

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011022\
 Data File : VN070549.D
 Acq On : 10 Jan 2022 17:44
 Operator : JC/MD
 Sample : N1015-04
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 20969

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: VN070549.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.585	205	222	280	rBV	12599721	23611795	6.67%	3.287%
2	4.100	749	787	790	rBV3	70402137	81156746	22.93%	11.297%
3	4.586	951	968	1025	rVB	1355136	5178715	1.46%	0.721%
4	6.729	1682	1767	1867	rBV3	52001764	353957564	100.00%	49.269%
5	7.340	1976	1995	2036	rVB	1527036	3986882	1.13%	0.555%
6	8.965	2587	2601	2627	rVB	2332648	4830677	1.36%	0.672%
7	9.531	2781	2812	2833	rVV4	1842664	4845194	1.37%	0.674%
8	10.441	3124	3151	3168	rBV3	3786893	7527632	2.13%	1.048%
9	10.604	3192	3212	3228	rBV3	39992415	73481568	20.76%	10.228%
10	10.682	3229	3241	3278	rVV	6759316	14526639	4.10%	2.022%
11	10.827	3279	3295	3328	rVV	4465855	8907226	2.52%	1.240%
12	11.090	3376	3393	3409	rBV	6257333	10345207	2.92%	1.440%
13	11.723	3608	3629	3668	rBV5	36667787	91650075	25.89%	12.757%
14	12.278	3820	3836	3857	rBV	2306974	4445013	1.26%	0.619%
15	12.728	3994	4004	4029	rVB	2150108	3905924	1.10%	0.544%
16	13.519	4277	4299	4323	rBV	13399145	22368488	6.32%	3.114%
17	13.672	4342	4356	4375	rBV	2094466	3691298	1.04%	0.514%

