

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062922\
 Data File : VN073239.D
 Acq On : 29 Jun 2022 13:41
 Operator : JC\MD
 Sample : N3504-03
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TRE-1615

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\82N062822W.M

Title : SW846 8260

Signal : TIC: VN073239.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.387	84	85	152	rBV	43014520	391209108	47.04%	27.048%
2	4.210	276	395	396	rBV2	32021041	831603015	100.00%	57.497%
3	4.869	486	507	553	rVB	3945258	12787191	1.54%	0.884%
4	5.551	603	623	669	rBV	9716043	37990208	4.57%	2.627%
5	6.669	790	813	854	rBV	1606849	8670003	1.04%	0.599%
6	6.998	856	869	899	rVB	4441172	15104191	1.82%	1.044%
7	7.363	911	931	960	rBV	12171813	40001095	4.81%	2.766%
8	8.198	1061	1073	1091	rBV	5230894	15733725	1.89%	1.088%
9	8.810	1164	1177	1188	rBV	4200784	16858922	2.03%	1.166%
10	9.157	1221	1236	1260	rBV	10109717	31436712	3.78%	2.174%
11	12.080	1722	1733	1742	rBV	8683822	14650262	1.76%	1.013%
12	13.710	2002	2010	2017	rVB	7135217	11328530	1.36%	0.783%
13	14.074	2064	2072	2082	rBV	12018380	18972231	2.28%	1.312%

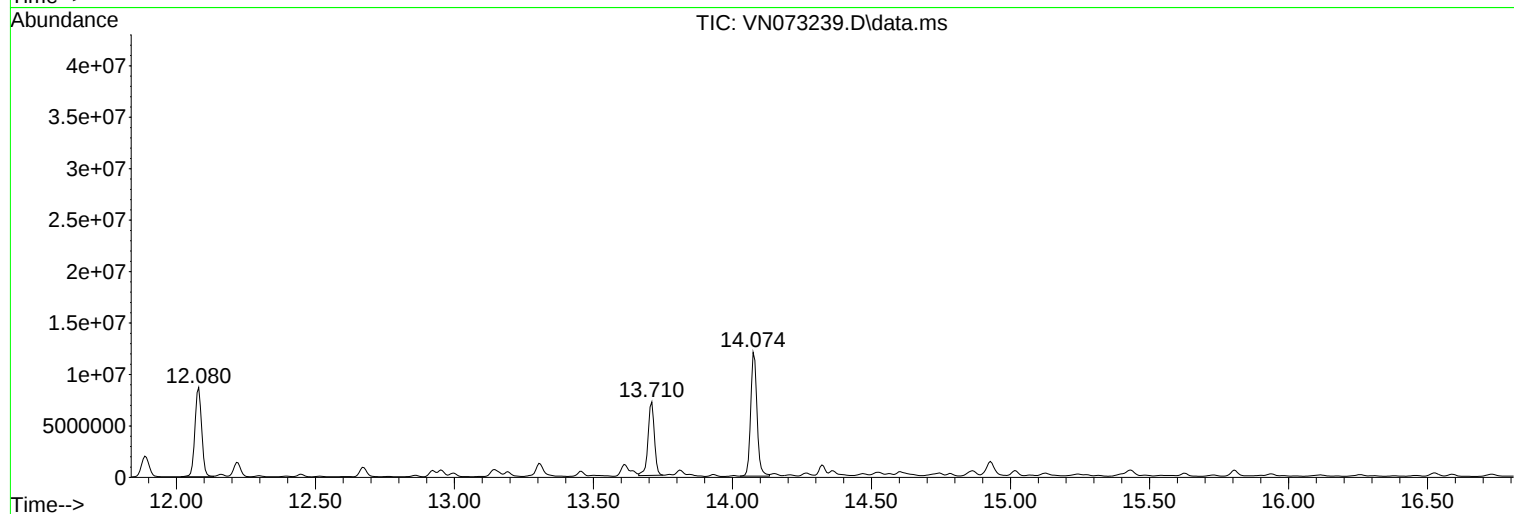
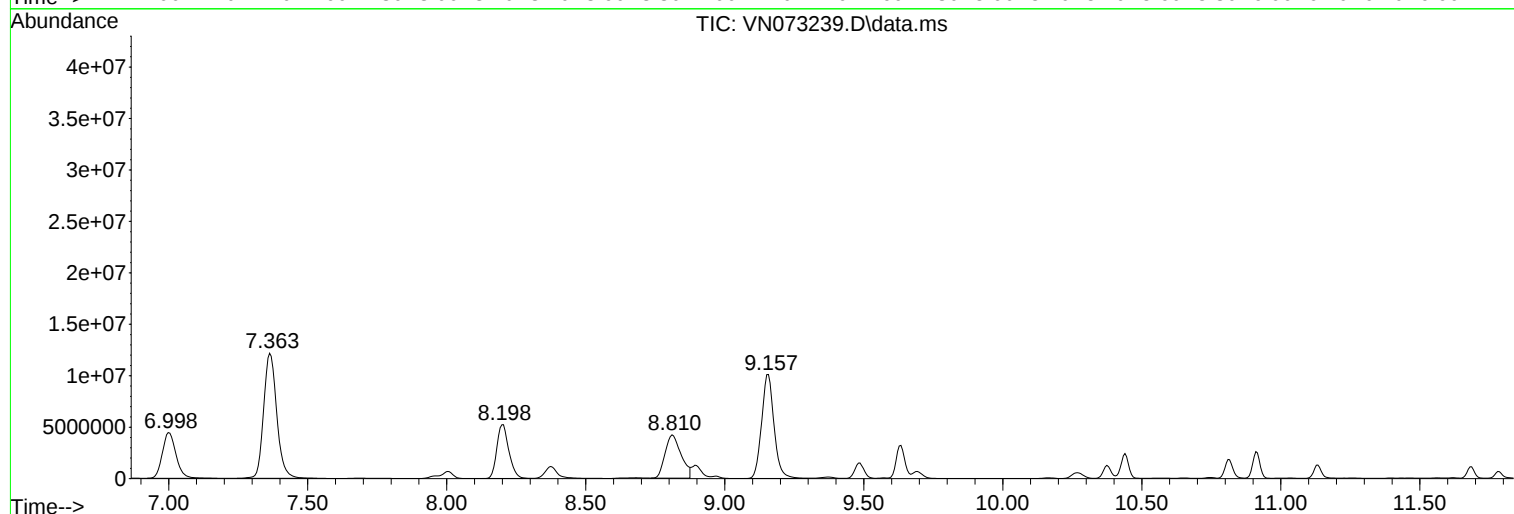
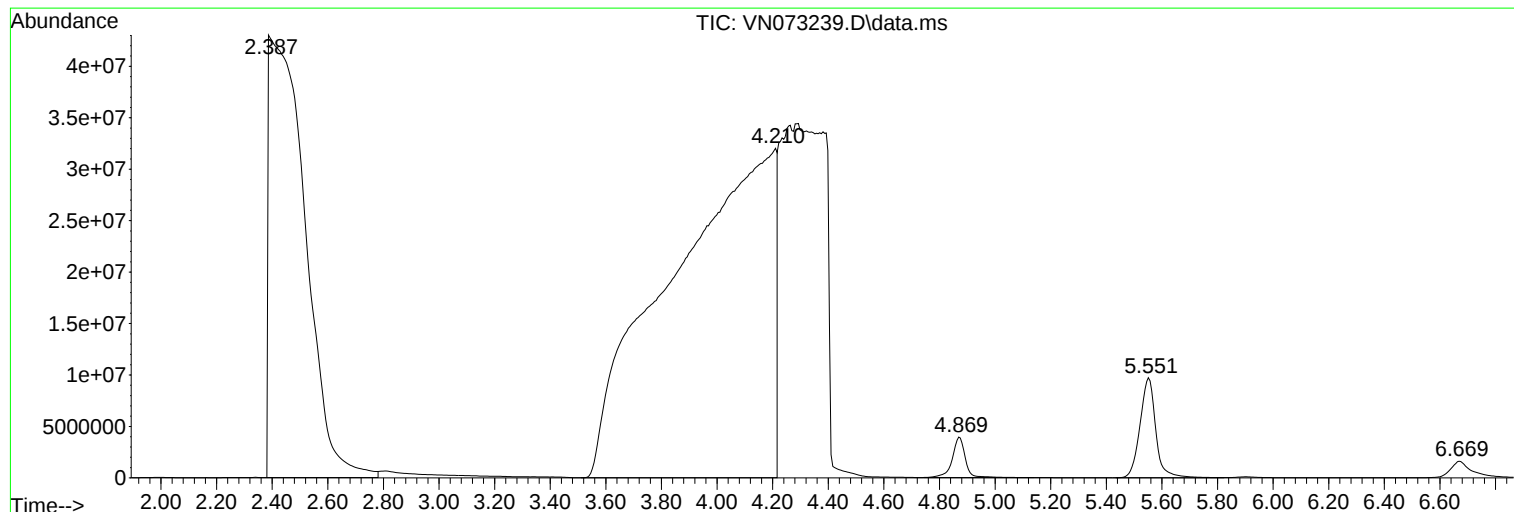
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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



