LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062922\
Data File : VN073238.D
Acq On : 29 Jun 2022 13:16
Operator : JC\MD
Sample : N3504-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TRE-1614

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: VN073238.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.381	83	84	231	rBV	42965849	392963043	43.54%	25.871%
2	4.252	278	402	407	rBV2	33409750	902518606	100.00%	59.417%
3	5.469	592	609	649	rBV	6707387	27126971	3.01%	1.786%
4	6.993	854	868	895	rBV	10740527	33990287	3.77%	2.238%
5	7.351	910	929	959	rVB	13731089	40025547	4.43%	2.635%
6	8.192	1060	1072	1091	rBV	5655950	14789243	1.64%	0.974%
7	8.792	1163	1174	1187	rBV	3312431	12616767	1.40%	0.831%
8	9.145	1218	1234	1260	rBV	12849961	38388485	4.25%	2.527%
9	12.075	1721	1732	1742	rBV	10356974	17250918	1.91%	1.136%
10	13.710	2001	2010	2019	rVV	10356008	16332019	1.81%	1.075%
11	14.074	2064	2072	2082	rBV	14659502	22956318	2.54%	1.511%

Sum of corrected areas: 1518958204

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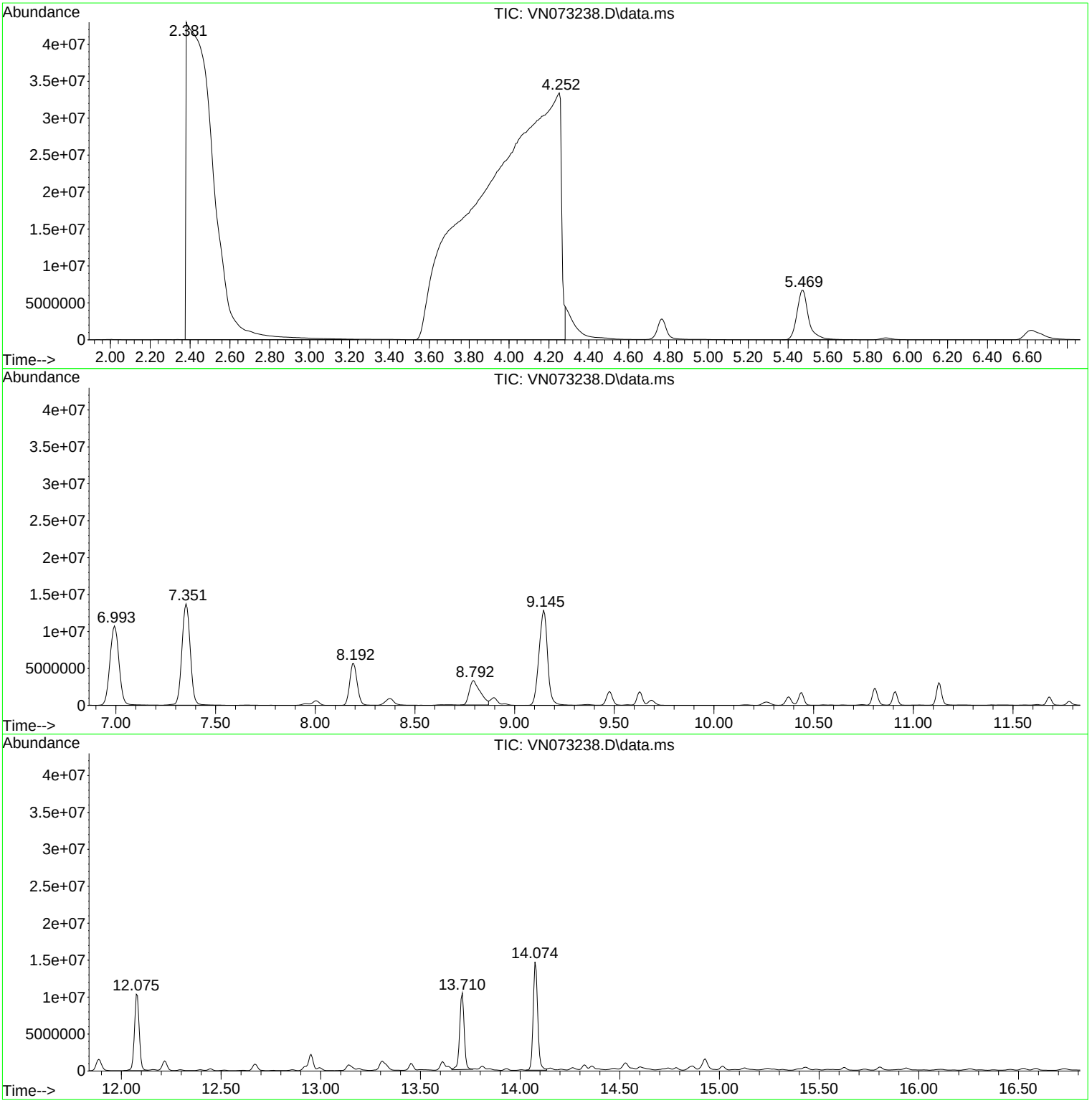
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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



