafluorobenzene	5.65

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol		46	C2H6O	000064-17-5	64
2	Dimethyl ether		46	C2H6O	000115-10-6	9
3	Methane, nitroso-		45	CH3NO	000865-40-7	4
4	Formic acid		46	CH2O2	000064-18-6	4
5	Oxalic acid		90	C2H2O4	000144-62-7	4



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COMP-5DL

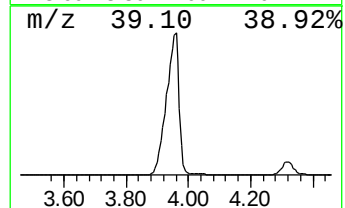
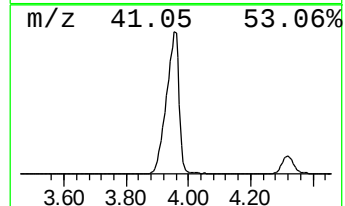
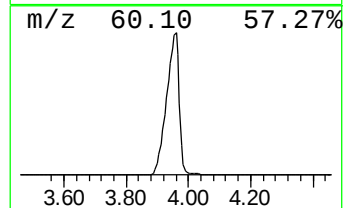
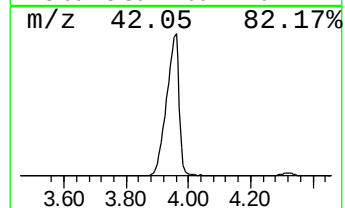
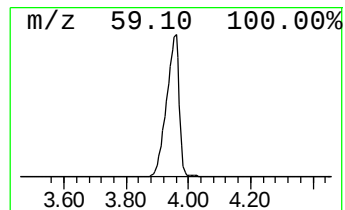
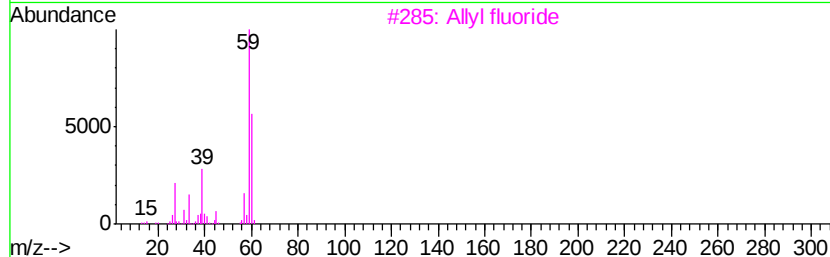
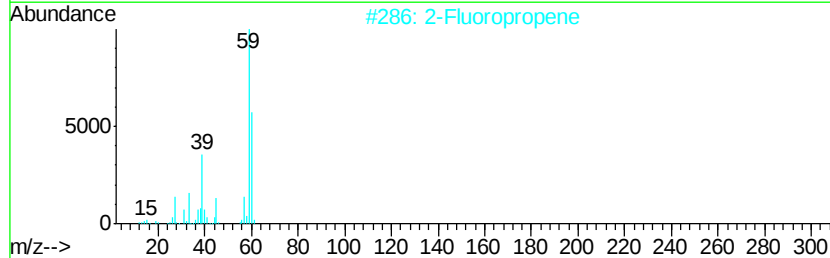
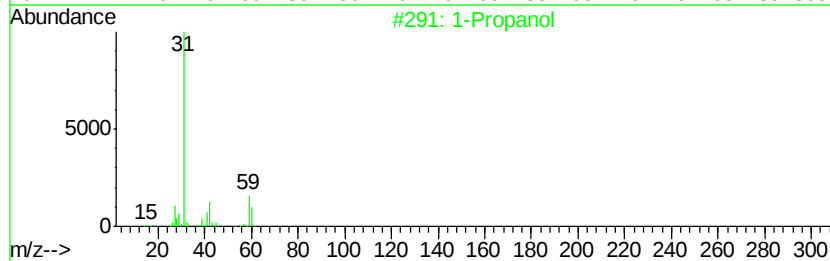
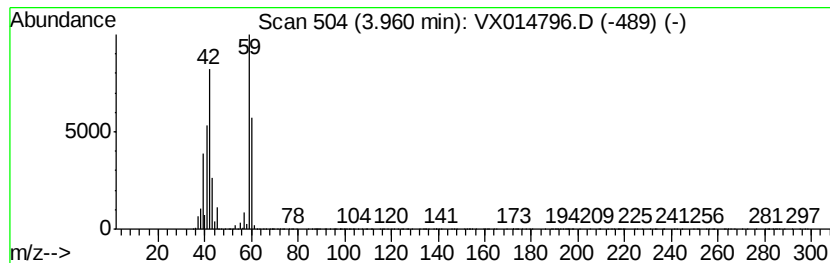
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.M
Quant Title : SW846 8260