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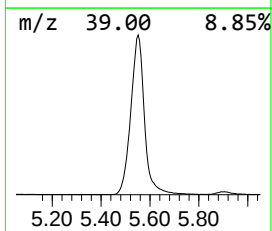
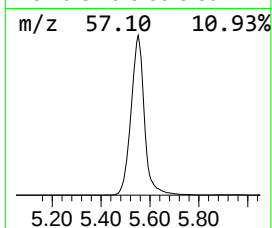
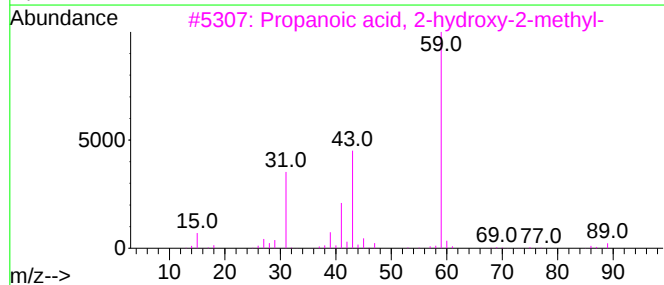
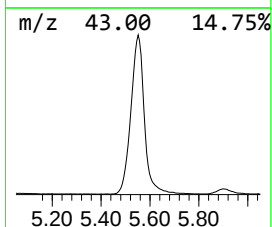
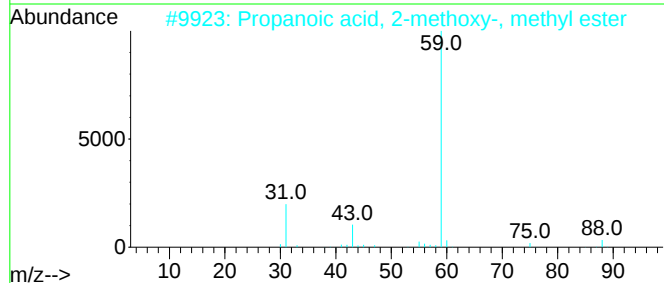
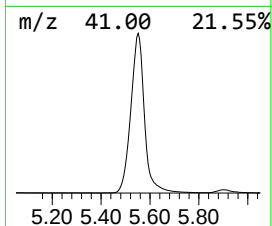
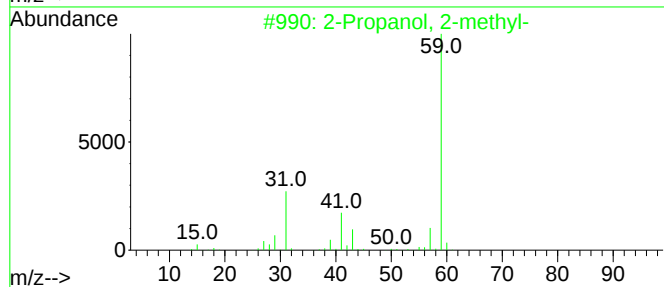
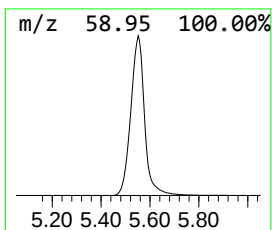
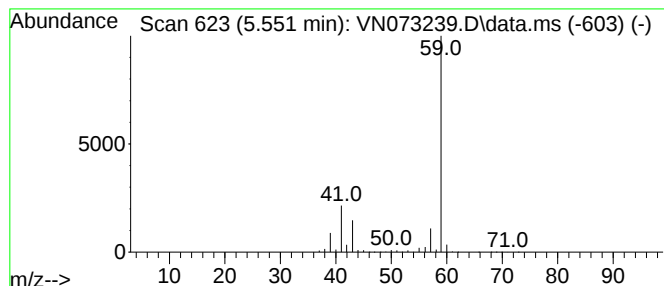
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Quant Title : SW846 8260