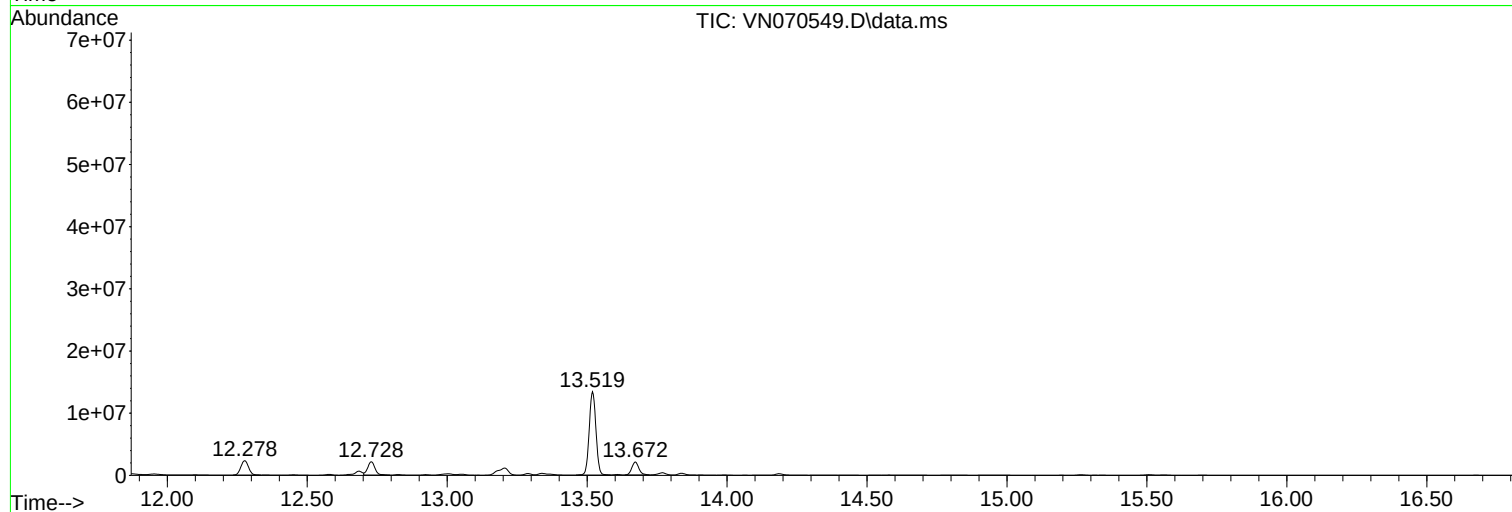
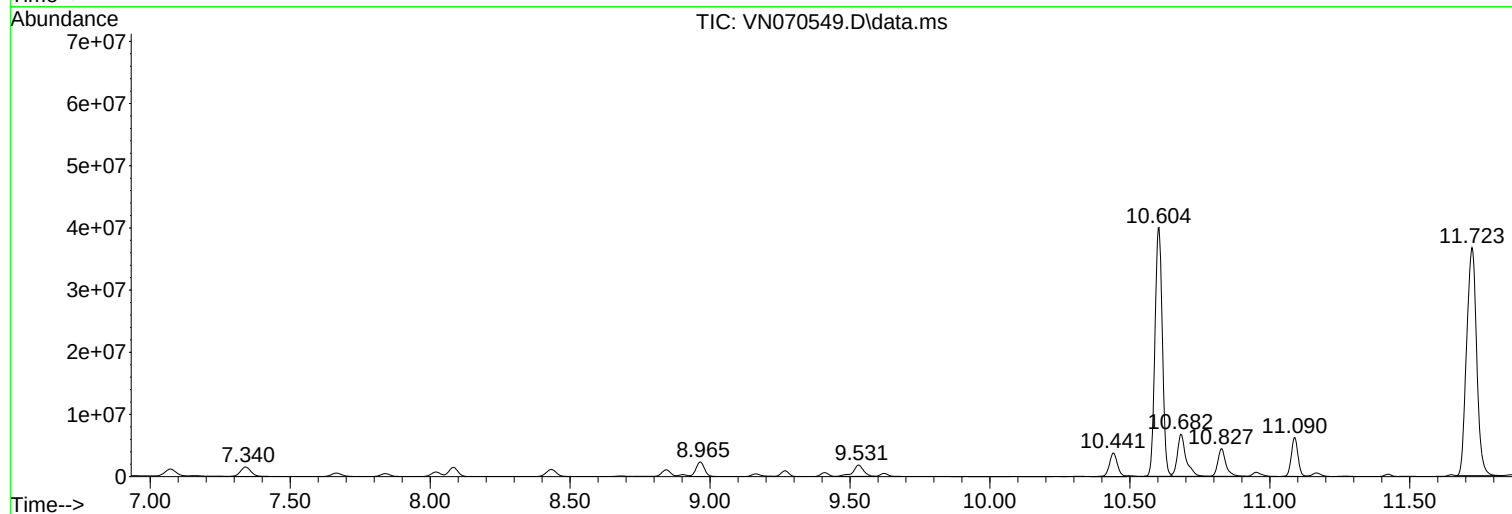
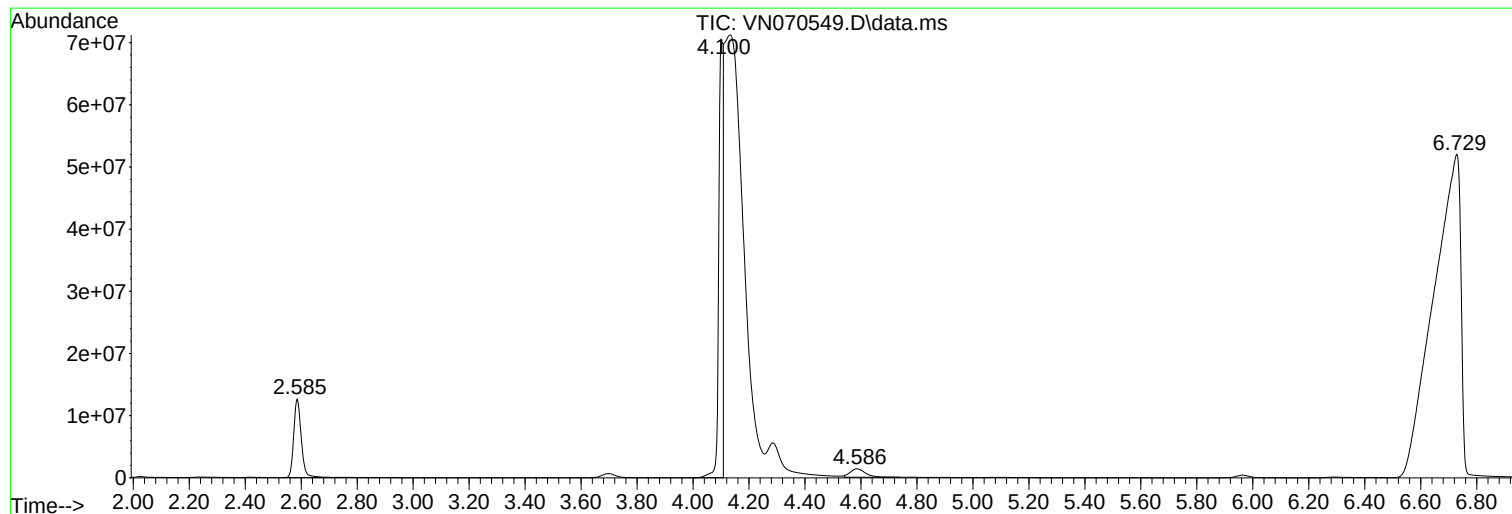
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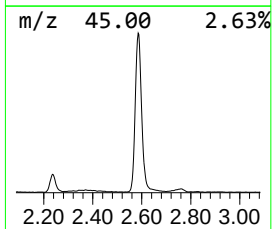
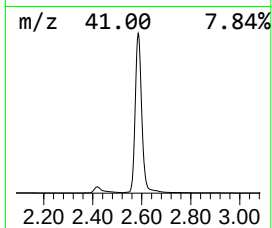
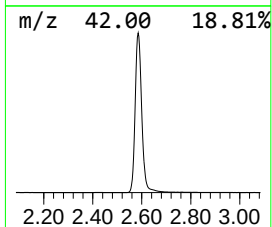
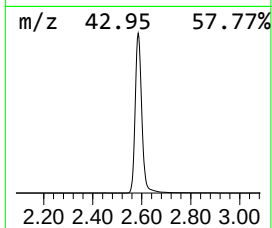
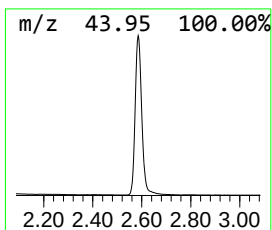
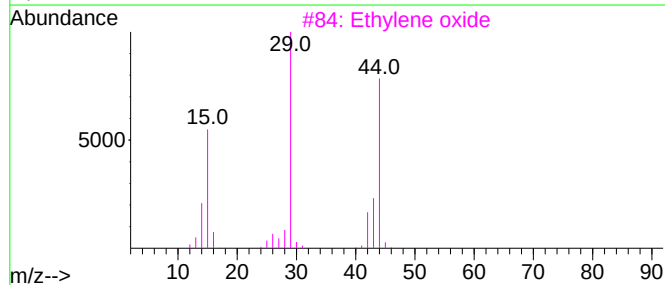
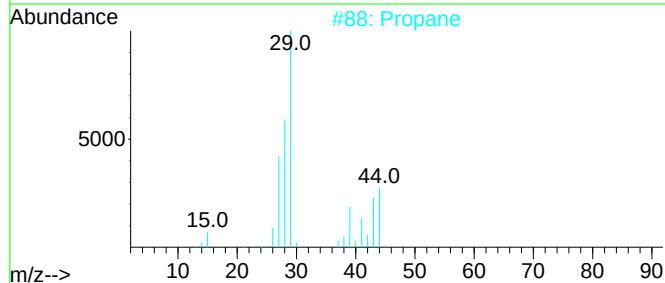
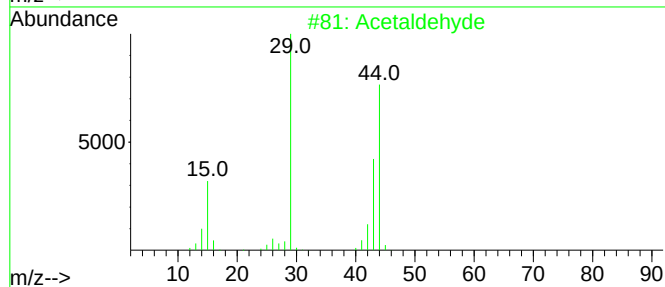
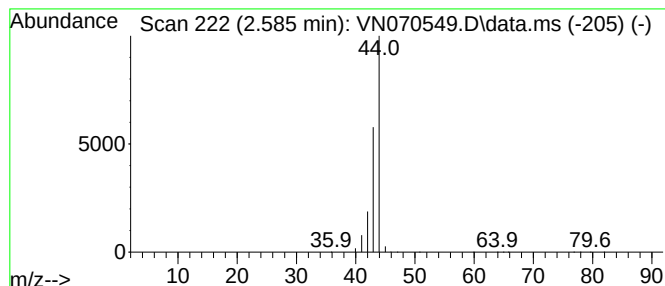
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Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.585	296.12 