

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011022\
 Data File : VN070551.D
 Acq On : 10 Jan 2022 18:35
 Operator : JC/MD
 Sample : N1015-09
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 31278

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\82N122721W.M

Title : SW846 8260

Signal : TIC: VN070551.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.582	204	221	290	rBV2	18053324	34818943	9.05%	3.393%
2	4.082	774	780	788	rBV2	71208929	124985172	32.47%	12.178%
3	6.678	1685	1748	1810	rBV	31195424	165892343	43.10%	16.164%
4	8.976	2586	2605	2662	rVB2	19586022	42771233	11.11%	4.168%
5	9.215	2667	2694	2706	rVV	10783615	22640157	5.88%	2.206%
6	9.268	2707	2714	2754	rVB	3793448	6983914	1.81%	0.680%
7	10.443	3134	3152	3169	rBV	3766758	7708016	2.00%	0.751%
8	10.615	3196	3216	3226	rBV	2640901	6401267	1.66%	0.624%
9	10.851	3286	3304	3309	rBV8	187430187	384919283	100.00%	37.506%
10	11.712	3609	3625	3666	rVB4	89103390	173732111	45.13%	16.928%
11	12.278	3819	3836	3858	rBV	4659466	8893117	2.31%	0.867%
12	12.685	3967	3988	3998	rBV	10693363	17783645	4.62%	1.733%
13	13.206	4161	4182	4201	rVB	2771402	5437354	1.41%	0.530%
14	13.519	4277	4299	4314	rBV	10995846	17839771	4.63%	1.738%
15	13.672	4343	4356	4372	rVB2	3297807	5492752	1.43%	0.535%

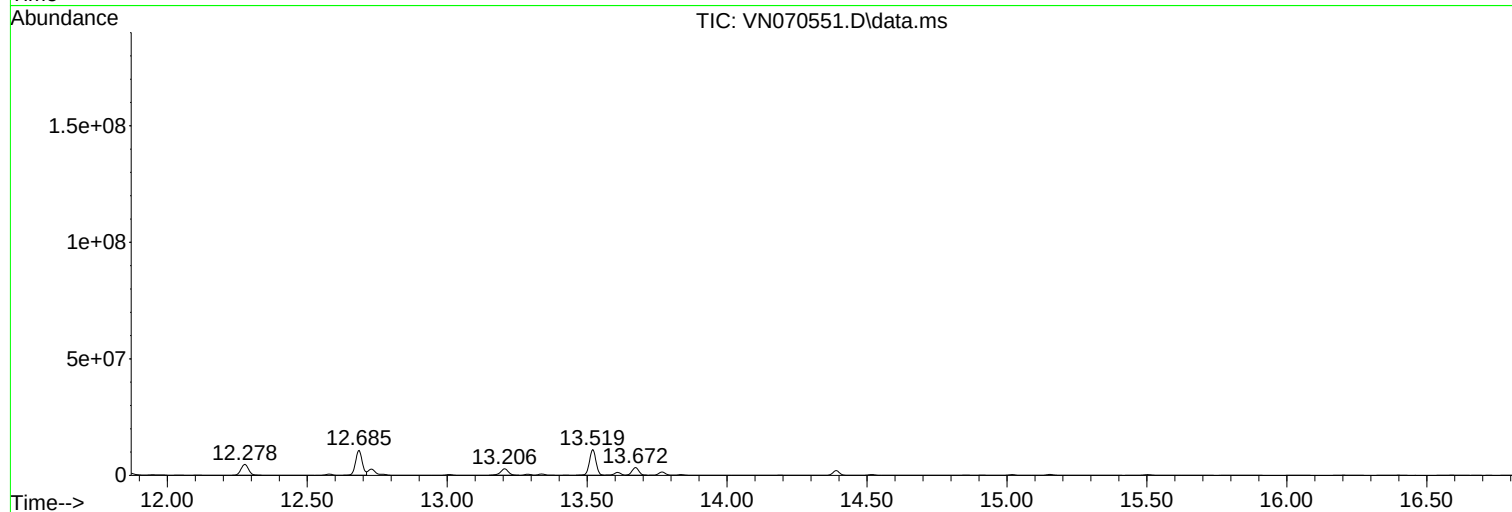
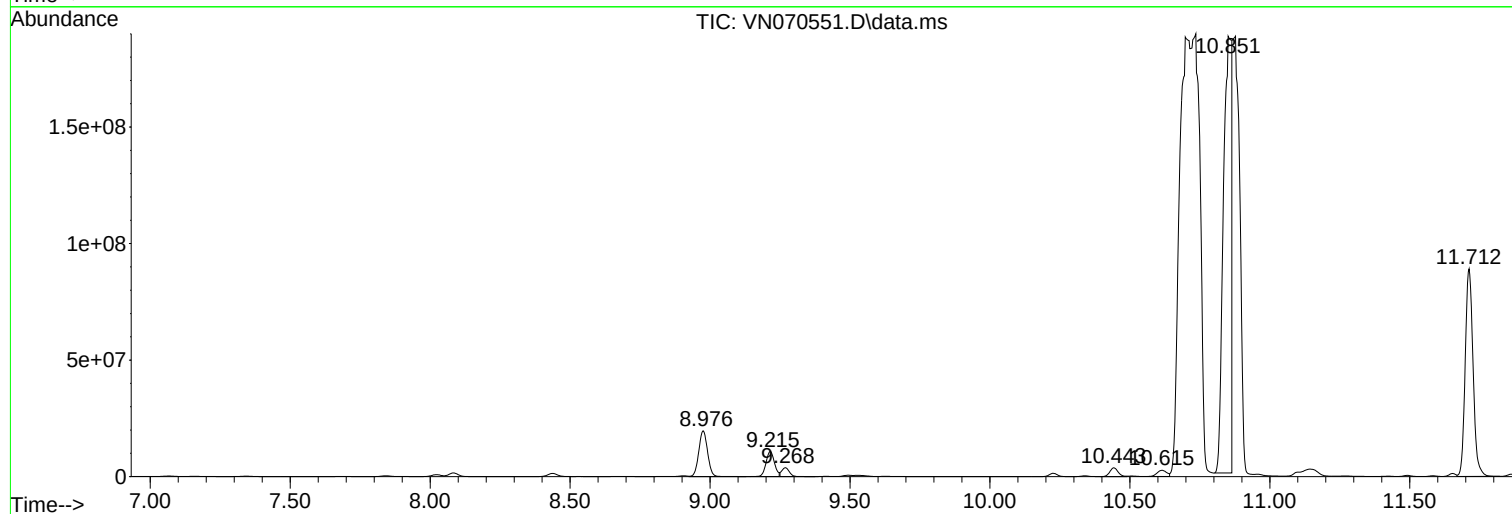
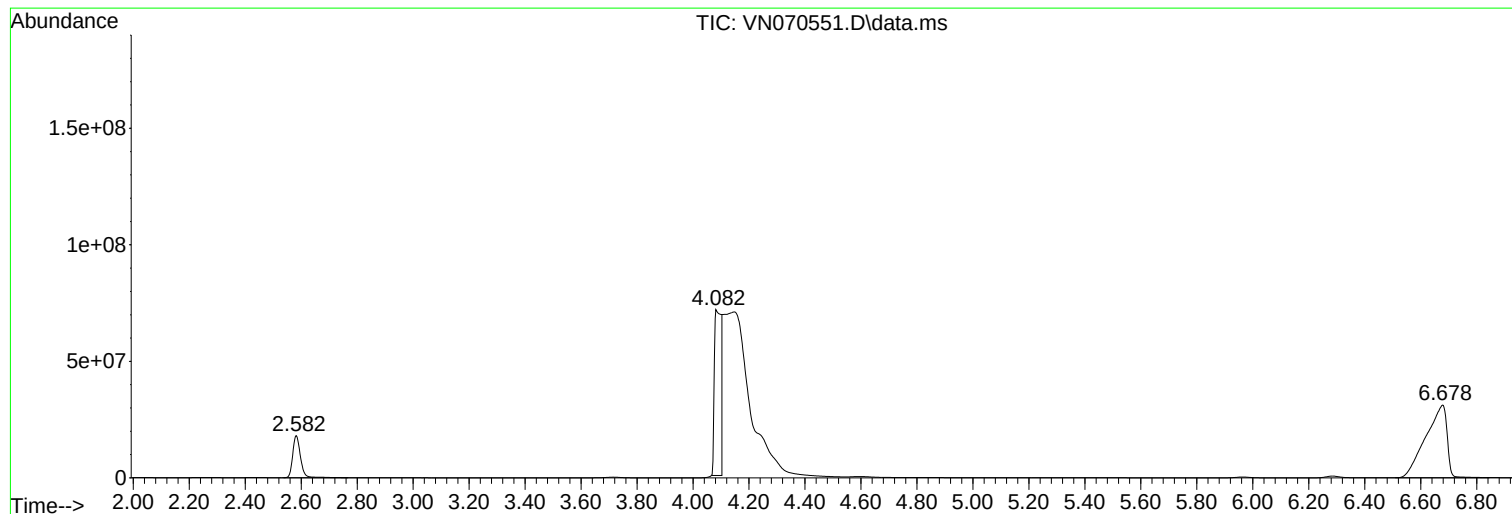
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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