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

Peak Number 3 2-Propanol, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.551	120.73 ug/l	37990200	Pentafluorobenzene	8.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 2-methyl-			74	C4H10O	000075-65-0	74
2	Propanoic acid, 2-methoxy-, meth...			118	C5H10O3	017639-76-8	9
3	Propanoic acid, 2-hydroxy-2-methyl-			104	C4H8O3	000594-61-6	9
4	4-Hydroxy-3-hexanone			116	C6H12O2	004984-85-4	9
5	Formamide, N-methyl-			59	C2H5NO	000123-39-7	5



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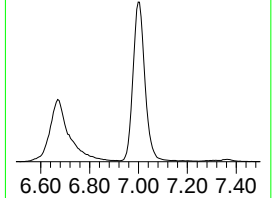
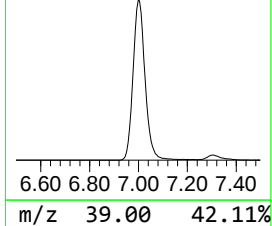
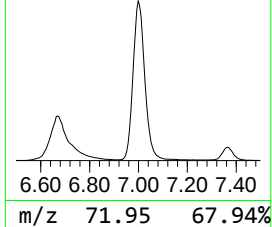
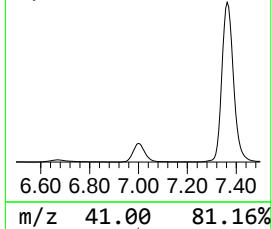
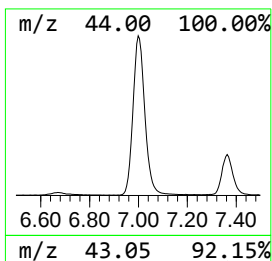
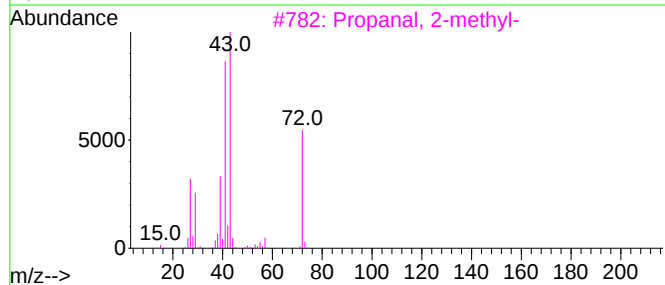
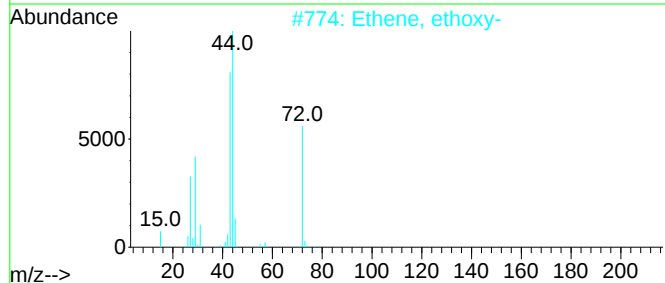
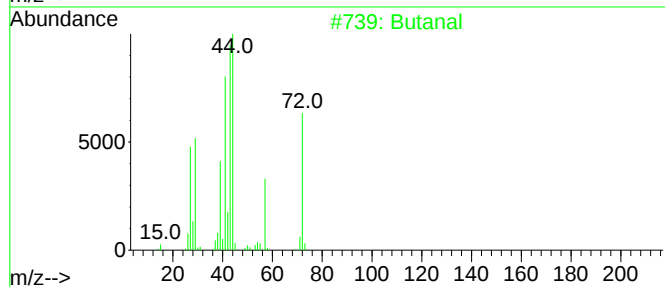
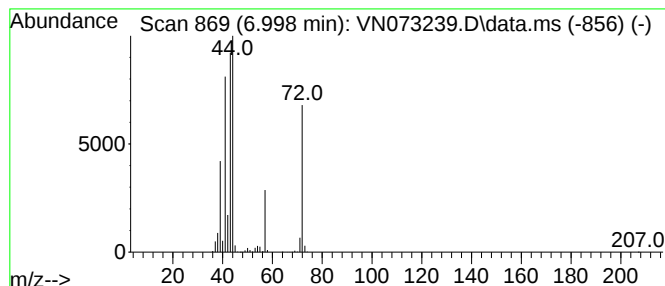
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Quant Title : SW846 8260