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

Peak Number 4 1-Propanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.96	353.64 ug/l	8486780	Pentafluorobenzene	5.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Propanol	60	C3H8O	000071-23-8	59
2		2-Fluoropropene	60	C3H5F	001184-60-7	47
3		Allyl fluoride	60	C3H5F	000818-92-8	38
4		Cyclopropane	42	C3H6	000075-19-4	25
5		Methanamine, N-hydroxy-N-methyl-	61	C2H7NO	005725-96-2	9



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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
COMP-5DL

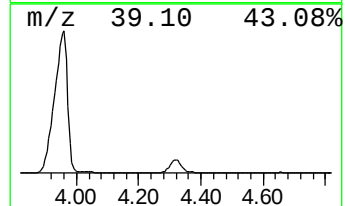
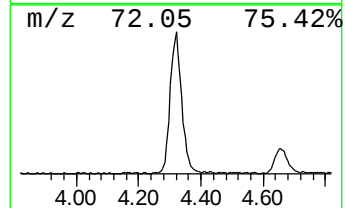
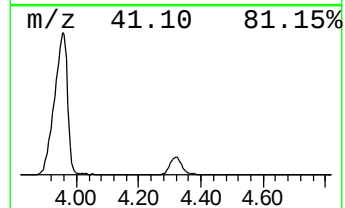
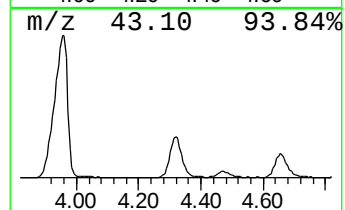
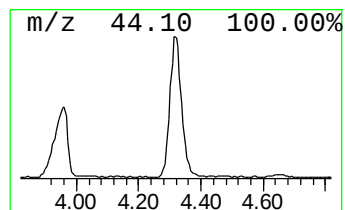
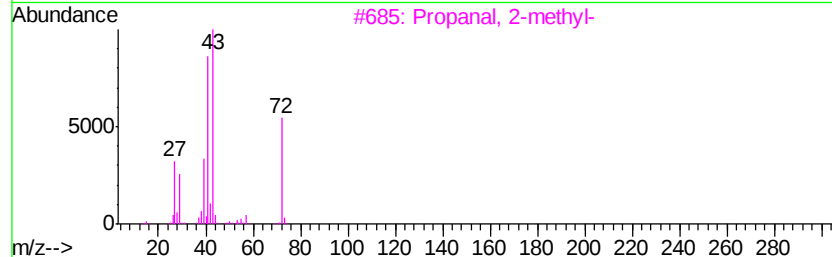
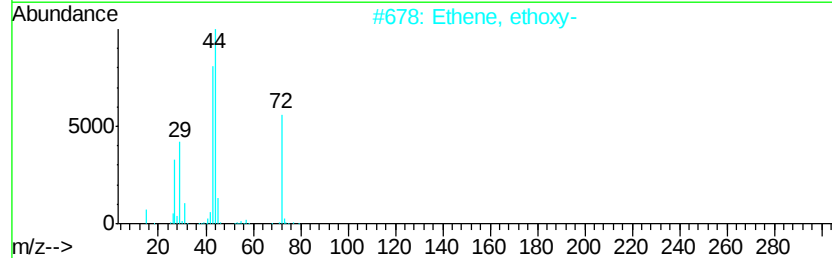
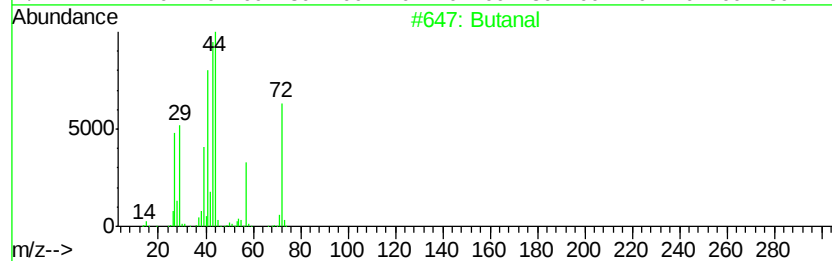
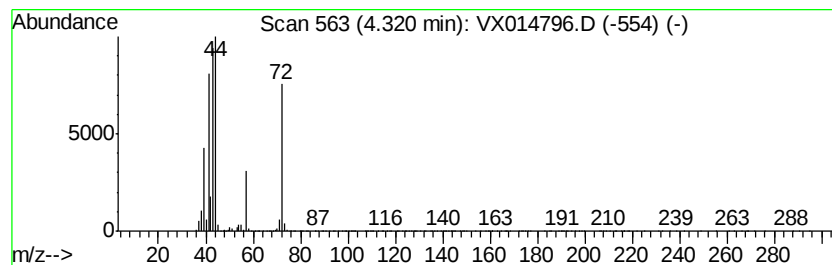
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Quant Title : SW846 8260