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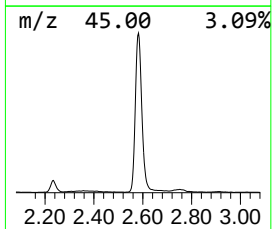
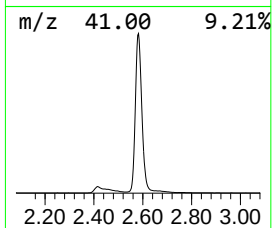
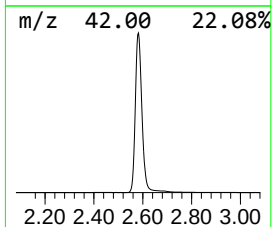
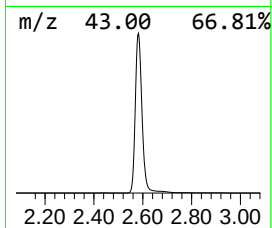
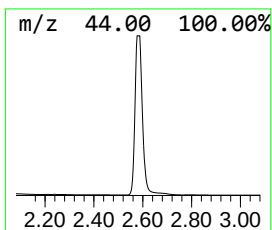
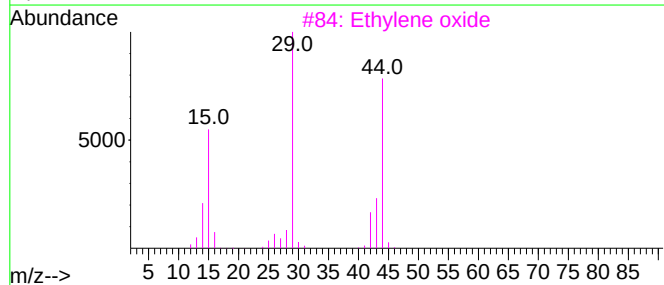
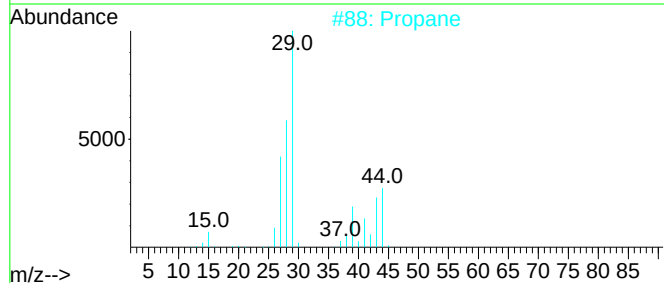
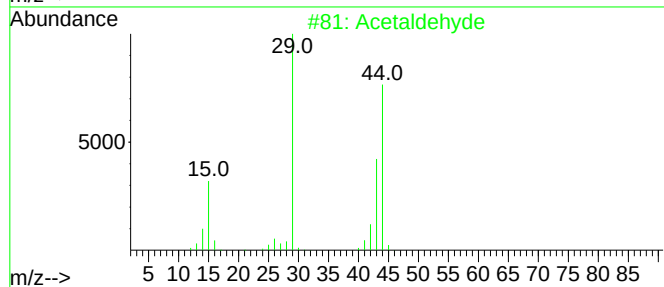
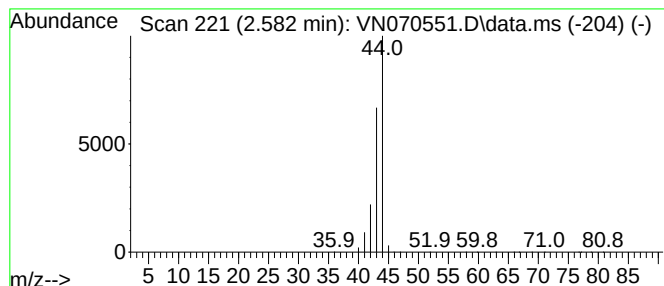
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Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.582	40.70 ug/l	34818900	Pentafluorobenzene	8.083