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Data File : VN073238.D
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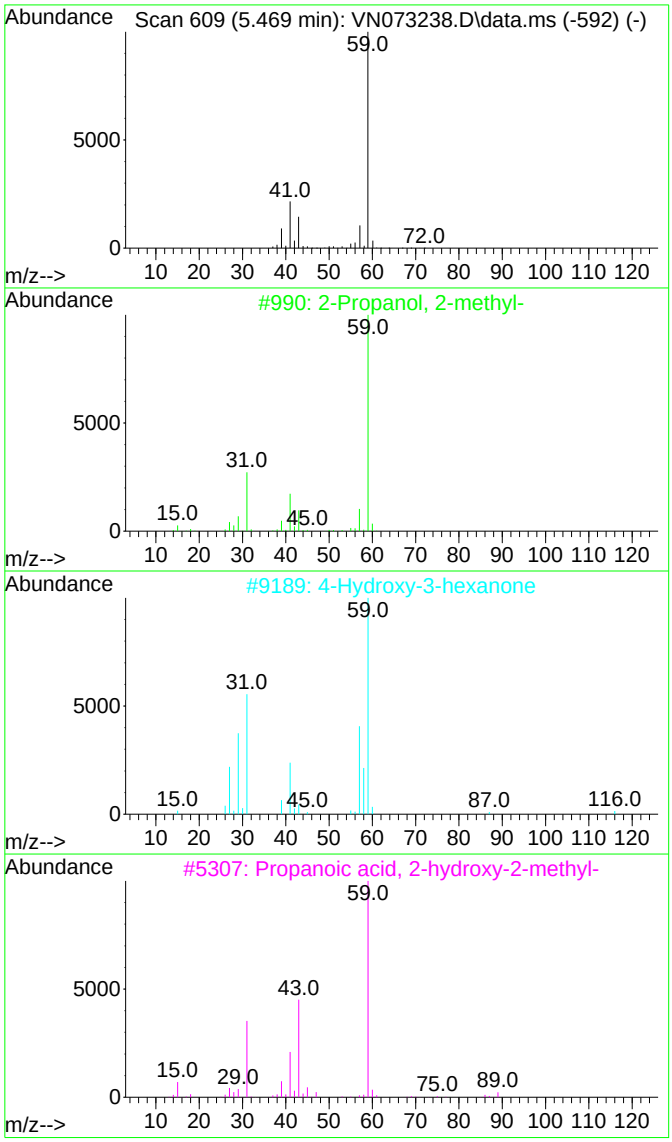
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

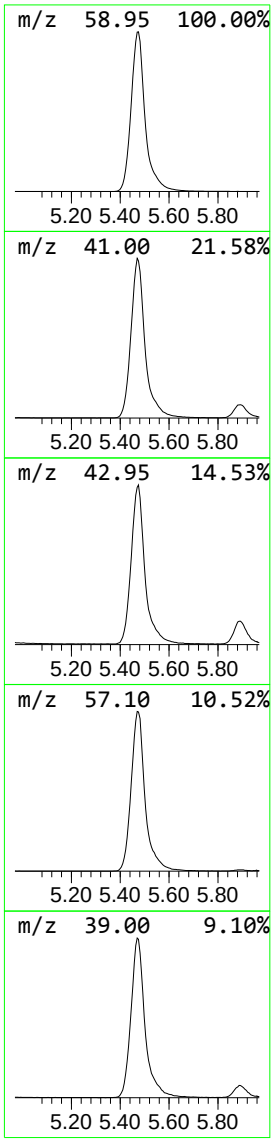
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Propanol, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.469	91.71 ug/l	27127000	Pentafluorobenzene	8.004

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	74
2	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	9
3	Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	9
4	Formamide, N-methyl-	59	C2H5NO	000123-39-7	5
5	Guanidine	59	CH5N3	000113-00-8	4





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Data File : VN073238.D
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Operator : JC\MD
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ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TRE-1614