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

Peak Number 5 Butanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.32	32.02 ug/l	768459	Pentafluorobenzene	5.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanal	72	C4H8O	000123-72-8	94
2		Ethene, ethoxy-	72	C4H8O	000109-92-2	58
3		Propanal, 2-methyl-	72	C4H8O	000078-84-2	58
4		1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	38
5		Isobutylene epoxide	72	C4H8O	000558-30-5	35



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Instrument :
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ClientSampleId :
COMP-5DL

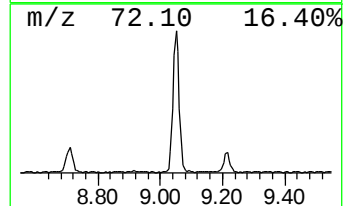
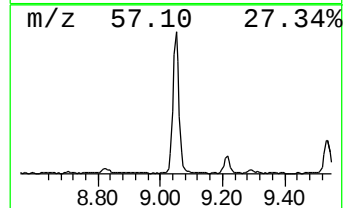
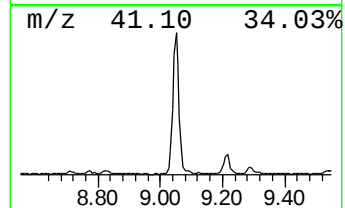
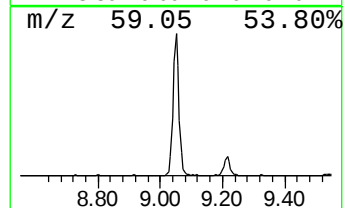
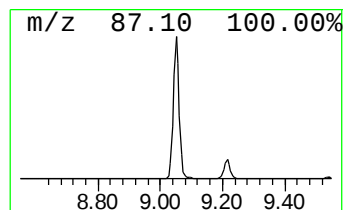
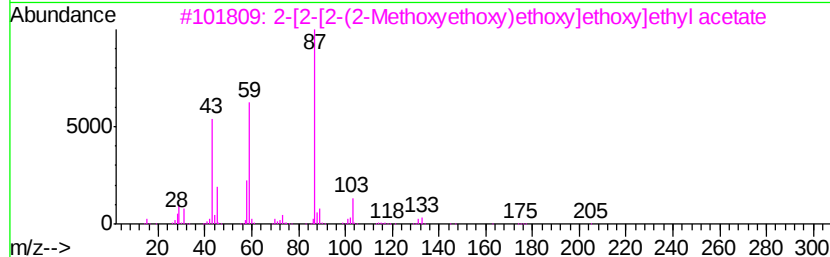
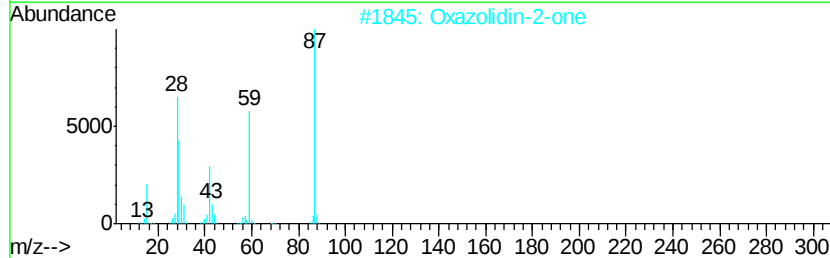
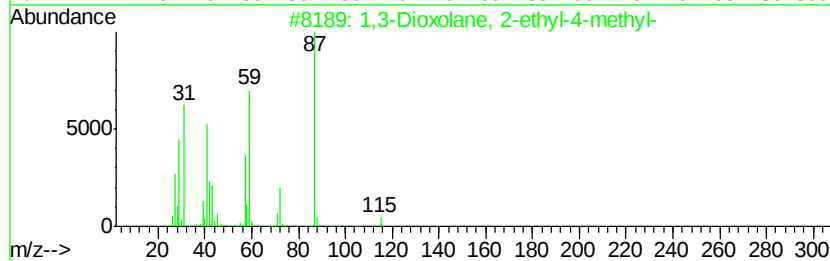
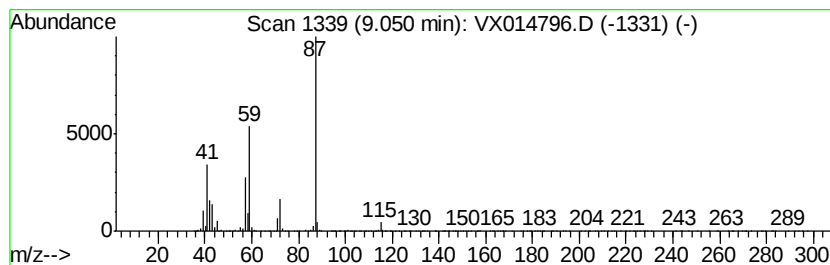
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Quant Title : SW846 8260

