

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062922\
Data File : VN073237.D
Acq On : 29 Jun 2022 12:52
Operator : JC\MD
Sample : N3504-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TRE-1613

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_N\methods\82N062822W.M

Title : SW846 8260

Signal : TIC: VN073237.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.428	90	92	204	rBV3	41963814	283490632	35.85%	22.316%
2	4.216	279	396	400	rBV2	30869090	790713315	100.00%	62.245%
3	4.269	400	405	468	rVV	4135783	20140942	2.55%	1.586%
4	5.451	588	606	645	rBV	5301136	22677864	2.87%	1.785%
5	6.992	852	868	907	rBV	6548667	20492404	2.59%	1.613%
6	7.345	909	928	954	rVV	11259149	32406873	4.10%	2.551%
7	8.186	1059	1071	1091	rBV	4434544	11225962	1.42%	0.884%
8	9.145	1217	1234	1260	rBV	12101296	34442474	4.36%	2.711%
9	12.074	1721	1732	1742	rBV	9374399	15574992	1.97%	1.226%
10	13.710	2001	2010	2018	rVV	11346442	17756156	2.25%	1.398%
11	14.074	2065	2072	2082	rBV	13423595	21397575	2.71%	1.684%

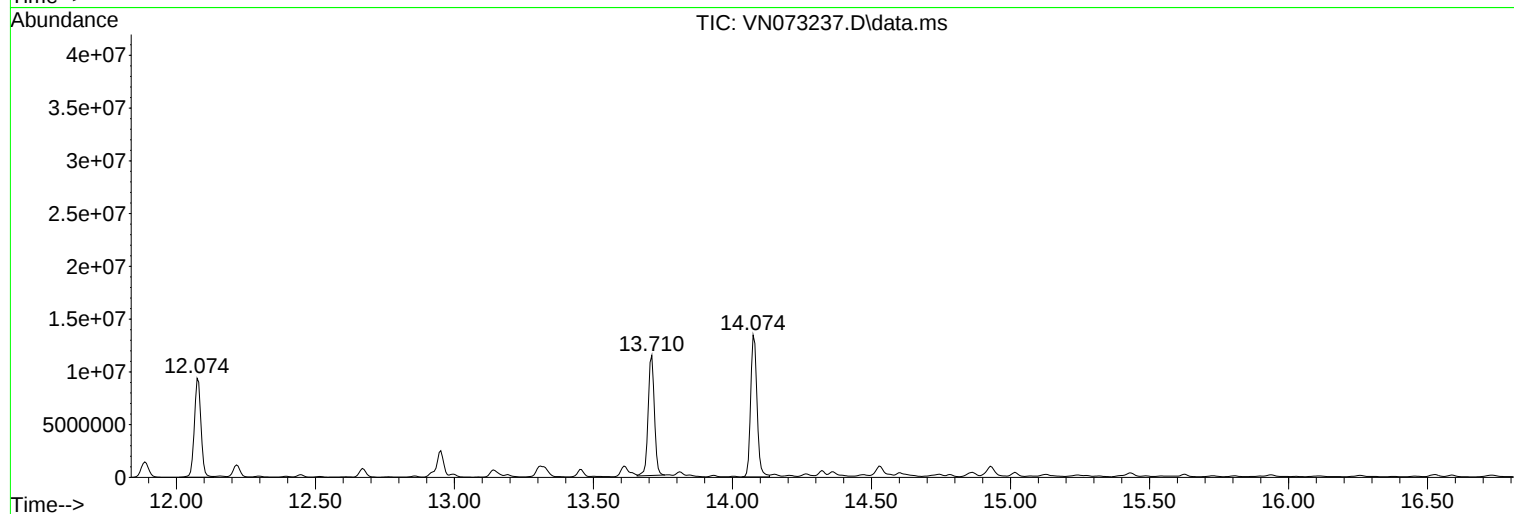
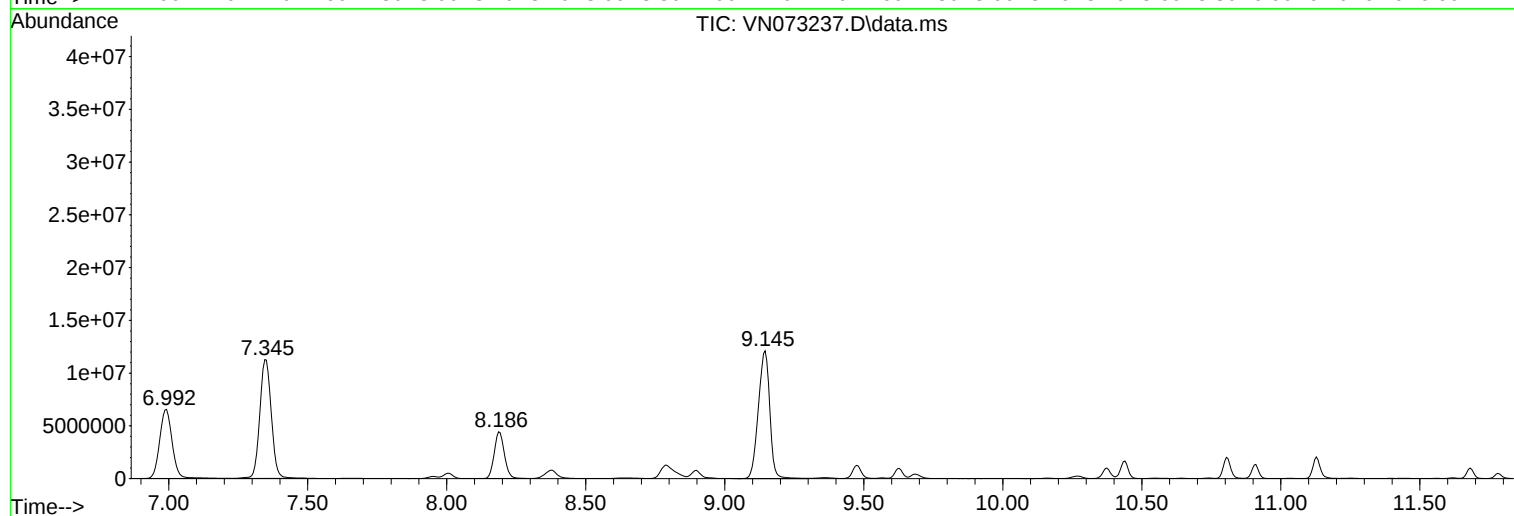
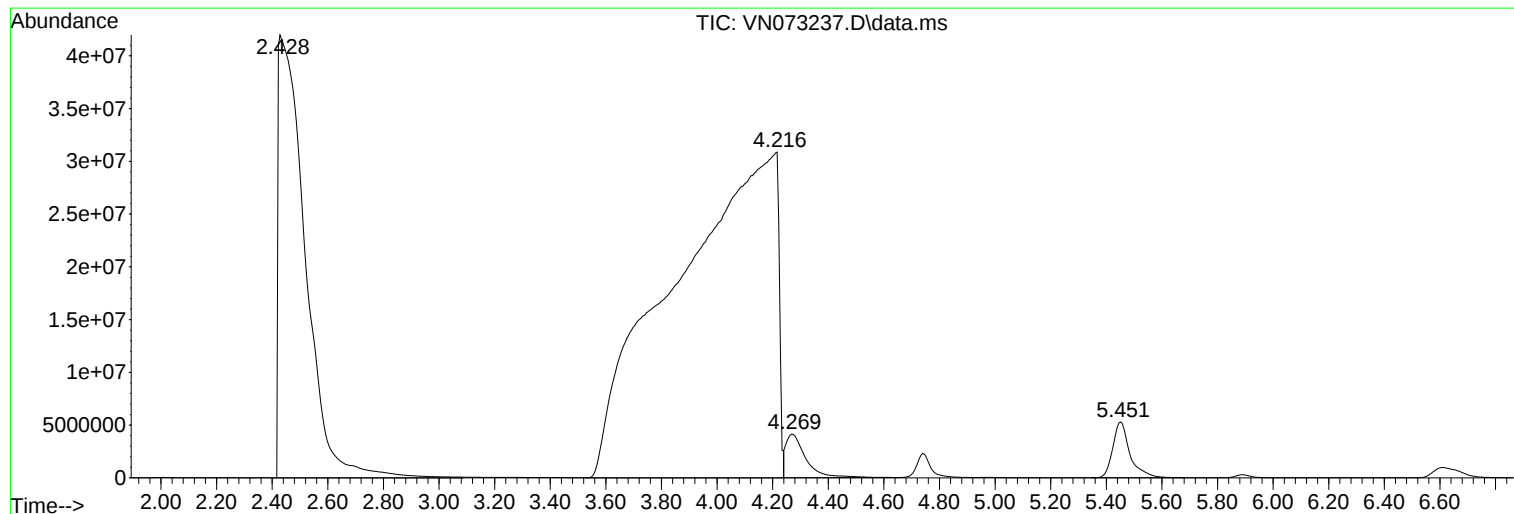
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Quant Title : SW846 8260