ug/l	23611800	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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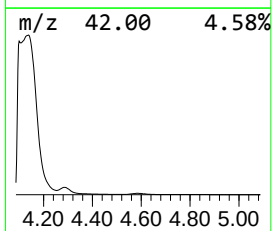
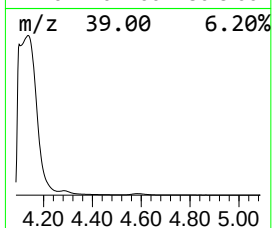
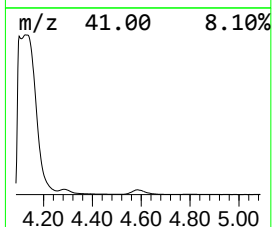
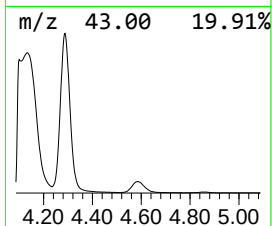
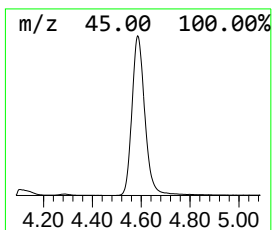
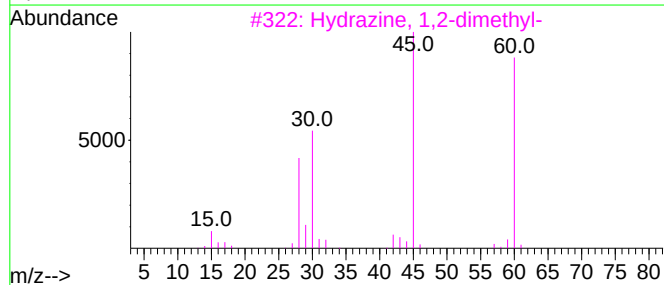
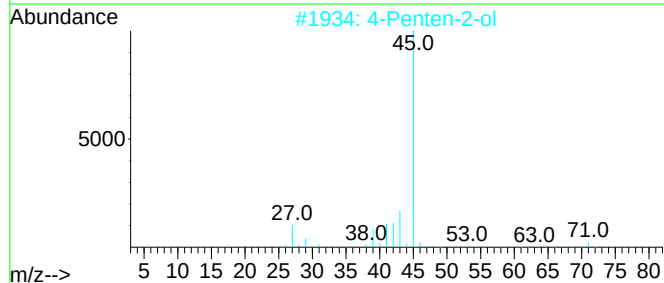
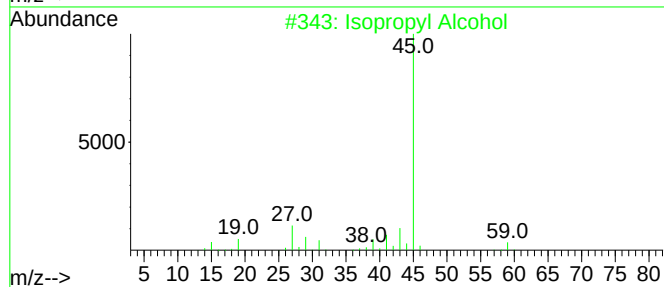
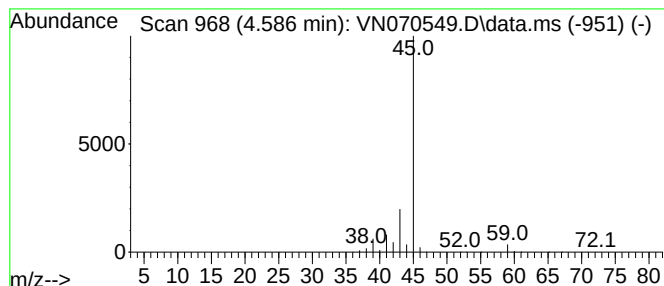
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 2 Isopropyl Alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.586	64.95 ug/l	5178720	Pentafluorobenzene	8.083