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Peak Number 4 Butanal Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.998	48.00 ug/l	15104200	Pentafluorobenzene	8.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	94
2			Ethene, ethoxy-	72	C4H8O	000109-92-2	52
3			Propanal, 2-methyl-	72	C4H8O	000078-84-2	52
4			2-Propen-1-ol, 2-methyl-, acetate	114	C6H10O2	000820-71-3	25
5			Isobutylene epoxide	72	C4H8O	000558-30-5	22



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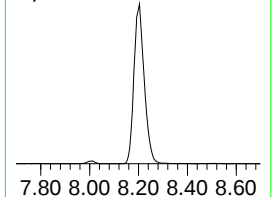
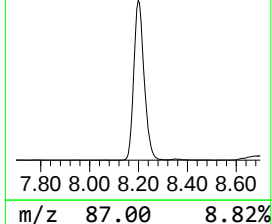
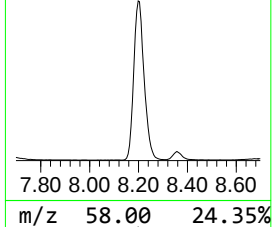
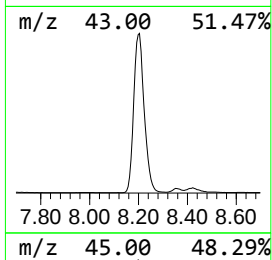
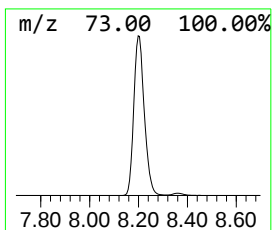
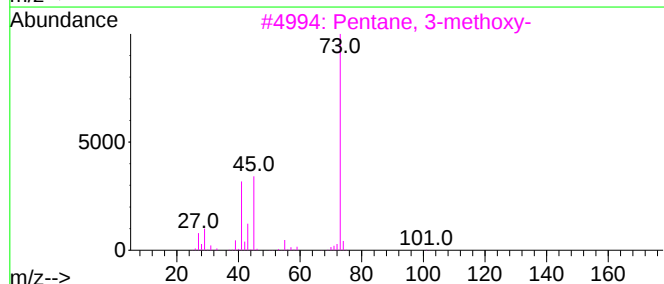
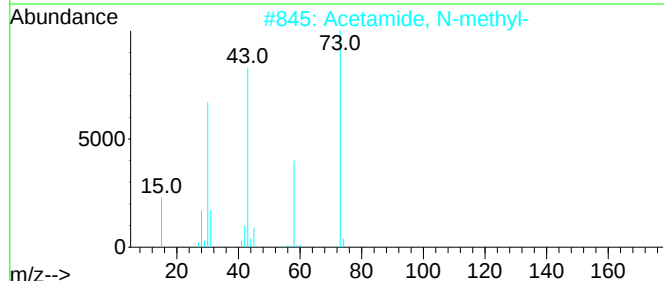
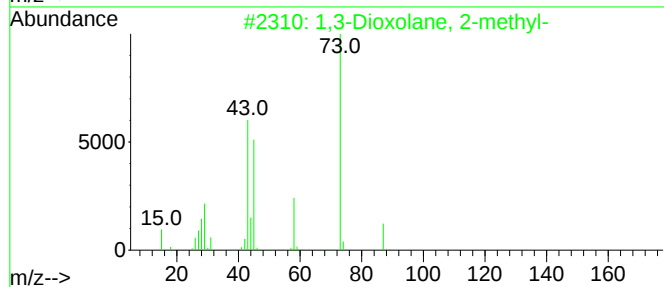
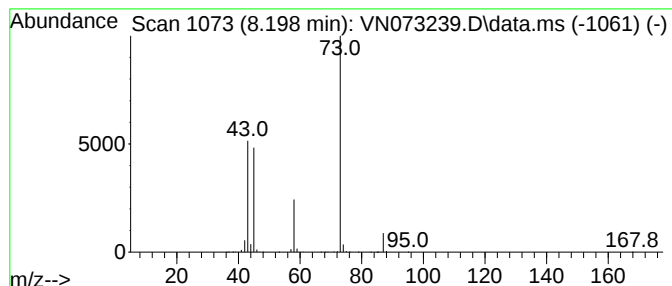
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 1,3-Dioxolane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.198	50.00 ug/l	15733700	Pentafluorobenzene	8.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	91
2			Acetamide, N-methyl-	73	C3H7NO	000079-16-3	35
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	28
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5			Acetone	58	C3H6O	000067-64-1	9