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

Peak Number 7 1,3-Dioxolane, 2-ethyl-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.05	21.23 ug/l	839483	Chlorobenzene-d5	10.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	95
2		Oxazolidin-2-one	87	C3H5NO2	000497-25-6	64
3		2-[2-[2-(2-Methoxyethoxy)ethoxy]ethoxy]ethyl acetate	250	C11H22O6	1000351-91-4	59
4		2-Propanone, O-methylloxime	87	C4H9NO	003376-35-0	52
5		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	50



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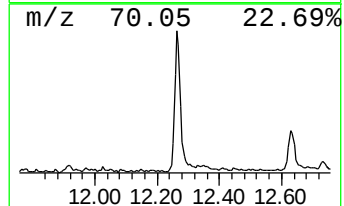
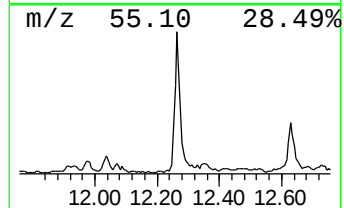
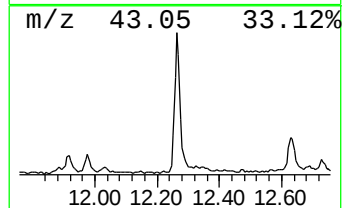
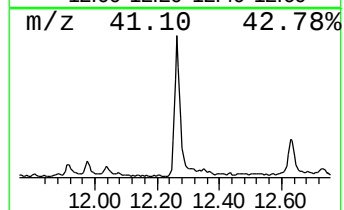
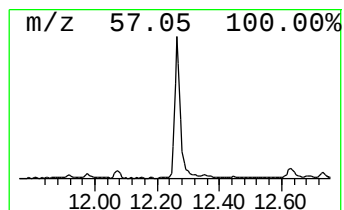
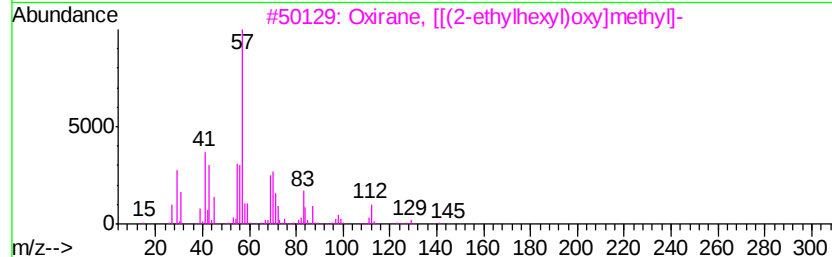
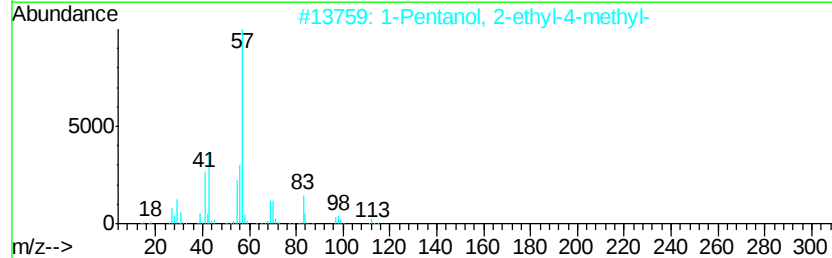
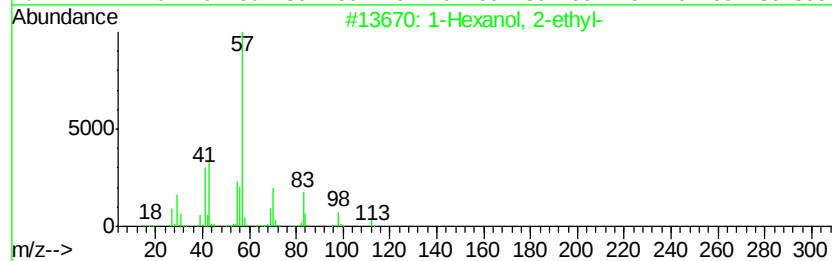
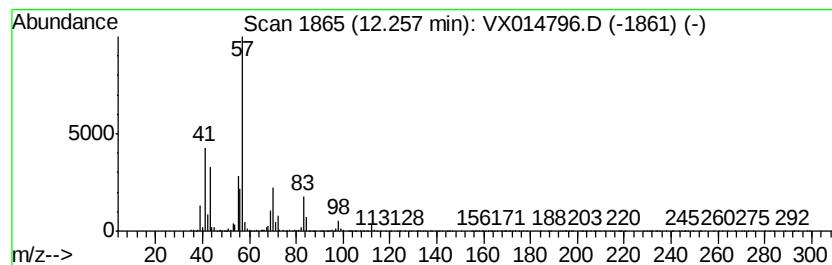
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 1-Hexanol, 2-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.26	10.70 ug/l	400842	1,4-Dichlorobenzene-d4	12.07		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	86
2		1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	64
3		Oxirane, [[(2-ethylhexyl)oxylmet...	186	C11H22O2	002461-15-6	56
4		Undec-10-enoic acid, t-butyl ester	240	C15H28O2	093757-41-6	53
5		2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	50