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	86
2			4-Penten-2-ol	86	C5H10O	000625-31-0	9
3			Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
4			Formamide	45	CH3NO	000075-12-7	5
5			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	4



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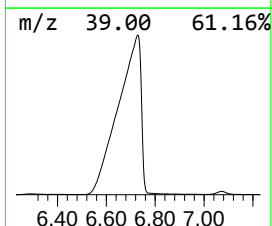
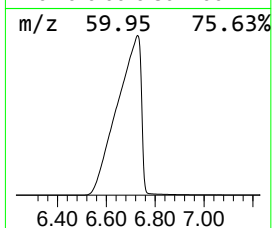
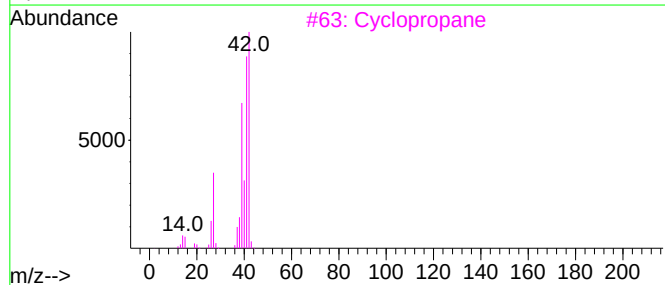
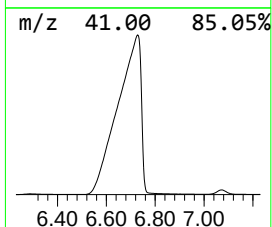
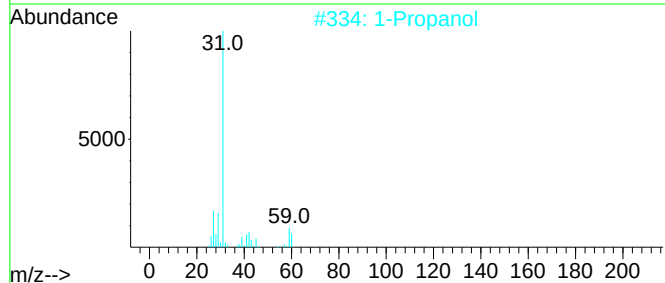
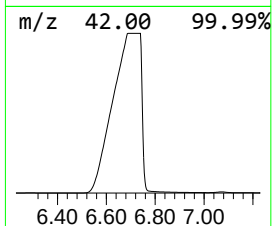
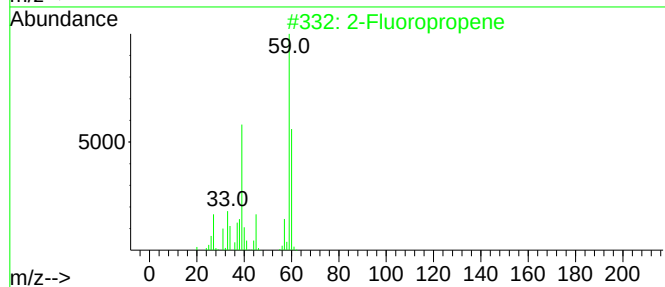
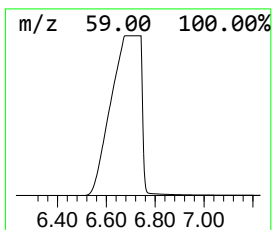
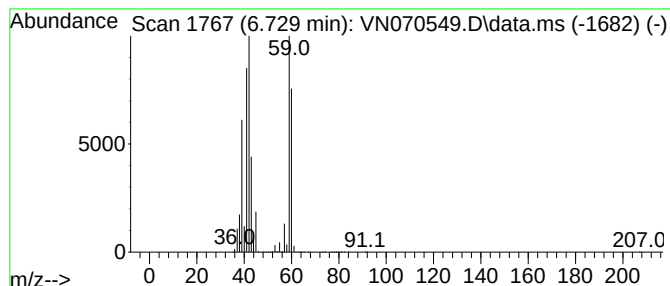
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Fluoropropene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.729	4439.03 ug/l	353958000	Pentafluorobenzene	8.083

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Fluoropropene	60	C3H5F	001184-60-7	53
2			1-Propanol	60	C3H8O	000071-23-8	50
3			Cyclopropane	42	C3H6	000075-19-4	38
4			Formamidoxime	60	CH4N2O	000624-82-8	35
5			Propene	42	C3H6	000115-07-1	25