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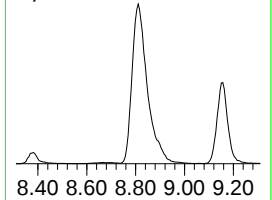
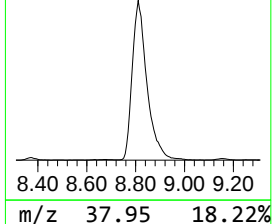
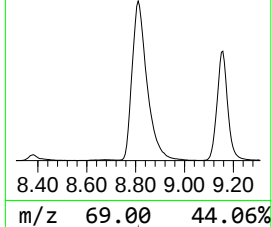
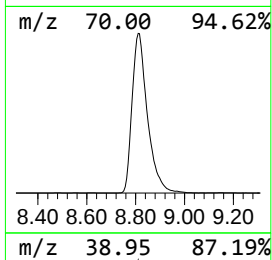
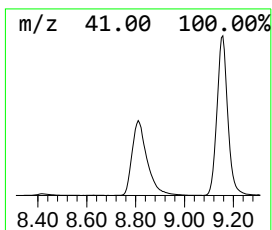
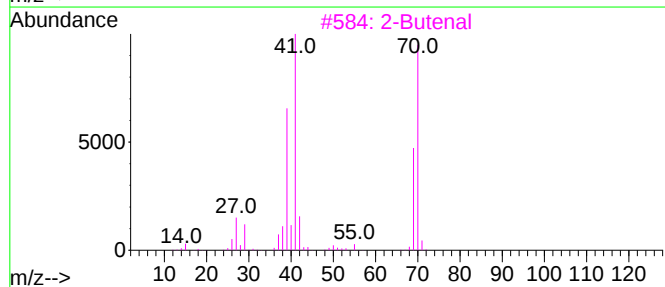
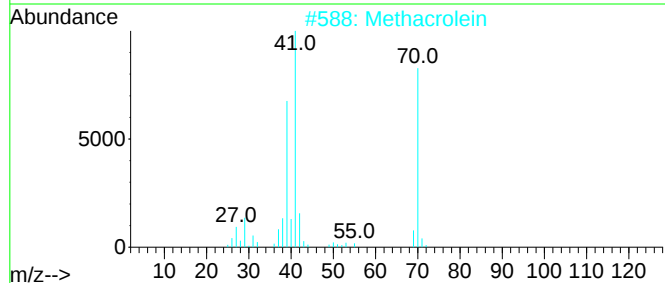
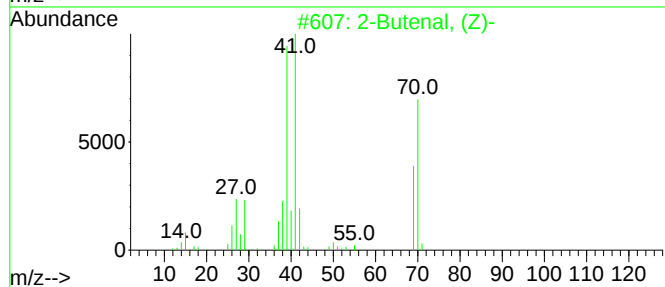
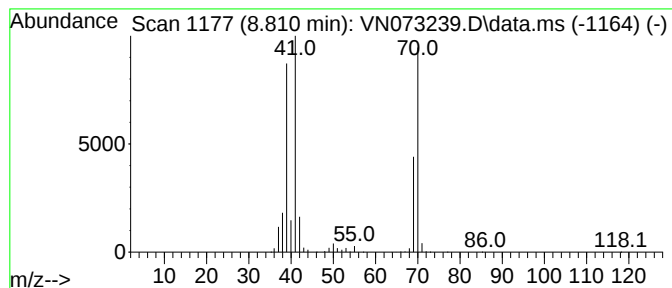
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Peak Number 6 2-Butenal, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.810	50.00 ug/l	16858900	1,4-Difluorobenzene	8.898

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenal, (Z)-	70	C4H6O	015798-64-8	91	
2	Methacrolein	70	C4H6O	000078-85-3	91	
3	2-Butenal	70	C4H6O	004170-30-3	91	
4	2-Butenal, (E)-	70	C4H6O	000123-73-9	91	
5	Furan, 2,3-dihydro-	70	C4H6O	001191-99-7	90	