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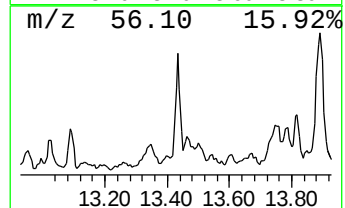
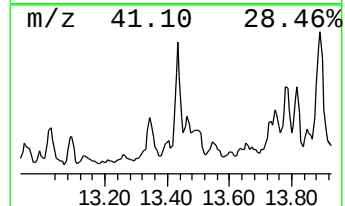
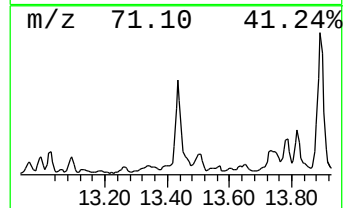
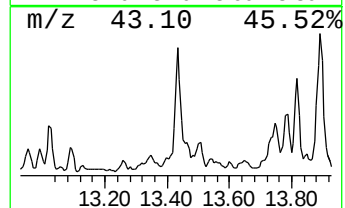
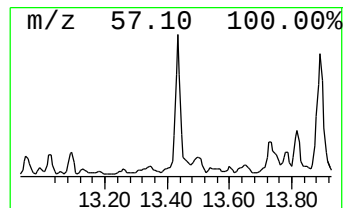
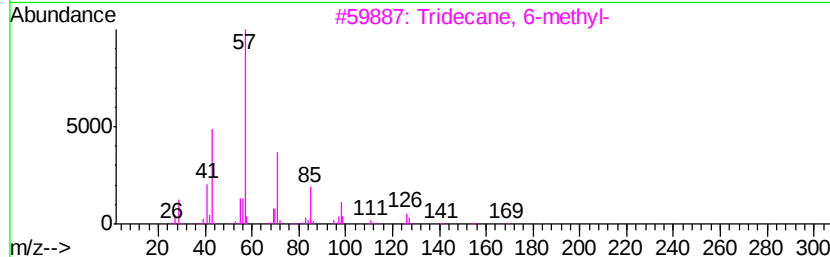
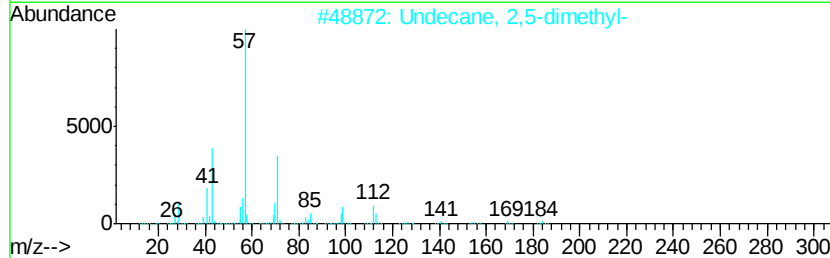
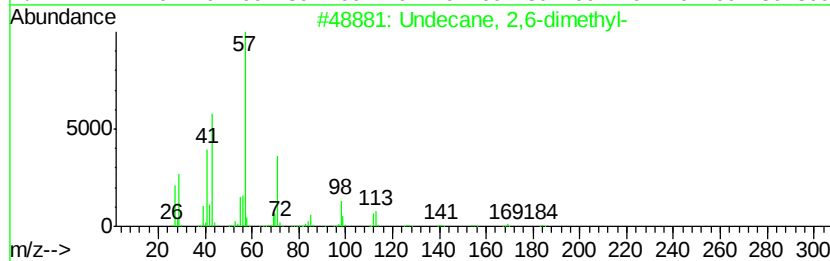
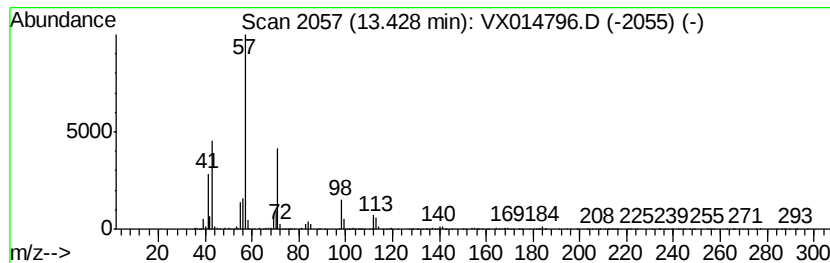
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Quant Title : SW846 8260