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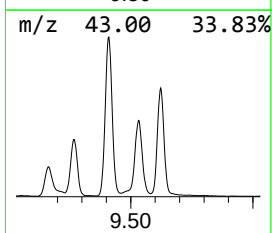
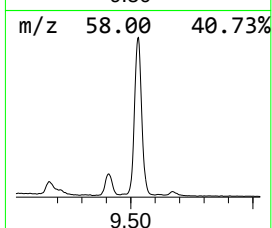
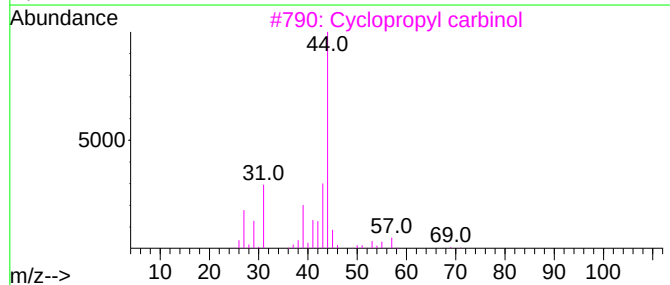
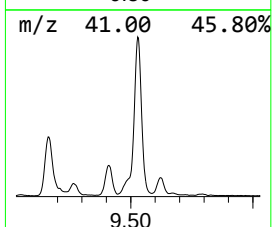
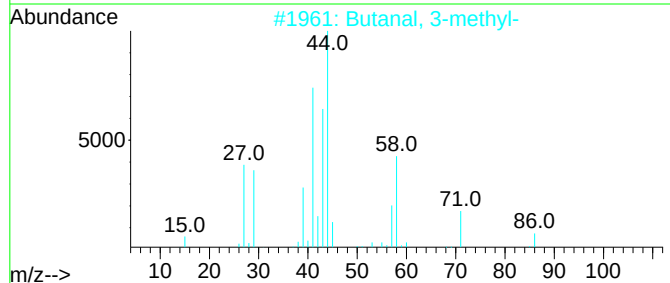
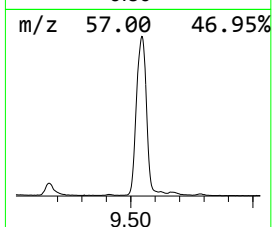
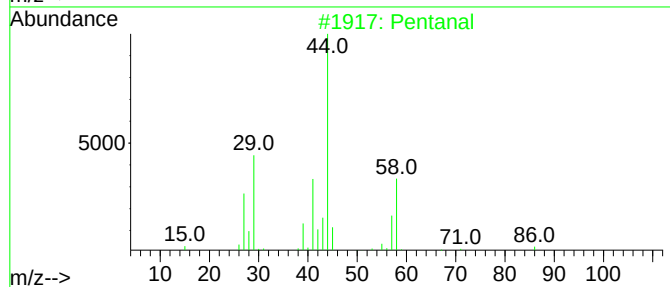
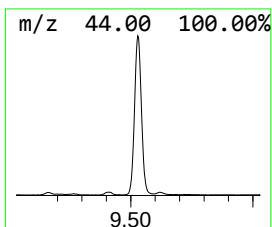
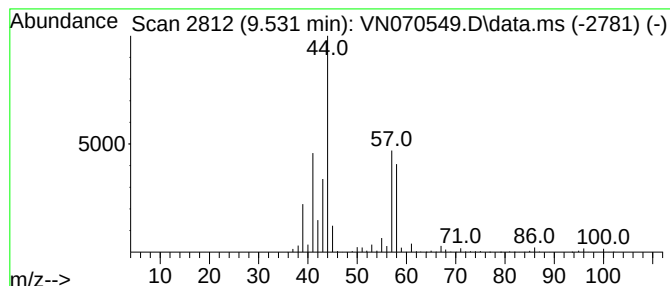
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Peak Number 4 Pentanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.531	50.15 ug/l	4845190	1,4-Difluorobenzene	8.965

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanal	86	C5H10O	000110-62-3	86
2			Butanal, 3-methyl-	86	C5H10O	000590-86-3	64
3			Cyclopropyl carbinol	72	C4H8O	002516-33-8	47
4			Carbonic acid, ethyl 2-propenyl ...	130	C6H10O3	001469-70-1	10
5			Cyclobutanol	72	C4H8O	002919-23-5	9