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	74
2			Propane	44	C3H8	000074-98-6	5
3			Ethylene oxide	44	C2H4O	000075-21-8	5
4			Alanine	89	C3H7NO2	000056-41-7	4
5			Hydrogen isocyanate	43	CHNO	000075-13-8	3



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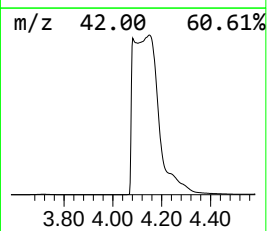
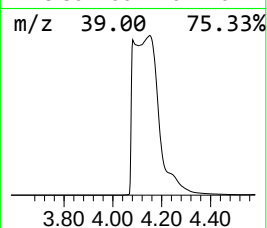
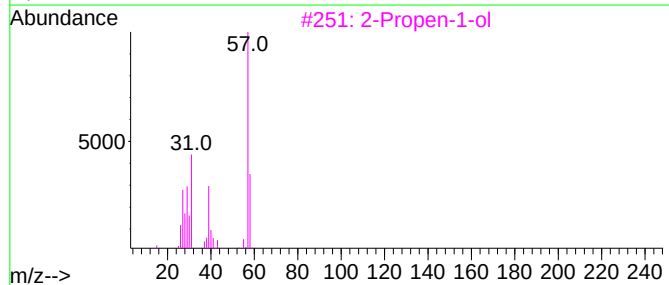
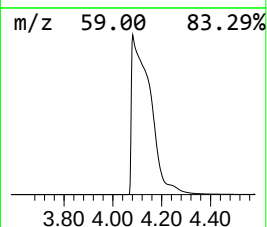
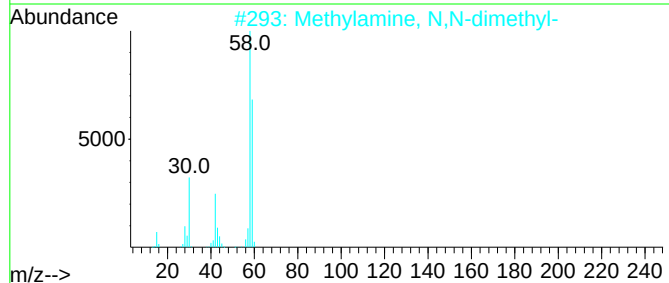
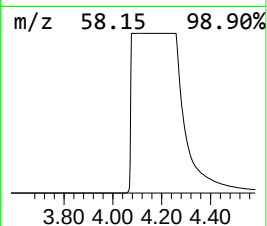
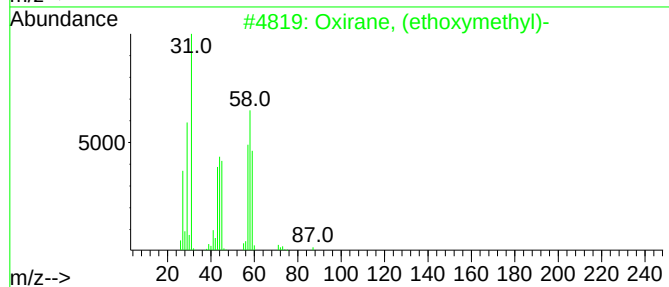
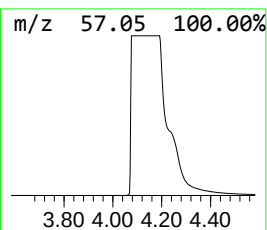
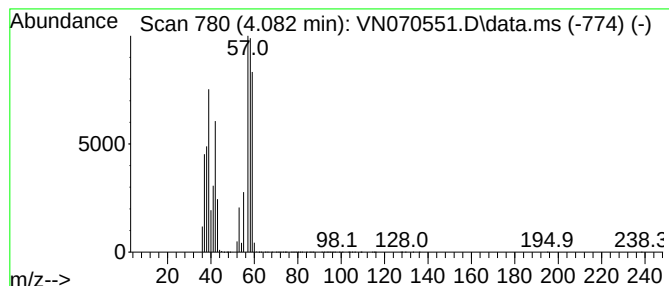
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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Peak Number 2 unknown4.082 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.082	146.11 ug/l	124985000	Pentafluorobenzene	8.083