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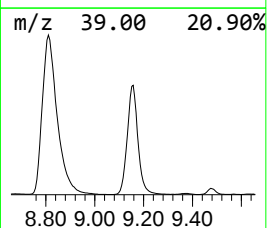
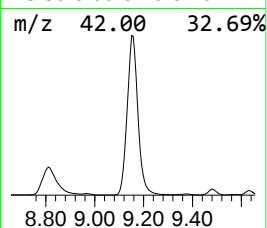
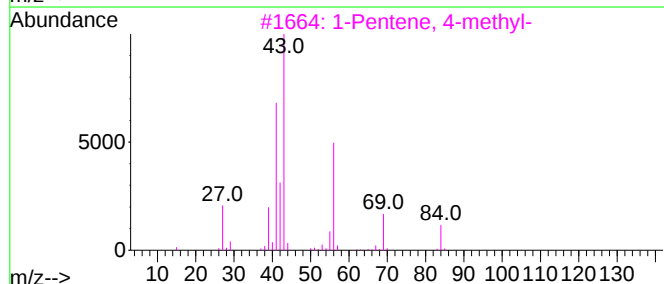
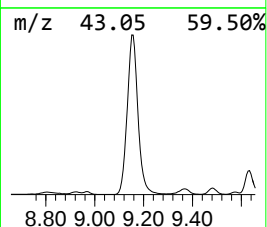
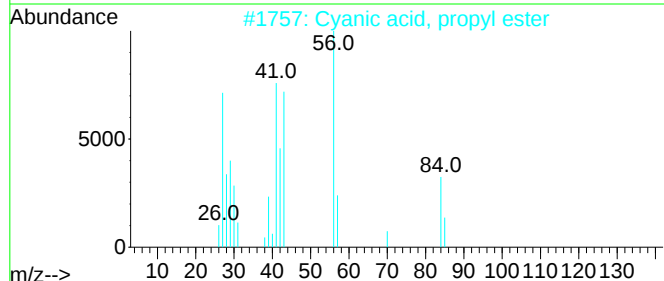
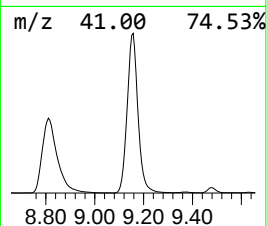
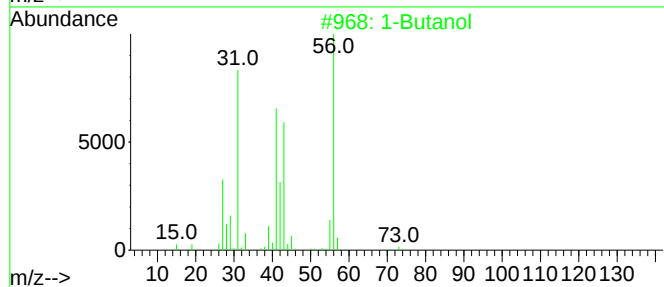
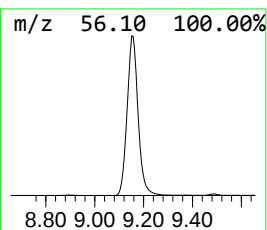
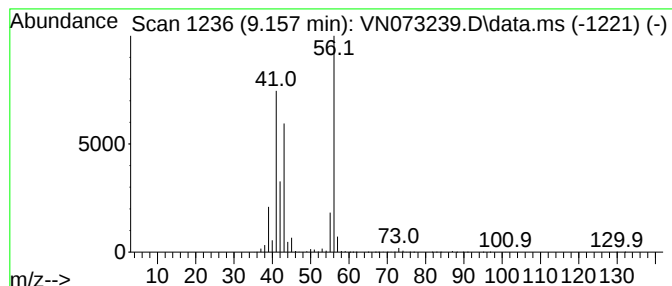
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Quant Title : SW846 8260

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

Peak Number 7 1-Butanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.157	93.23 ug/l	31436700	1,4-Difluorobenzene	8.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol	74	C4H10O	000071-36-3	91
2			Cyanoic acid, propyl ester	85	C4H7NO	001768-36-1	56
3			1-Pentene, 4-methyl-	84	C6H12	000691-37-2	40
4			1-Hexanol	102	C6H14O	000111-27-3	39
5			1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	12



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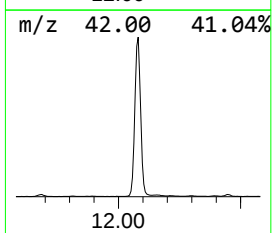
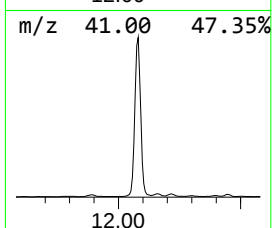
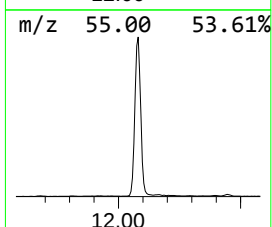
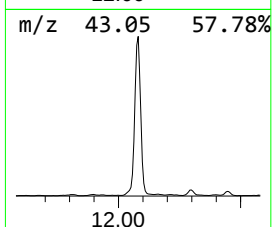
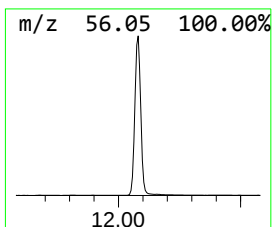
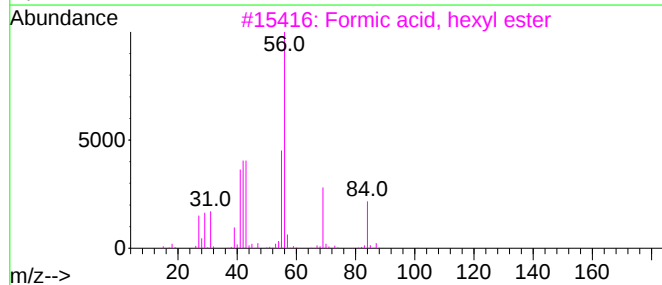
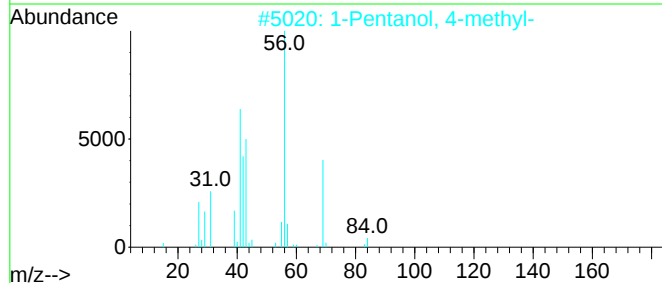
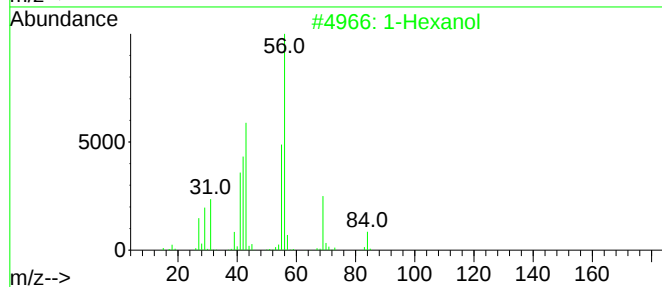
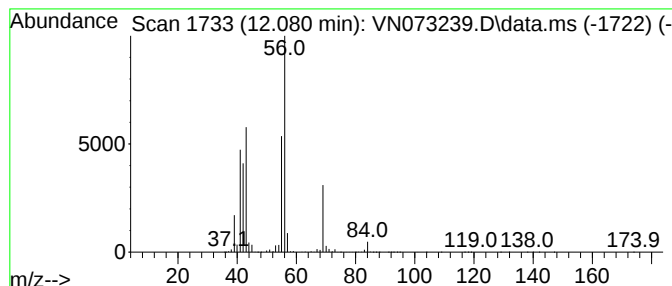
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Quant Title : SW846 8260