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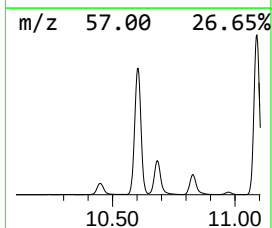
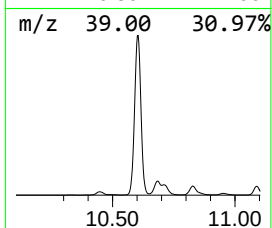
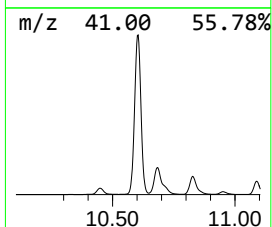
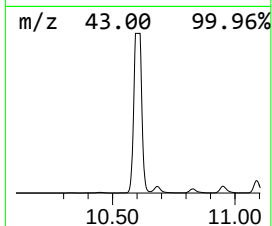
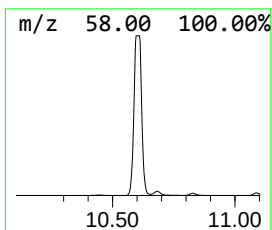
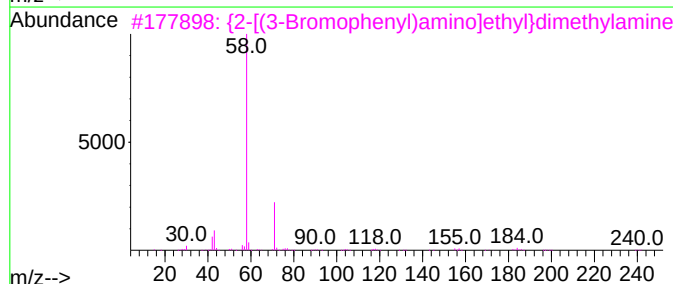
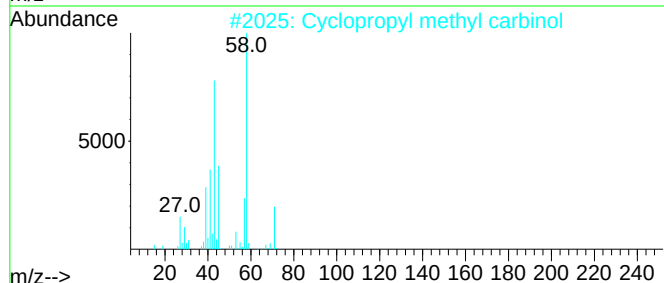
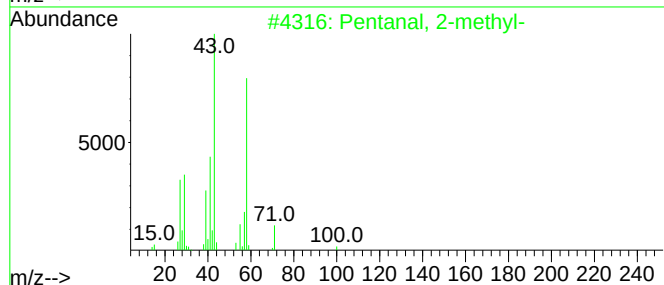
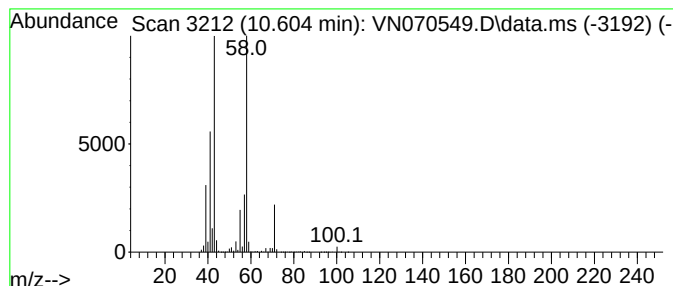
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Quant Title : SW846 8260

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

Peak Number 5 Pentanal, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.604	40.09 ug/l	73481600	Chlorobenzene-d5	11.741

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanal, 2-methyl-	100	C6H12O	000123-15-9	83
2			Cyclopropyl methyl carbinol	86	C5H10O	000765-42-4	64
3			{2-[(3-Bromophenyl)amino]ethyl}d...	284	C12H17BrN2O	1010506-64-8	45
4			Pentane, 1-(2-propenyloxy)-	128	C8H16O	023186-70-1	40
5			[2-(3-Bromophenoxy)ethyl]dimethy...	243	C10H14BrNO	221915-84-0	40



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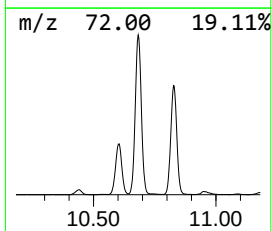
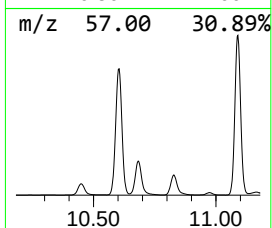
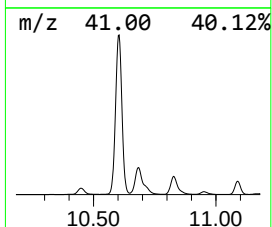
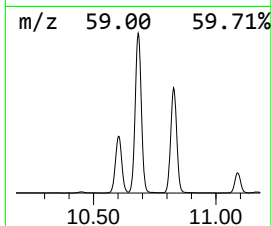
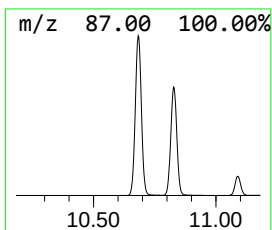
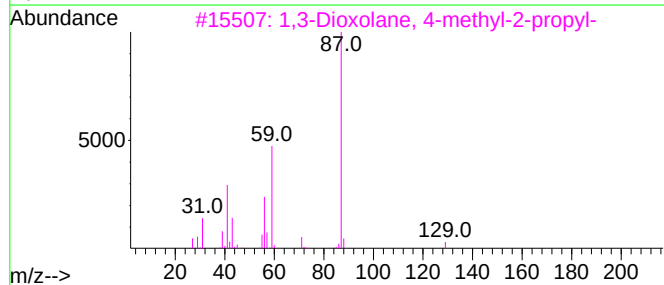
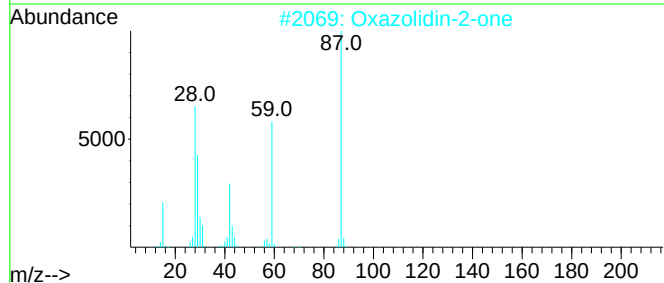
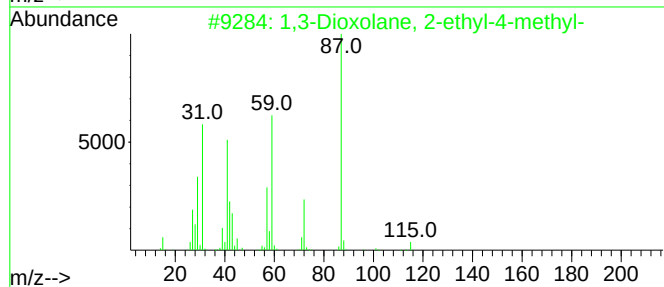
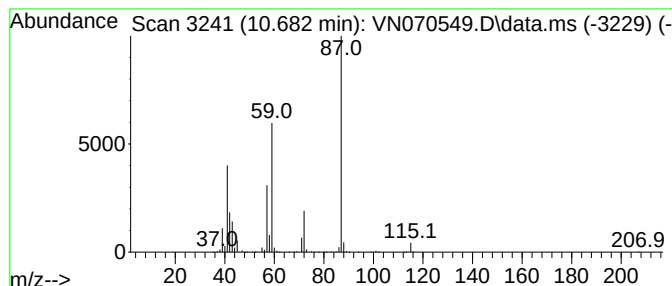
Instrument :
MSVOA_N
ClientSampleId :
20969