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

Peak Number 9 Undecane, 2,6-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.43	8.95 ug/l	335478	1,4-Dichlorobenzene-d4	12.07

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	94
2			Undecane, 2,5-dimethyl-	184	C13H28	017301-22-3	91
3			Tridecane, 6-methyl-	198	C14H30	013287-21-3	64
4			Sulfurous acid, butyl 2-ethylhex...	250	C12H26O3S	1000309-18-8	64
5			Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	59



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX020320\
Data File : VX014796.D
Acq On : 03 Feb 2020 15:34
Operator : JC/SP
Sample : L1329-19DL 4X
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-5DL

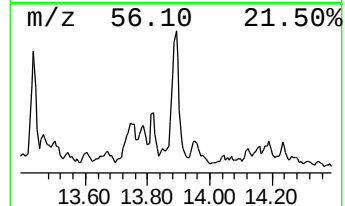
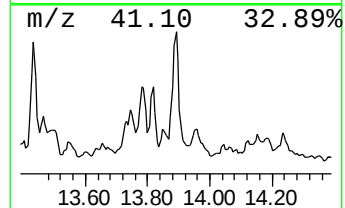
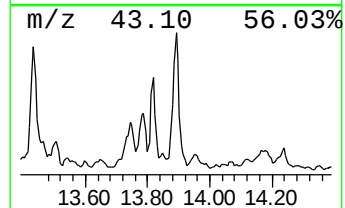
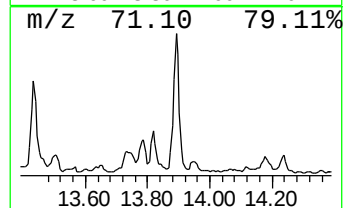
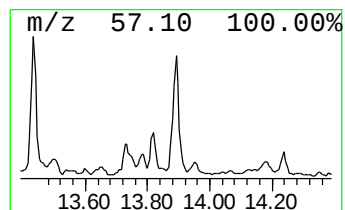
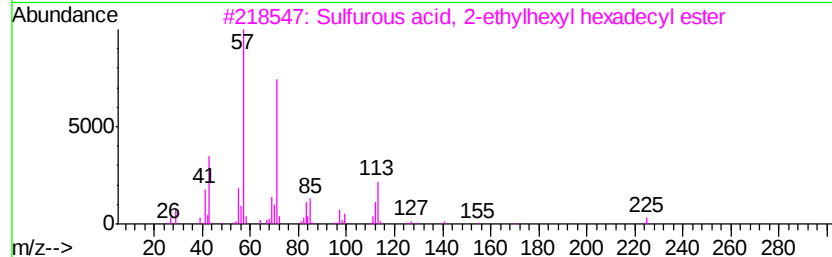
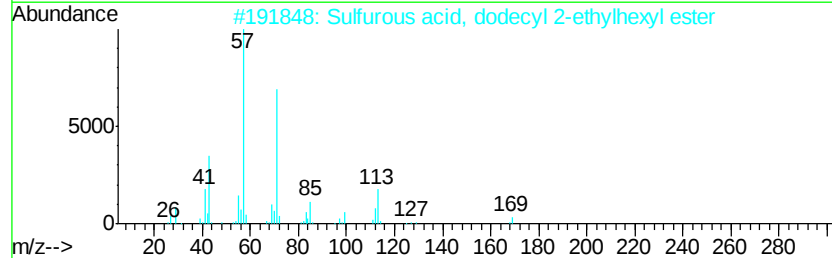
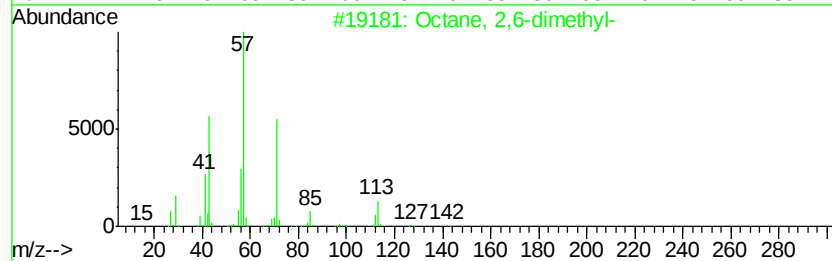
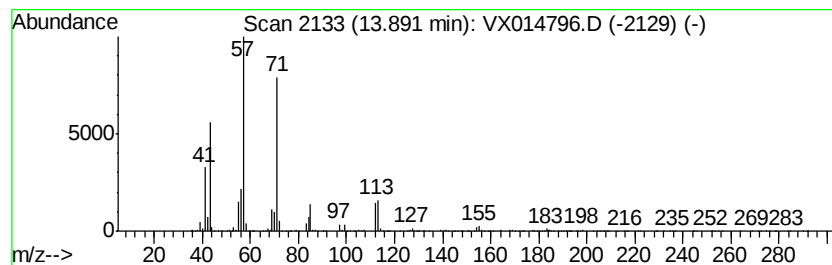
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.M
Quant Title : SW846 8260

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