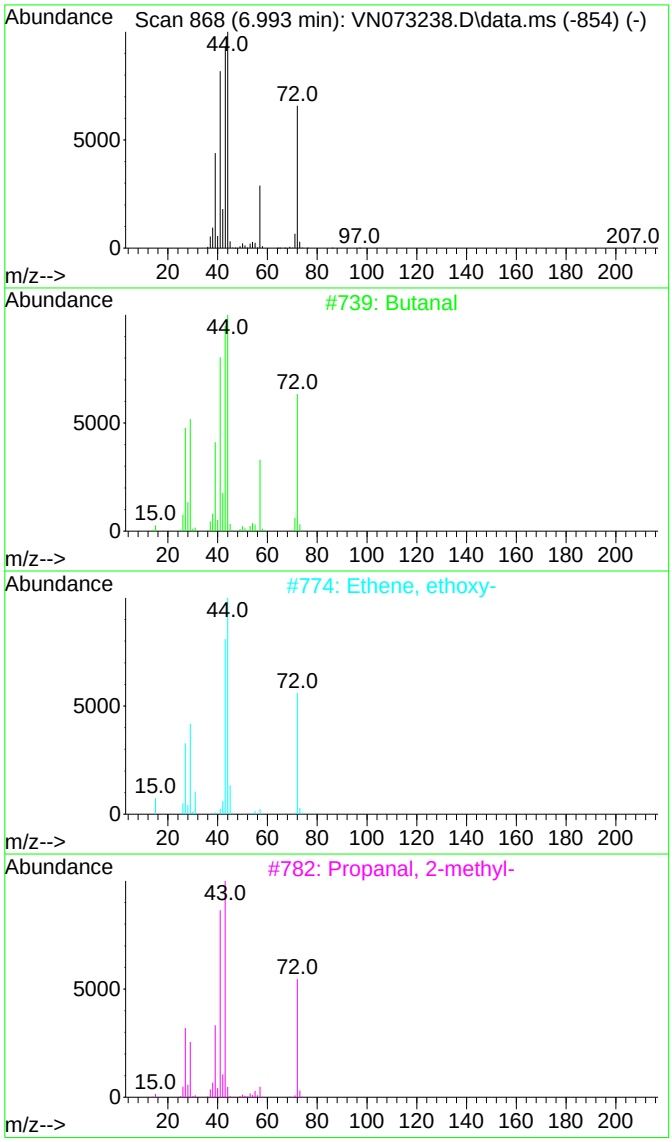
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

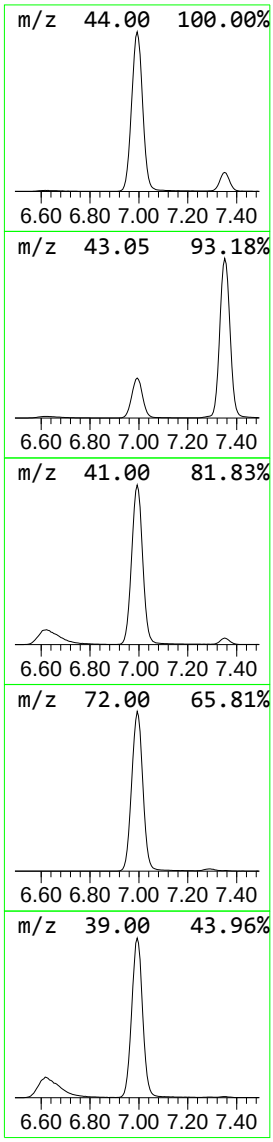
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Butanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.993	114.92 ug/l	33990300	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	49
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
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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Data File : VN073238.D
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Operator : JC\MD
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TRE-1614

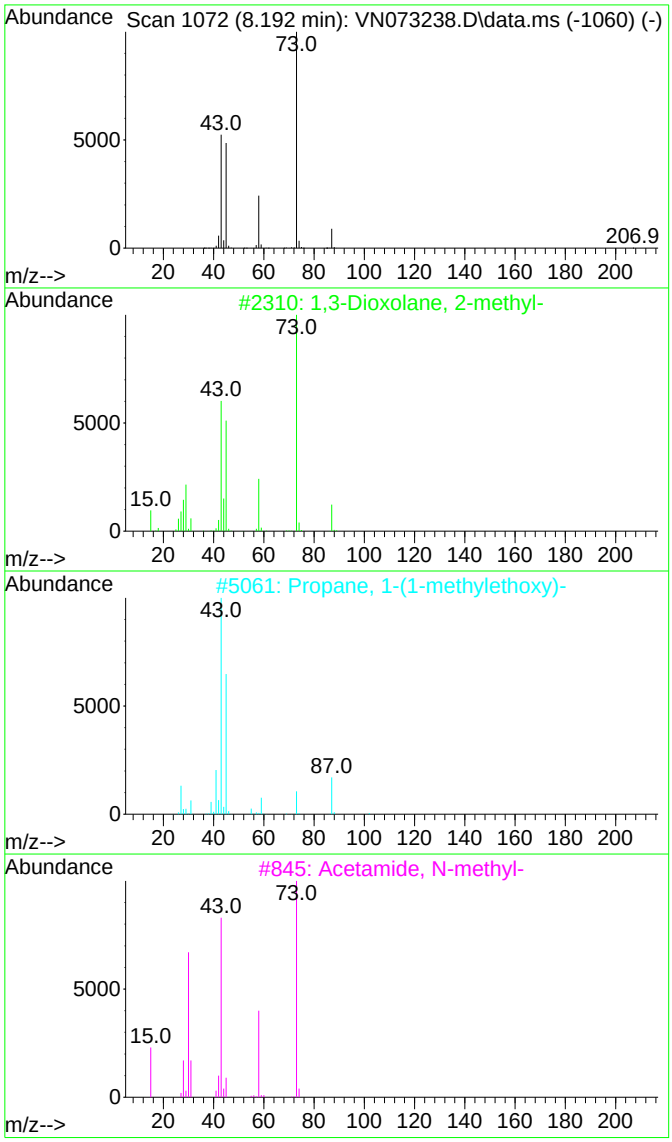
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