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

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

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.682	7.93 ug/l	14526600	Chlorobenzene-d5		11.741	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-ethyl-4-methyl-		116	C6H12O2	004359-46-0	91
2	Oxazolidin-2-one		87	C3H5NO2	000497-25-6	64
3	1,3-Dioxolane, 4-methyl-2-propyl-		130	C7H14O2	004352-99-2	64
4	Acetamide, N-ethyl-		87	C4H9NO	000625-50-3	53
5	2-Propanone, O-methyloxime		87	C4H9NO	003376-35-0	52



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011022\
Data File : VN070549.D
Acq On : 10 Jan 2022 17:44
Operator : JC/MD
Sample : N1015-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
20969

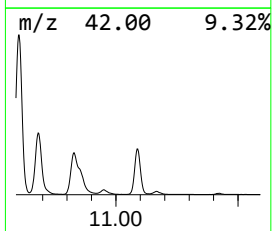
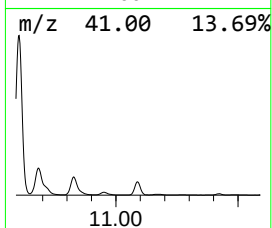
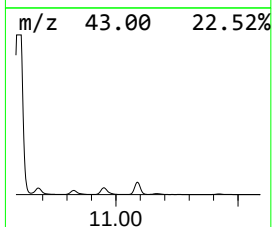
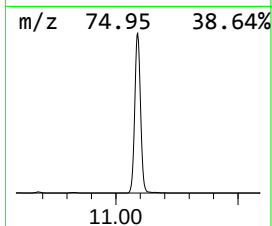
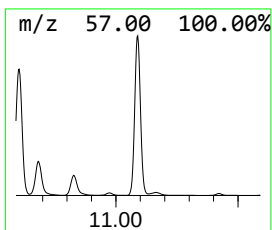
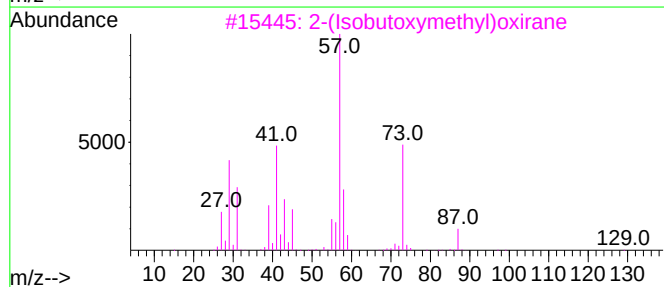
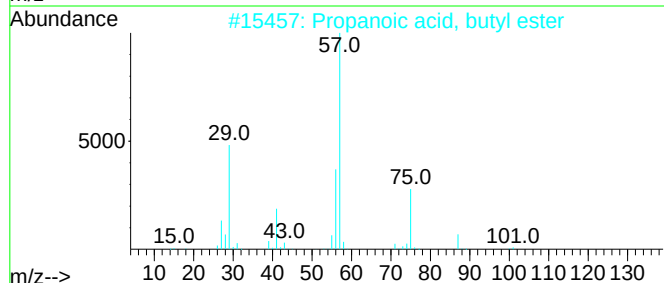
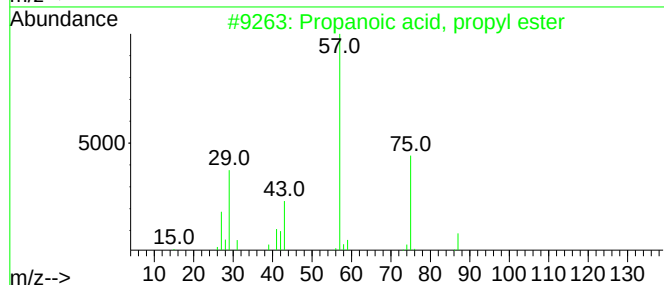
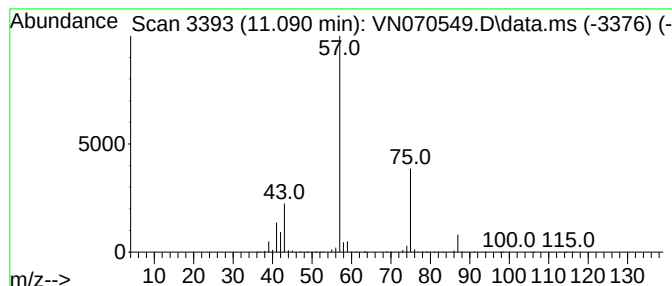
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Quant Title : SW846 8260

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

Peak Number 7 Propanoic acid, propyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.090	5.64 ug/l	10345200	Chlorobenzene-d5	11.741