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



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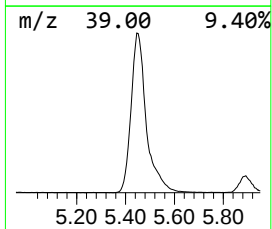
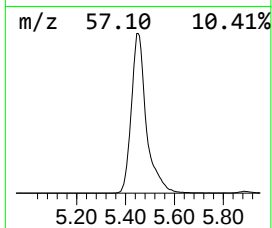
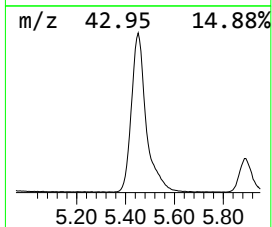
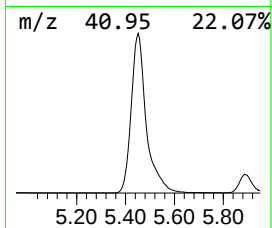
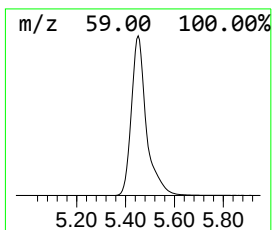
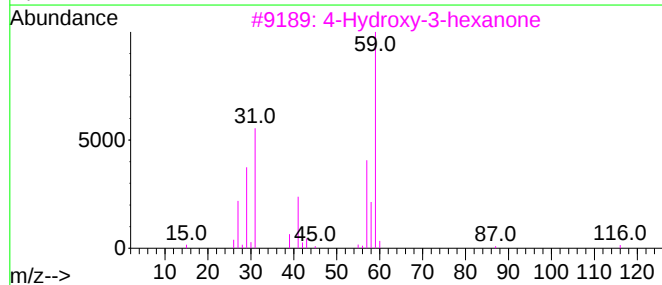
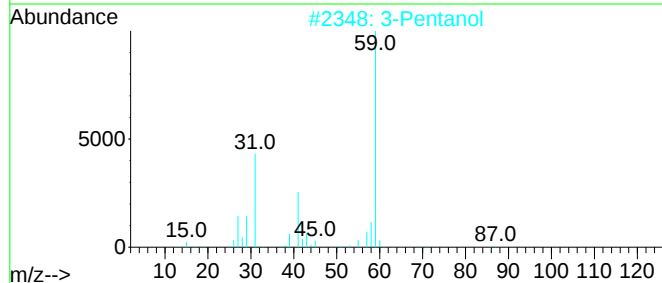
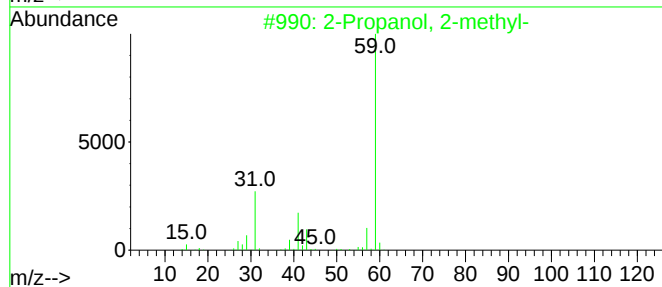
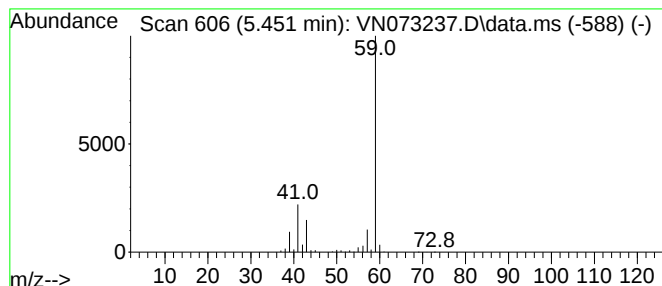
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.451	101.01 ug/l	22677900	Pentafluorobenzene	8.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 2-methyl-			74	C4H10O	000075-65-0	83
2	3-Pentanol			88	C5H12O	000584-02-1	9
3	4-Hydroxy-3-hexanone			116	C6H12O2	004984-85-4	9
4	Propanoic acid, 2-hydroxy-2-methyl-			104	C4H8O3	000594-61-6	9
5	Formamide, N-methyl-			59	C2H5NO	000123-39-7	5



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MSVOA_N
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TRE-1613