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

Peak Number 8 1-Hexanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.080	50.00 ug/l	14650300	Chlorobenzene-d5	11.680

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol	102	C6H14O	000111-27-3	86
2			1-Pentanol, 4-methyl-	102	C6H14O	000626-89-1	78
3			Formic acid, hexyl ester	130	C7H14O2	000629-33-4	72
4			Hexyl chloroformate	164	C7H13ClO2	006092-54-2	72
5			Cyclopropane, propyl-	84	C6H12	002415-72-7	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062922\
Data File : VN073239.D
Acq On : 29 Jun 2022 13:41
Operator : JC\MD
Sample : N3504-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TRE-1615

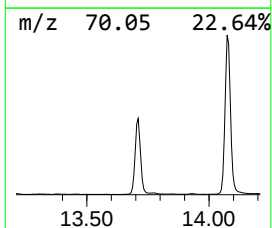
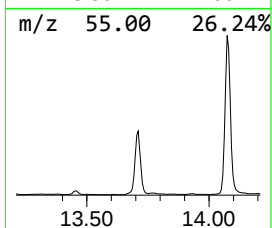
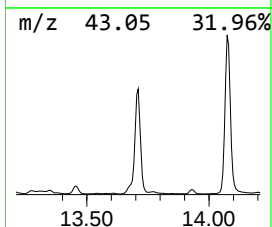
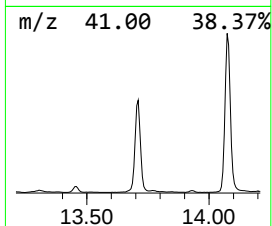
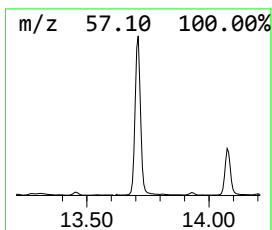
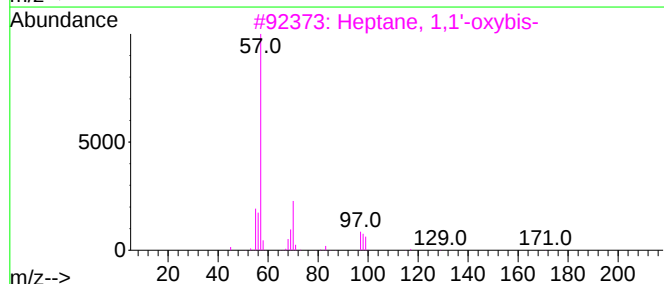
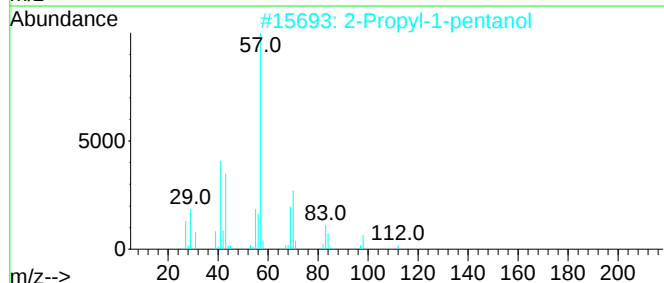
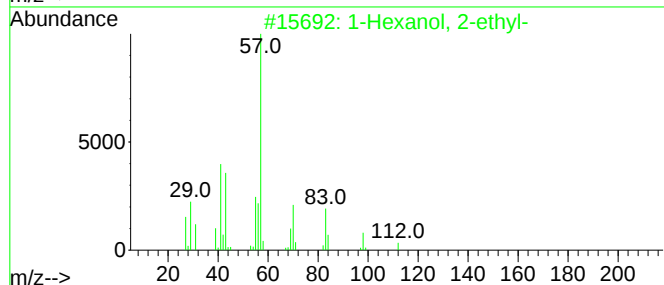
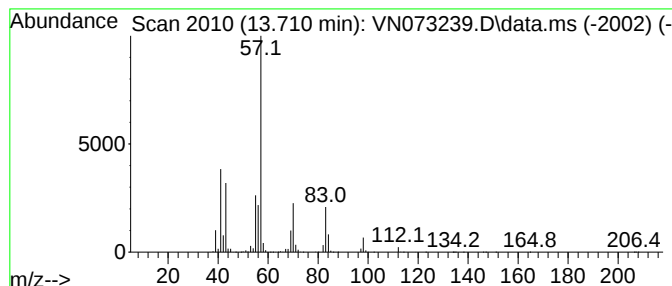
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.710	50.00 ug/l	11328500	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
3			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
4			Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	50
5			2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062922\
Data File : VN073239.D
Acq On : 29 Jun 2022 13:41
Operator : JC\MD
Sample : N3504-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TRE-1615