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, (ethoxymethyl)-		102	C5H10O2		004016-11-9	9
2	Methylamine, N,N-dimethyl-		59	C3H9N		000075-50-3	7
3	2-Propen-1-ol		58	C3H6O		000107-18-6	4
4	Propanal		58	C3H6O		000123-38-6	4
5	Methylenecyclopropane		54	C4H6		006142-73-0	2



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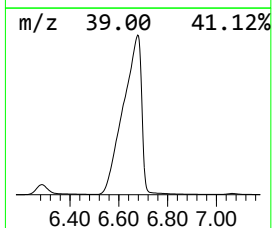
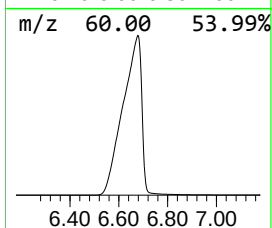
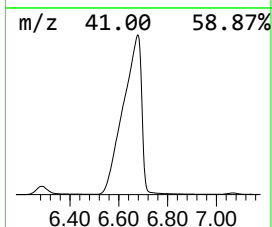
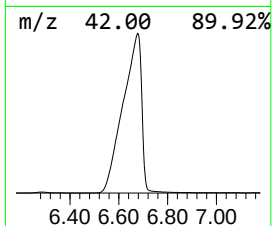
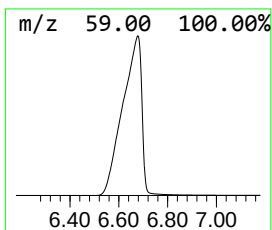
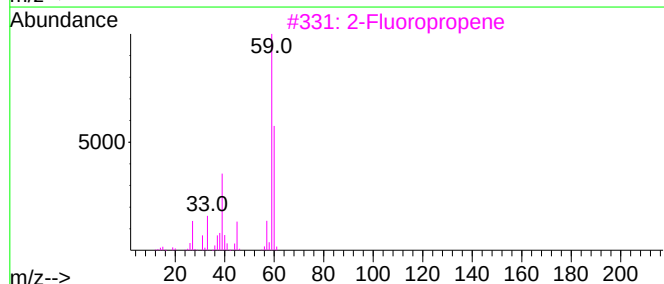
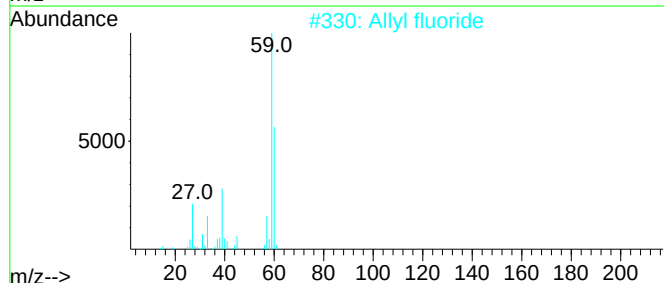
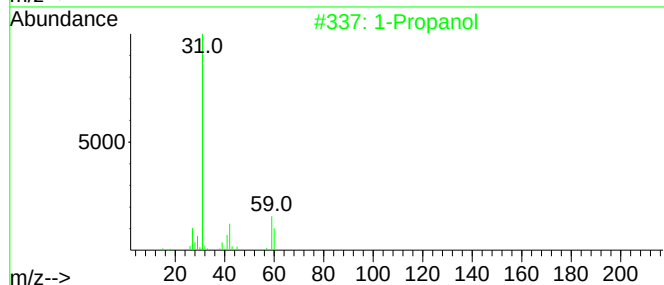
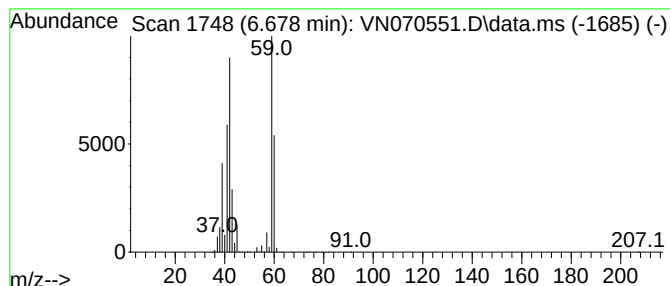
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Quant Title : SW846 8260

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Peak Number 3 1-Propanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.678	193.93 ug/l	165892000	Pentafluorobenzene	8.083

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Propanol	60	C3H8O	000071-23-8	64
2		Allyl fluoride	60	C3H5F	000818-92-8	32
3		2-Fluoropropene	60	C3H5F	001184-60-7	27
4		Cyclopropane	42	C3H6	000075-19-4	25
5		Formamidoxime	60	CH4N2O	000624-82-8	9