Peak Number 10 Octane, 2,6-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	12.27 ug/l	459826	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	87
2		Sulfurous acid, dodecyl 2-ethylh...	362	C20H42O3S	1000309-19-5	80
3		Sulfurous acid, 2-ethylhexyl hex...	418	C24H50O3S	1000309-19-9	72
4		Heptane, 3-[(ethenvloxy)methyl]-	156	C10H20O	000103-44-6	64
5		Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	59



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX020320\
Data File : VX014796.D
Acq On : 03 Feb 2020 15:34
Operator : JC/SP
Sample : L1329-19DL 4X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-5DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol	2.10	42.8	ug/l	1025930	1	5.65	1199940	50.0
1-Propanol	3.96	353.6	ug/l	8486780	1	5.65	1199940	50.0
Butanal	4.32	32.0	ug/l	768459	1	5.65	1199940	50.0
1,3-Dioxane, 2-me...	6.95	12.5	ug/l	398827	2	6.85	1597400	50.0
1,3-Dioxolane, 2-...	9.05	21.2	ug/l	839483	3	10.11	1977200	50.0
1-Hexanol, 2-ethyl-	12.26	10.7	ug/l	400842	4	12.07	1873480	50.0
Undecane, 2,6-dim...	13.43	8.9	ug/l	335478	4	12.07	1873480	50.0
Octane, 2,6-dimet...	13.89	12.3	ug/l	459826	4	12.07	1873480	50.0