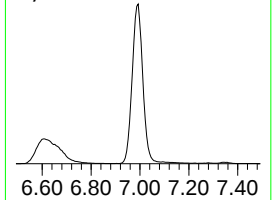
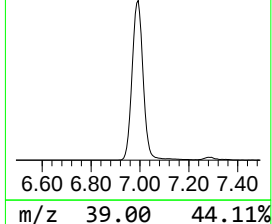
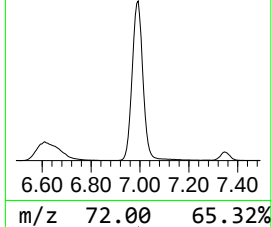
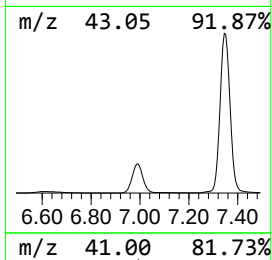
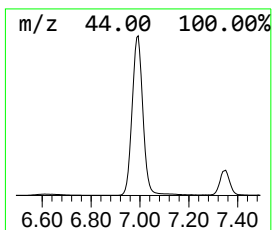
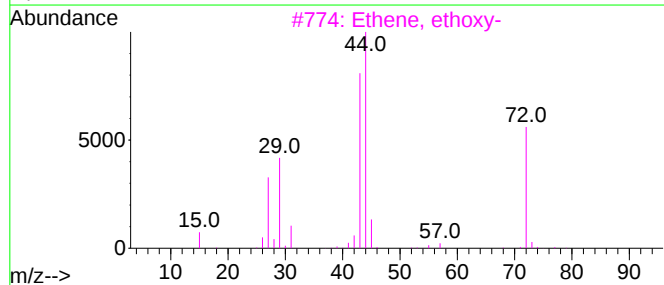
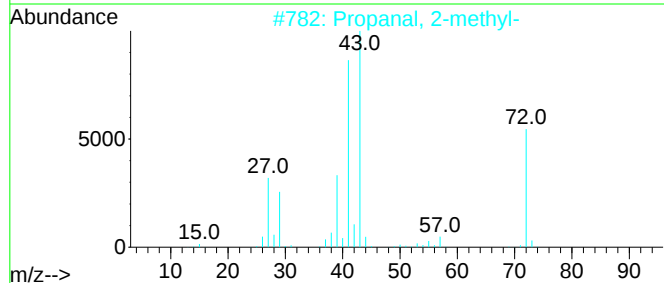
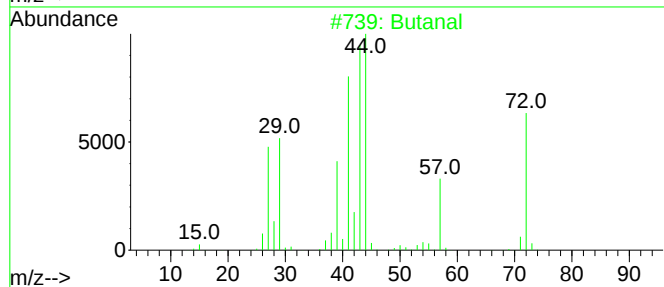
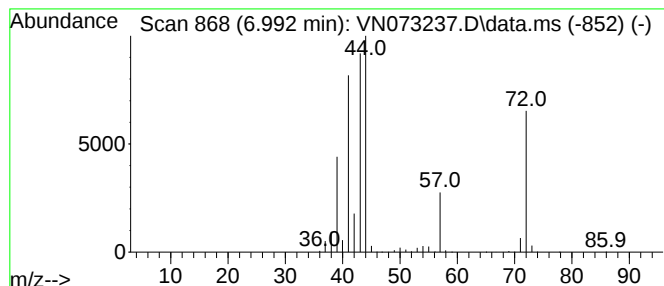
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

Peak Number 4 Butanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.992	91.27 ug/l	20492400	Pentafluorobenzene	8.004

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butanal	72	C4H8O	000123-72-8	94
2		Propanal, 2-methyl-	72	C4H8O	000078-84-2	52
3		Ethene, ethoxy-	72	C4H8O	000109-92-2	49
4		2-Propanone, hydrazone	72	C3H8N2	005281-20-9	35
5		2-Propen-1-ol, 2-methyl-, acetate	114	C6H10O2	000820-71-3	23