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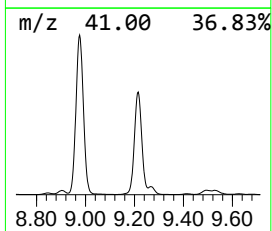
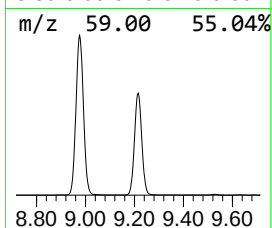
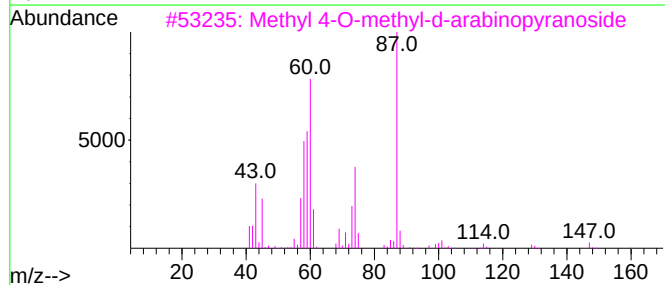
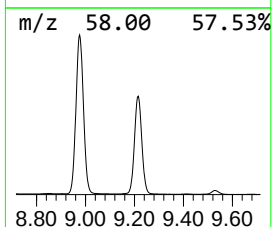
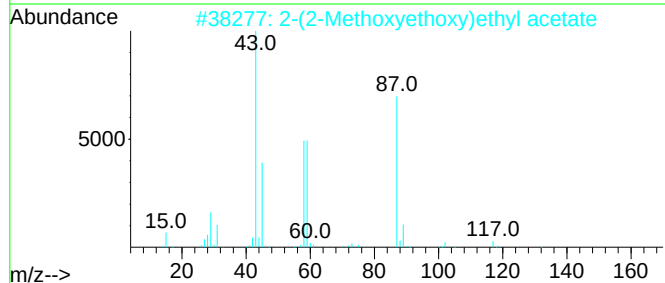
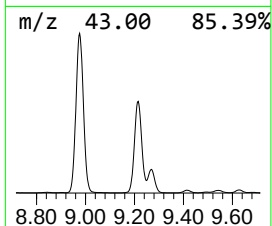
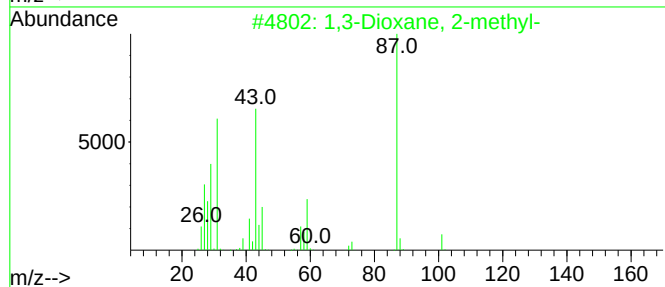
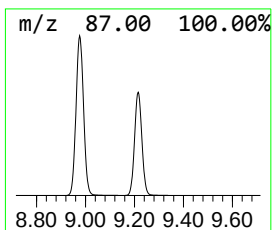
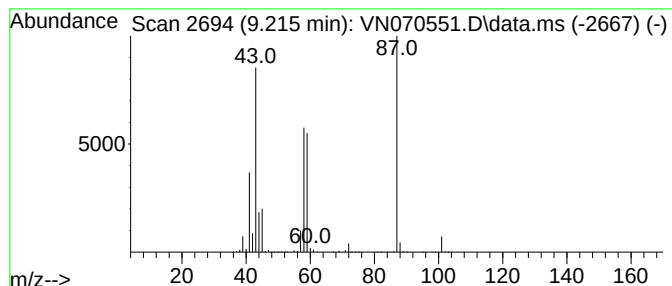
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 1,3-Dioxane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.215	26.47 ug/l	22640200	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	53
2			2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	39
3			Methyl 4-O-methyl-d-arabinopyran...	178	C7H14O5	1000129-79-9	38
4			Oxazolidin-2-one	87	C3H5NO2	000497-25-6	37
5			1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	37