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
2			Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	25
3			2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9
4			1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	7
5			1-Penten-3-ol	86	C5H10O	000616-25-1	4



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011022\
Data File : VN070549.D
Acq On : 10 Jan 2022 17:44
Operator : JC/MD
Sample : N1015-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
20969

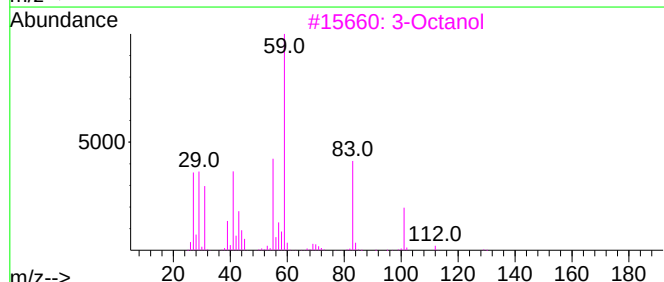
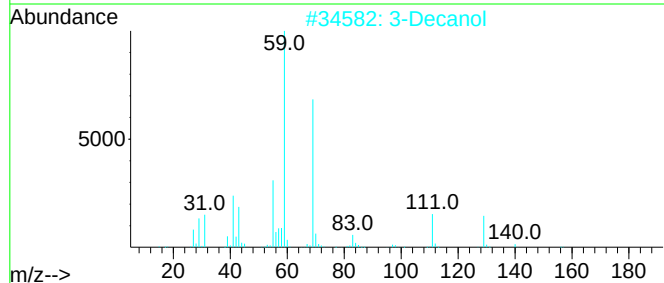
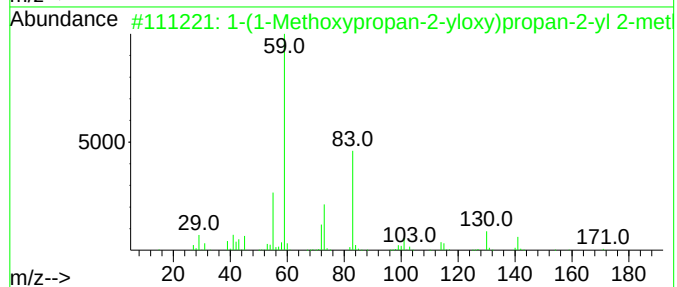
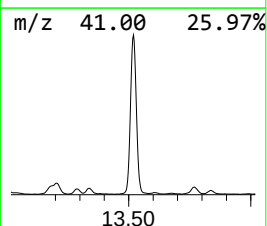
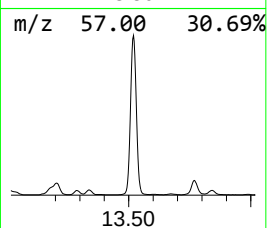
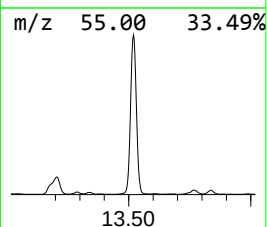
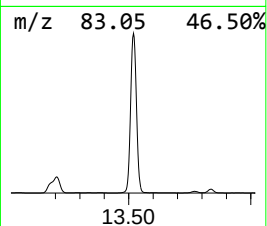
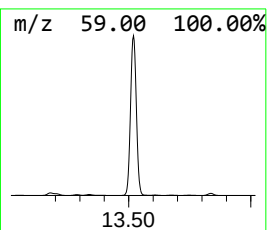
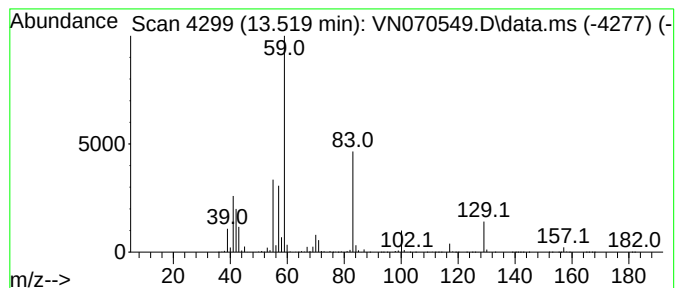
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 8 unknown13.519 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.519	302.99 ug/l	22368500	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	45		
2	3-Decanol	158	C10H22O	001565-81-7	43		
3	3-Octanol	130	C8H18O	000589-98-0	42		
4	3-Heptanol, 6-methyl-	130	C8H18O	018720-66-6	36		
5	1-(1-Methoxypropan-2-yloxy)propa...	232	C12H24O4	1000367-11-4	32		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011022\
Data File : VN070549.D
Acq On : 10 Jan 2022 17:44
Operator : JC/MD
Sample : N1015-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
20969

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	2.585	296.1	ug/l	23611800	1	8.083	3986880	50.0
Isopropyl Alcohol	4.586	65.0	ug/l	5178720	1	8.083	3986880	50.0
2-Fluoropropene	6.729	4439.0	ug/l	353958000	1	8.083	3986880	50.0
Pentanal	9.531	50.1	ug/l	4845190	2	8.965	4830680	50.0
Pentanal, 2-met...	10.604	40.1	ug/l	73481600	3	11.741	91650100	50.0
1,3-Dioxolane, ...	10.682	7.9	ug/l	14526600	3	11.741	91650100	50.0
Propanoic acid,...	11.090	5.6	ug/l	10345200	3	11.741	91650100	50.0
unknown13.519	13.519	303.0	ug/l	22368500	4	13.672	3691300	50.0