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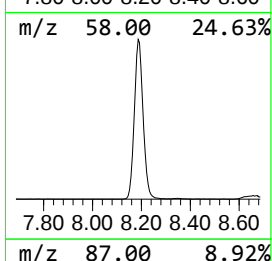
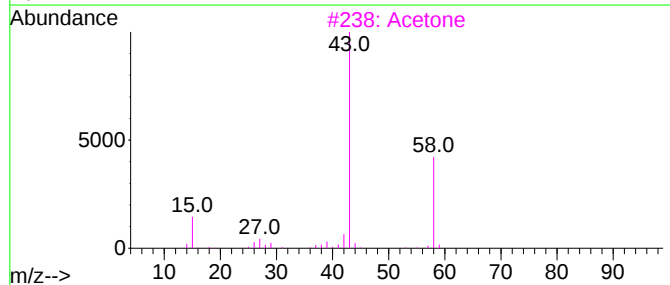
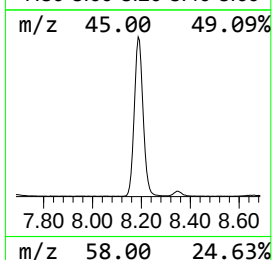
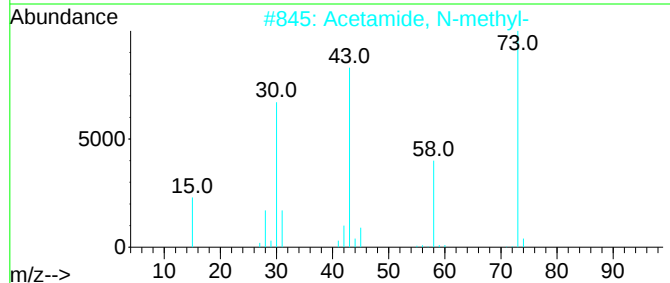
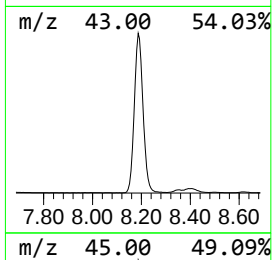
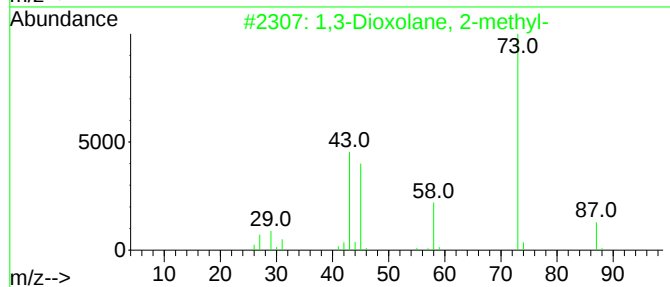
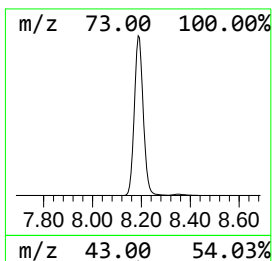
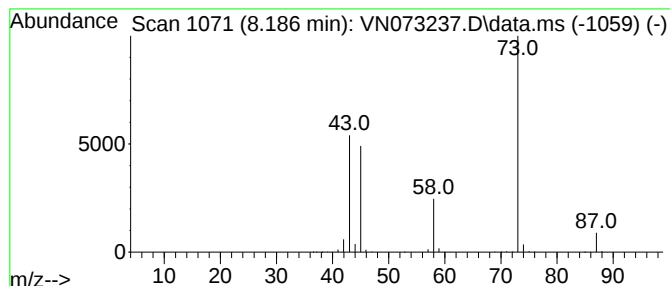
Instrument :
MSVOA_N
ClientSampleId :
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Peak Number 5 1,3-Dioxolane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
8.186	50.00 ug/l	11226000	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	37
3	Acetone	58	C3H6O	000067-64-1	12
4	1-Methoxy-2-propyl acetate	132	C6H12O3	000108-65-6	9
5	2,2'-Bi-1,3-dioxolane	146	C6H10O4	006705-89-1	9



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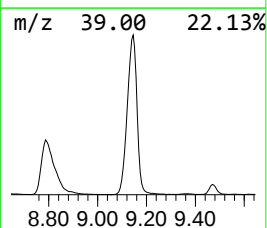
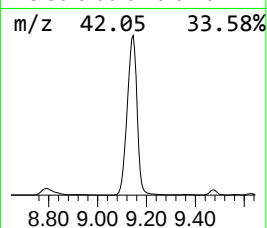
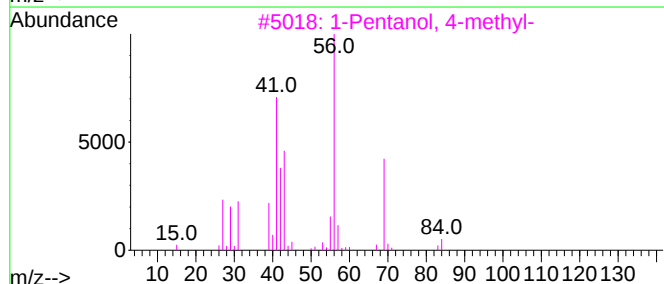
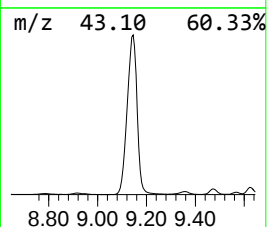
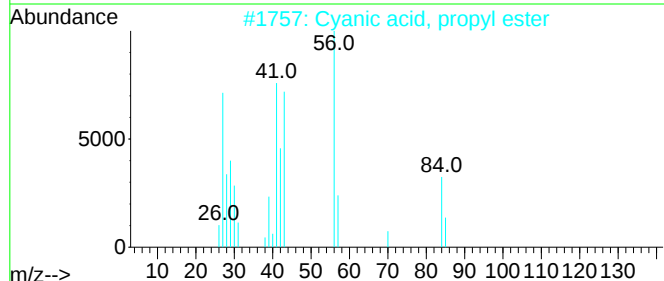
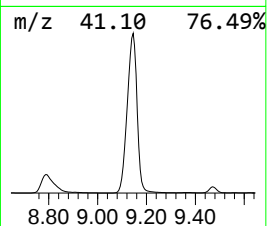
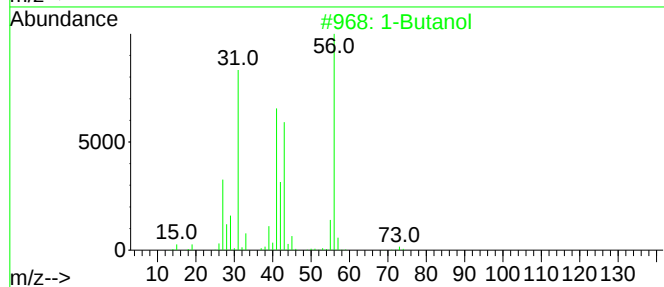
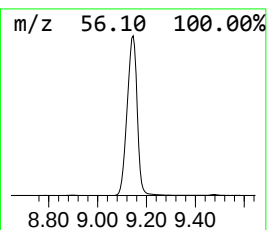
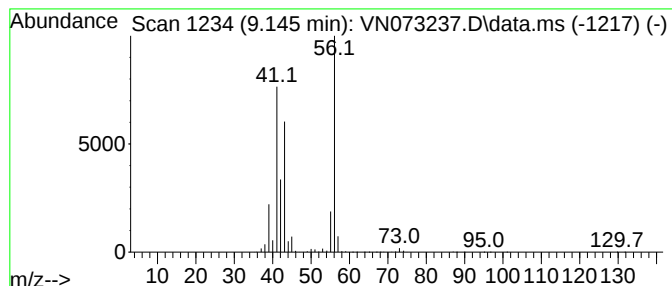
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Butanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.145	50.00 ug/l	34442500	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-Pentanol, 4-methyl-	102	C6H14O	000626-89-1	40
4			1-Hexanol	102	C6H14O	000111-27-3	39
5			Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	38