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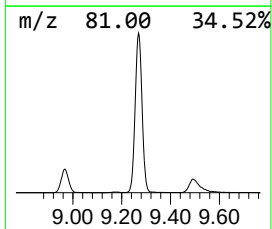
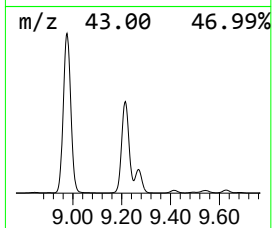
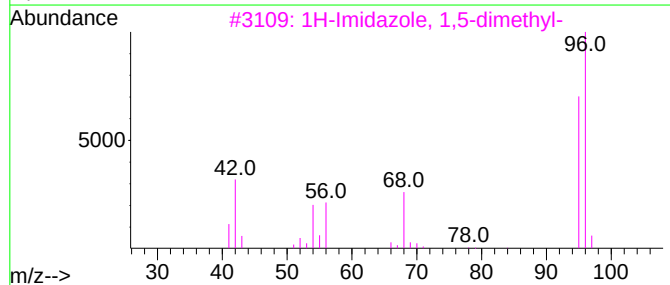
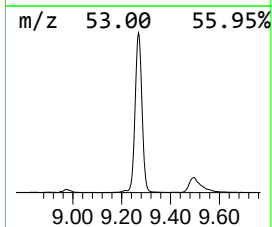
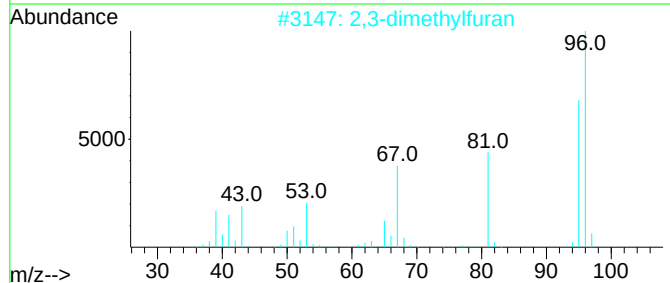
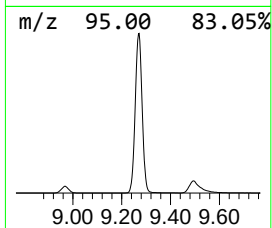
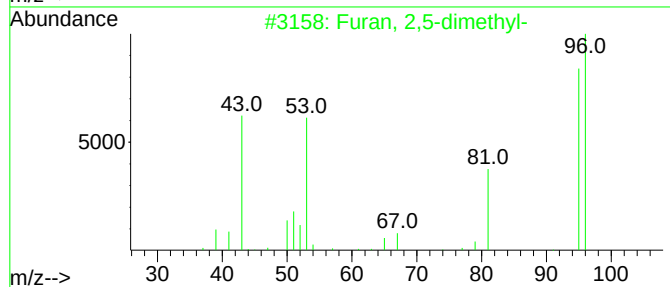
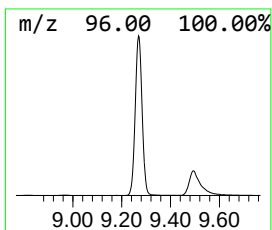
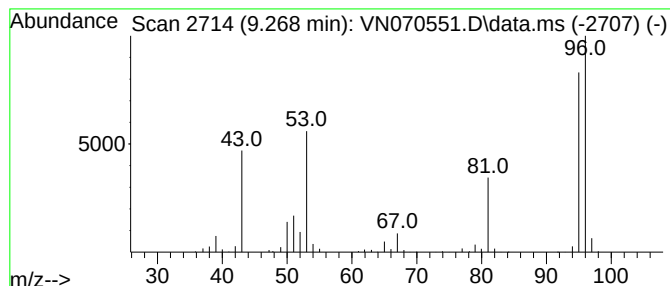
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Furan, 2,5-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.268	8.16 ug/l	6983910	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, 2,5-dimethyl-	96	C6H8O	000625-86-5	96
2			2,3-dimethylfuran	96	C6H8O	1000458-49-9	46
3			1H-Imidazole, 1,5-dimethyl-	96	C5H8N2	010447-93-5	38
4			1H-Pyrazole, 1,5-dimethyl-	96	C5H8N2	000694-31-5	38
5			1-Butyne, 3-methyl-	68	C5H8	000598-23-2	38



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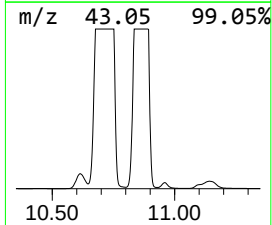
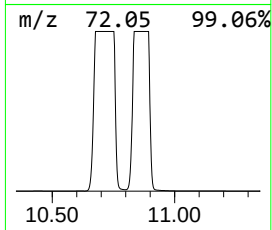
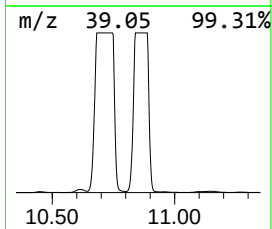
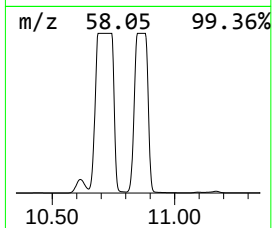
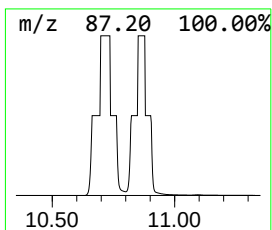
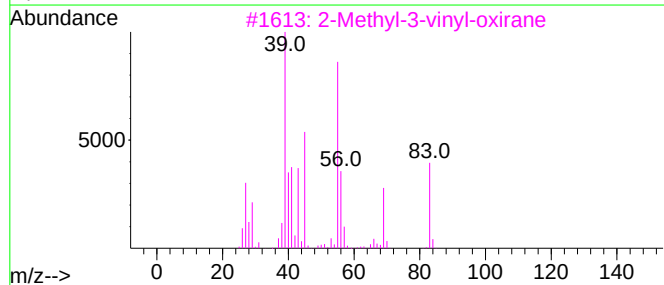
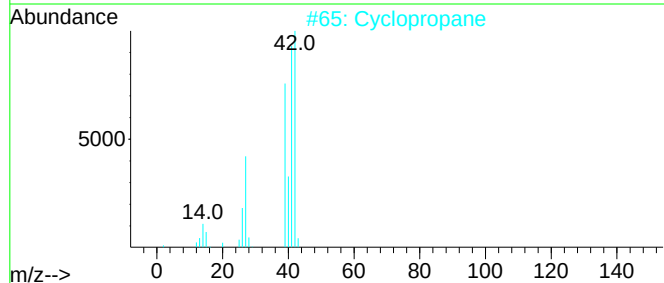
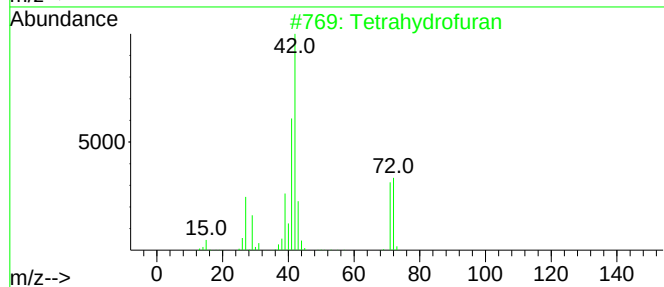
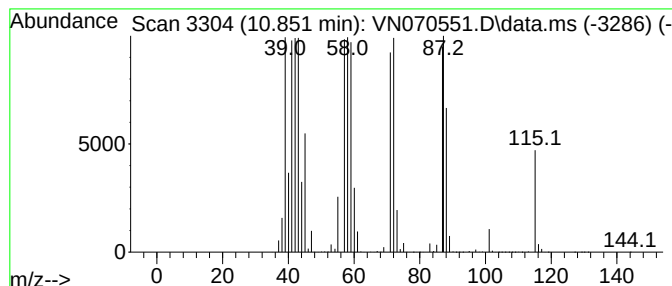
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown10.851 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.851	110.78 ug/l	384919000	Chlorobenzene-d5	11.744