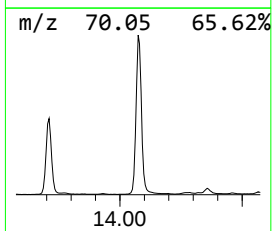
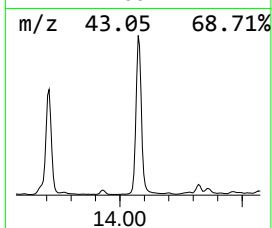
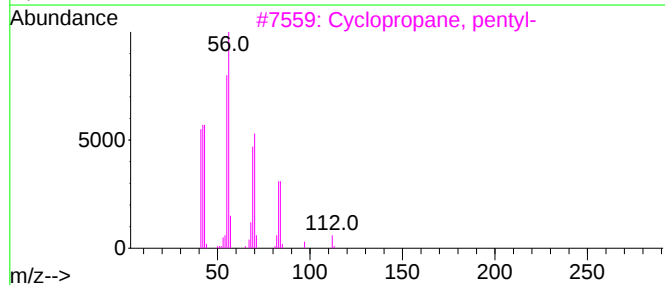
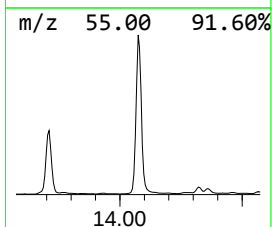
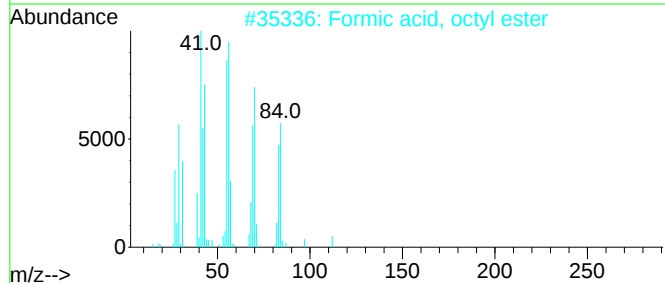
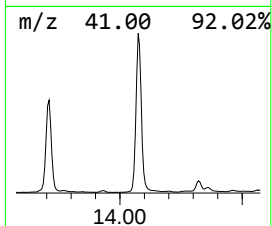
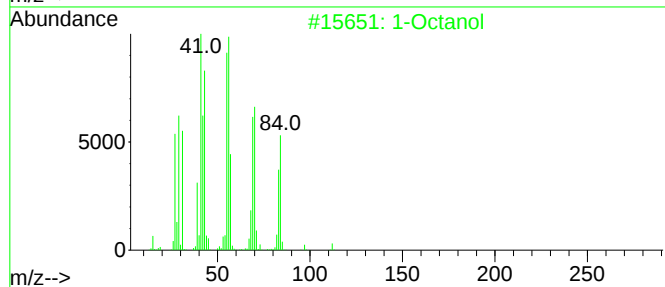
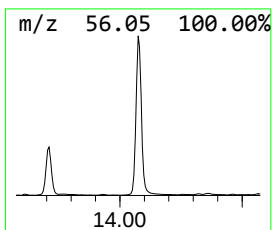
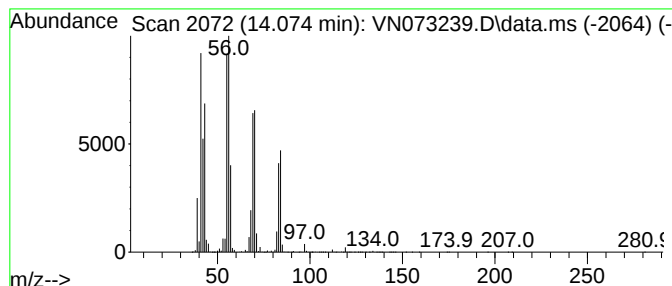
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Quant Title : SW846 8260

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

Peak Number 10 1-Octanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.074	83.74 ug/l	18972200	1,4-Dichlorobenzene-d4	13.610

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Octanol	130	C8H18O	000111-87-5	91
2		Formic acid, octyl ester	158	C9H18O2	000112-32-3	90
3		Cyclopropane, pentyl-	112	C8H16	002511-91-3	78
4		Cyclobutane, 1,2-diethyl-, cis-	112	C8H16	061141-50-2	64
5		1-Hexanol, 3-methyl-	116	C7H16O	013231-81-7	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062922\
Data File : VN073239.D
Acq On : 29 Jun 2022 13:41
Operator : JC\MD
Sample : N3504-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TRE-1615

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.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
2-Propanol, 2-m...	5.551	120.7	ug/l	37990200	1	8.004	15733700	50.0
Butanal	6.998	48.0	ug/l	15104200	1	8.004	15733700	50.0
1,3-Dioxolane, ...	8.198	50.0	ug/l	15733700	1	8.004	15733700	50.0
2-Butenal, (Z)-	8.810	50.0	ug/l	16858900	2	8.898	16858900	50.0
1-Butanol	9.157	93.2	ug/l	31436700	2	8.898	16858900	50.0
1-Hexanol	12.080	50.0	ug/l	14650300	3	11.680	14650300	50.0
1-Hexanol, 2-et...	13.710	50.0	ug/l	11328500	4	13.610	11328500	50.0
1-Octanol	14.074	83.7	ug/l	18972200	4	13.610	11328500	50.0