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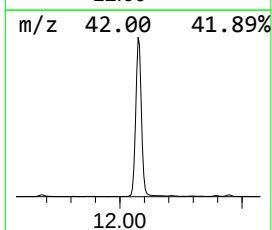
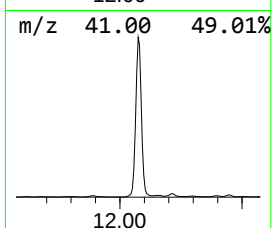
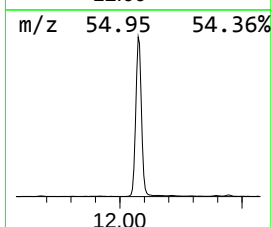
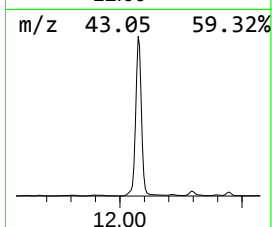
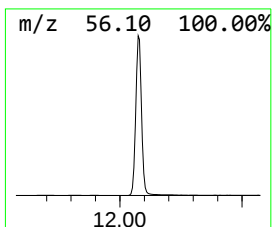
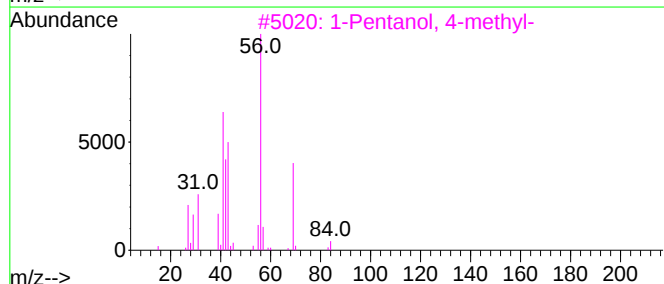
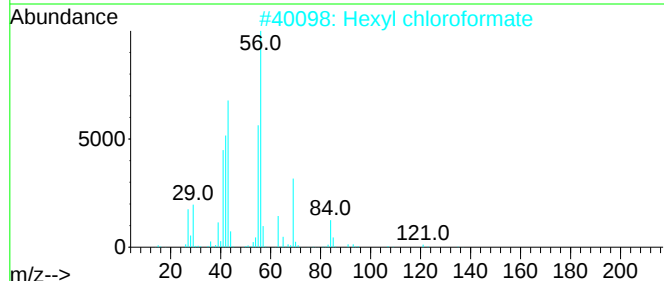
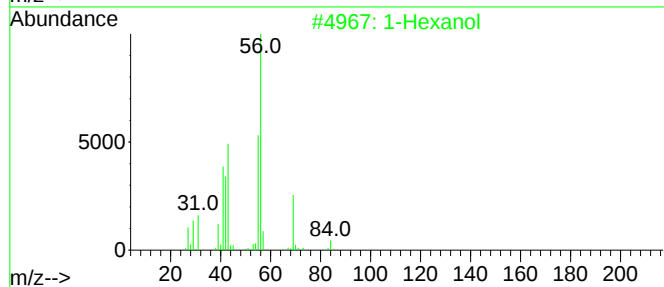
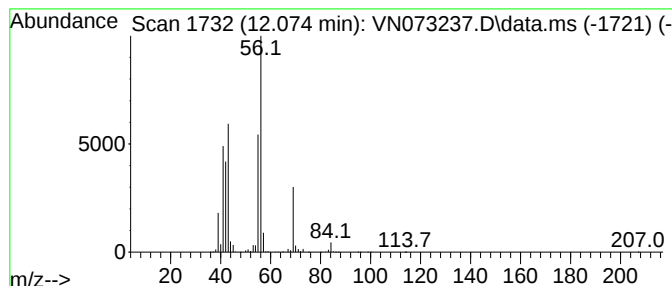
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 1-Hexanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.074	50.00 ug/l	15575000	Chlorobenzene-d5	11.680	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol	102	C6H14O	000111-27-3	83
2	Hexyl chloroformate	164	C7H13ClO2	006092-54-2	83
3	1-Pentanol, 4-methyl-	102	C6H14O	000626-89-1	78
4	Formic acid, hexyl ester	130	C7H14O2	000629-33-4	72
5	Cyclopropane, propyl-	84	C6H12	002415-72-7	64