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetrahydrofuran	72	C4H8O	000109-99-9	38
2			Cyclopropane	42	C3H6	000075-19-4	35
3			2-Methyl-3-vinyl-oxirane	84	C5H8O	006790-37-0	12
4			Ethane, isothiocyanato-	87	C3H5NS	000542-85-8	11
5			Propane, 2,2'-[methylenebis(oxy)...	160	C9H20O2	002568-93-6	10



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011022\
Data File : VN070551.D
Acq On : 10 Jan 2022 18:35
Operator : JC/MD
Sample : N1015-09
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31278

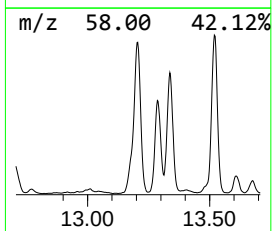
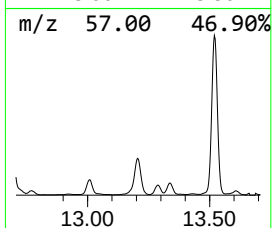
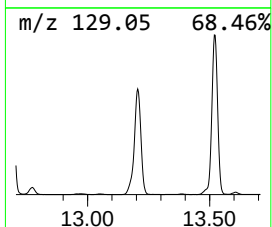
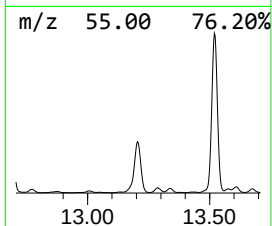
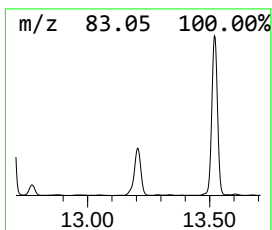
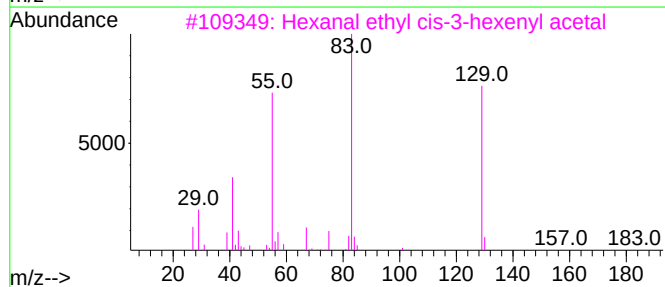
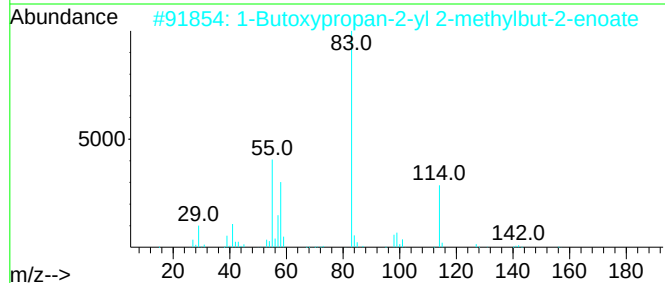
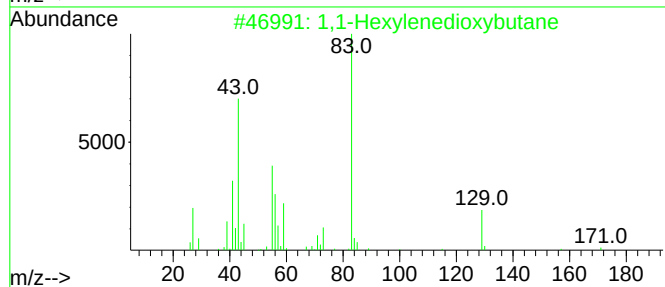
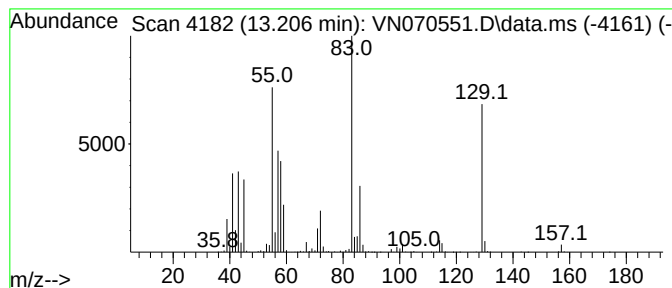
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Quant Title : SW846 8260

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

Peak Number 7 unknown13.206 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.206	49.50 ug/l	5437350	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,1-Hexylenedioxybutane	172	C10H20O2	1000249-77-4	43
2			1-Butoxypropan-2-yl 2-methylbut-...	214	C12H22O3	1000367-09-3	32
3			Hexanal ethyl cis-3-hexenyl acetal	228	C14H28O2	1000431-42-9	32
4			Cyclohexanecarboxylic acid, 2-me...	184	C11H20O2	037139-85-8	32
5			1,4-Pentadien-3-ol	84	C5H8O	000922-65-6	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011022\
Data File : VN070551.D
Acq On : 10 Jan 2022 18:35
Operator : JC/MD
Sample : N1015-09
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31278