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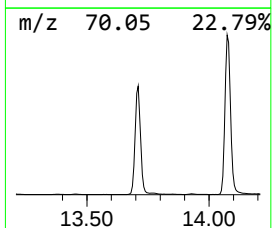
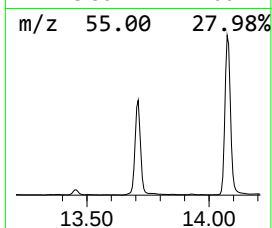
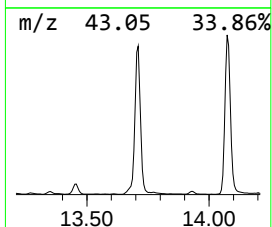
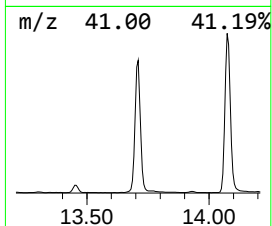
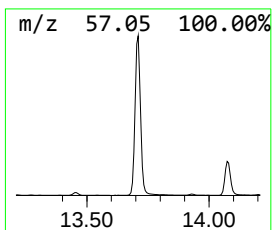
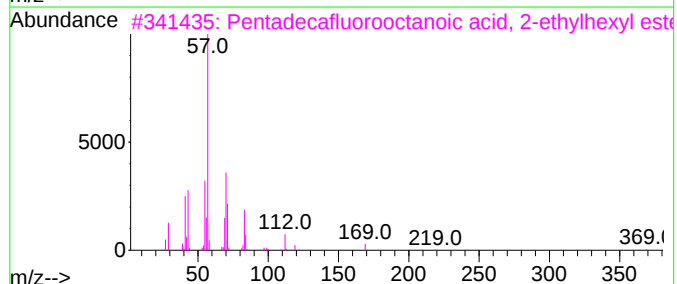
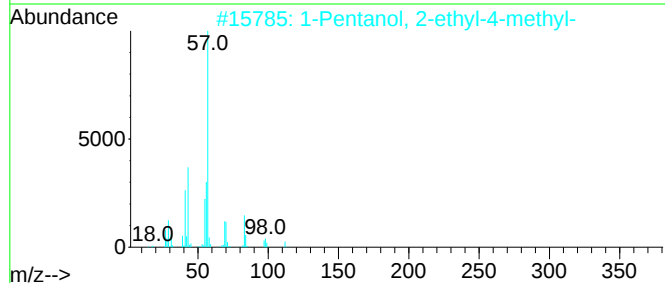
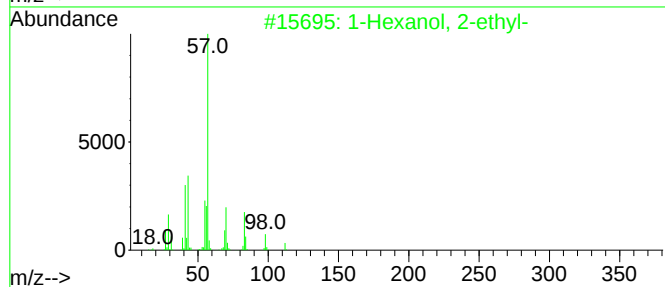
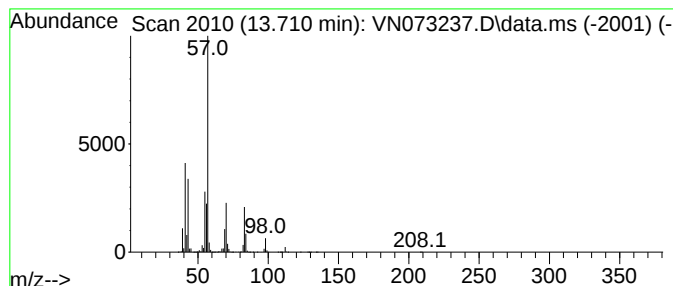
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.710	50.00 ug/l	17756200	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			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3			Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	50
4			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	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 : VN073237.D
Acq On : 29 Jun 2022 12:52
Operator : JC\MD
Sample : N3504-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TRE-1613