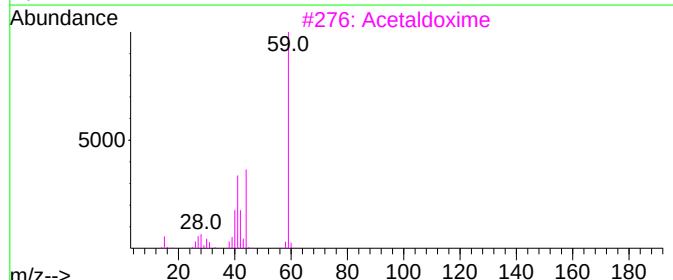
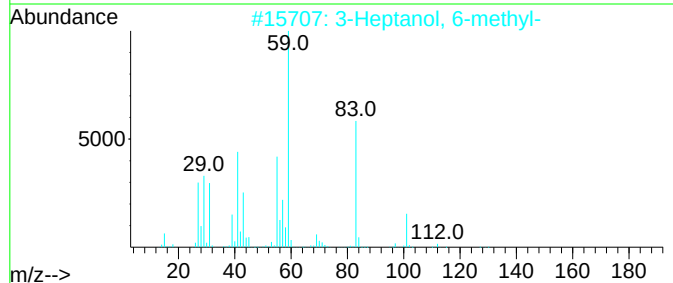
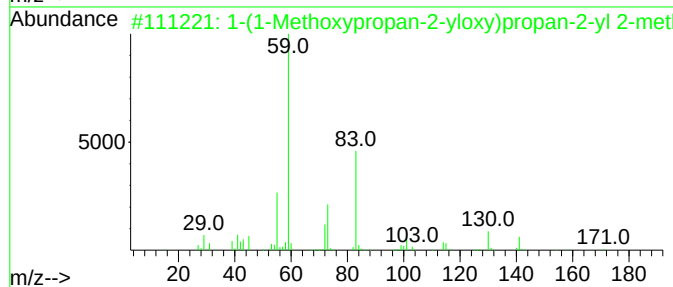
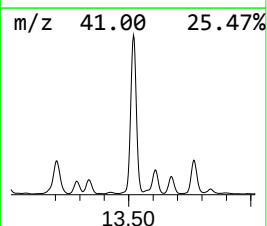
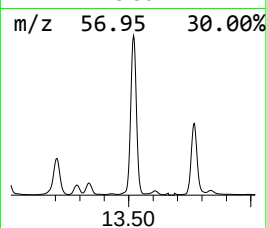
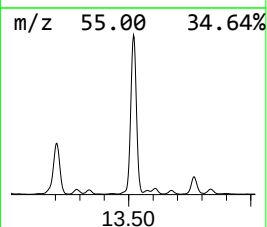
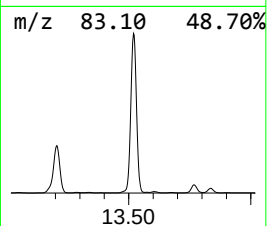
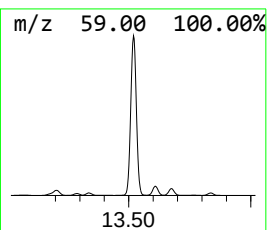
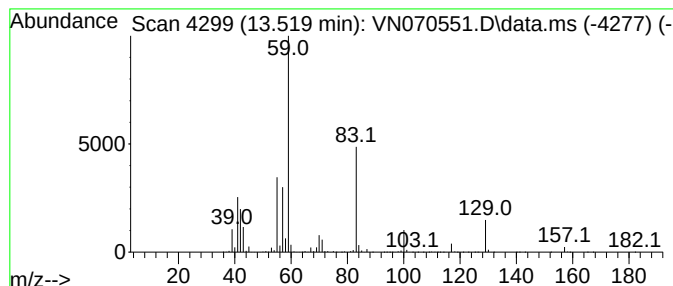
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Quant Title : SW846 8260

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

Peak Number 8 unknown13.519 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.519	162.39 ug/l	17839800	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(1-Methoxypropan-2-yloxy)propa...	230	C12H22O4	1000367-11-3	42		
2	3-Heptanol, 6-methyl-	130	C8H18O	018720-66-6	40		
3	Acetaldoxime	59	C2H5NO	000107-29-9	37		
4	6-Methyl-2-heptanol, methyl ether	144	C9H20O	1000365-52-0	32		
5	1-(1-Methoxypropan-2-yloxy)propa...	232	C12H24O4	1000367-11-4	32		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011022\
Data File : VN070551.D
Acq On : 10 Jan 2022 18:35
Operator : JC/MD
Sample : N1015-09
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31278

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	2.582	40.7	ug/l	34818900	1	8.083	42771200	50.0
unknown4.082	4.082	146.1	ug/l	124985000	1	8.083	42771200	50.0
1-Propanol	6.678	193.9	ug/l	165892000	1	8.083	42771200	50.0
1,3-Dioxane, 2-...	9.215	26.5	ug/l	22640200	2	8.968	42771200	50.0
Furan, 2,5-dime...	9.268	8.2	ug/l	6983910	2	8.968	42771200	50.0
unknown10.851	10.851	110.8	ug/l	384919000	3	11.744	173732000	50.0
unknown13.206	13.206	49.5	ug/l	5437350	4	13.672	5492750	50.0
unknown13.519	13.519	162.4	ug/l	17839800	4	13.672	5492750	50.0