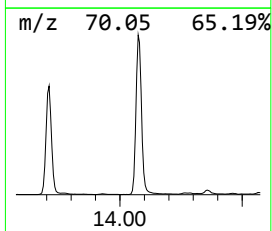
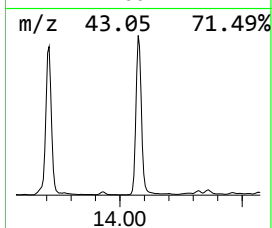
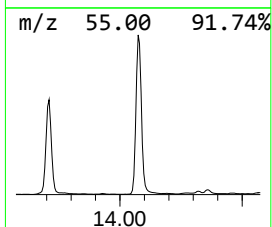
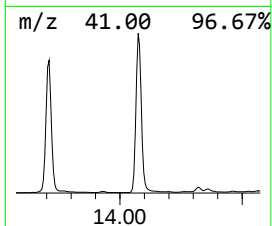
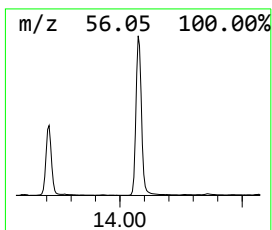
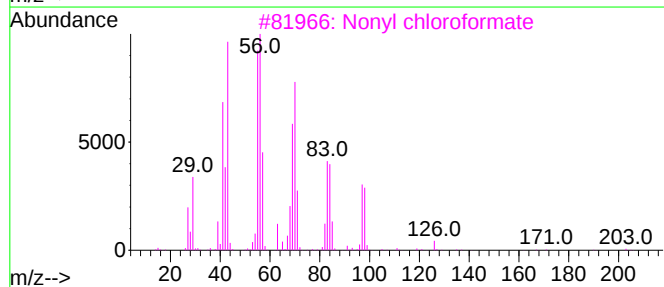
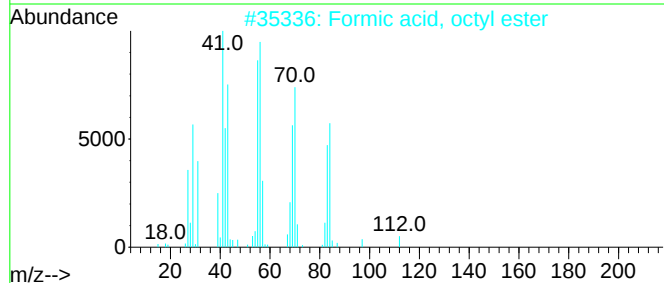
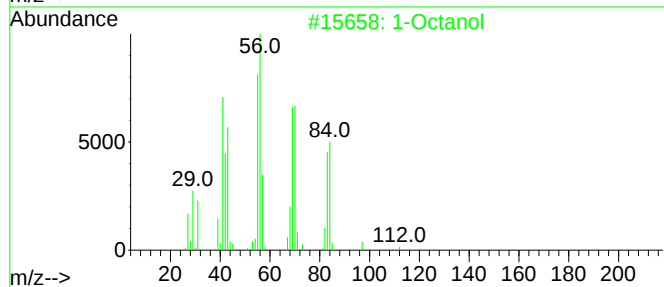
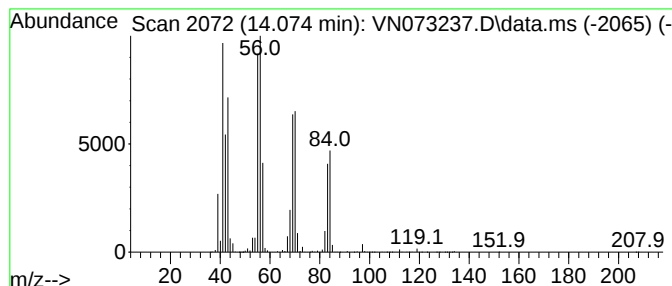
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Quant Title : SW846 8260

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

Peak Number 9 1-Octanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.074	60.25 ug/l	21397600	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	Nonyl chloroformate			206	C10H19ClO2	057045-82-6	78
4	Cyclopropane, pentyl-			112	C8H16	002511-91-3	78
5	1-Nonanol			144	C9H20O	000143-08-8	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062922\
Data File : VN073237.D
Acq On : 29 Jun 2022 12:52
Operator : JC\MD
Sample : N3504-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TRE-1613

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...	5.451	101.0	ug/l	22677900	1	8.004	11226000	50.0
Butanal	6.992	91.3	ug/l	20492400	1	8.004	11226000	50.0
1,3-Dioxolane, ...	8.186	50.0	ug/l	11226000	1	8.004	11226000	50.0
1-Butanol	9.145	50.0	ug/l	34442500	2	8.898	34442500	50.0
1-Hexanol	12.074	50.0	ug/l	15575000	3	11.680	15575000	50.0
1-Hexanol, 2-et...	13.710	50.0	ug/l	17756200	4	13.610	17756200	50.0
1-Octanol	14.074	60.3	ug/l	21397600	4	13.610	17756200	50.0