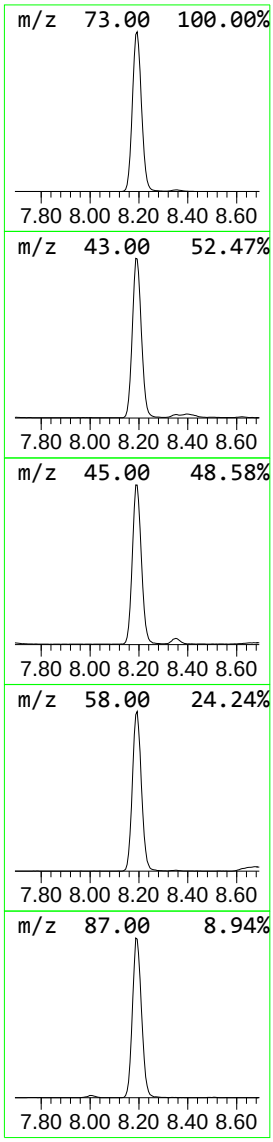
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1,3-Dioxolane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.192	50.00 ug/l	14789200	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	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	33
3	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	32
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5	Acetone	58	C3H6O	000067-64-1	9





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ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TRE-1614

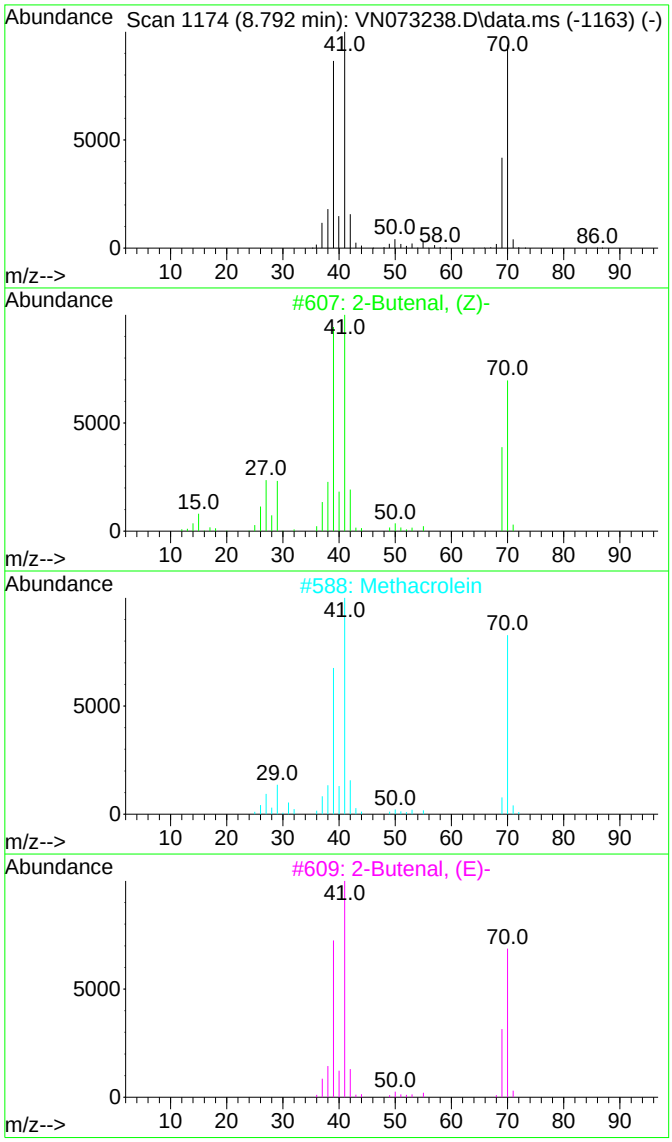
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

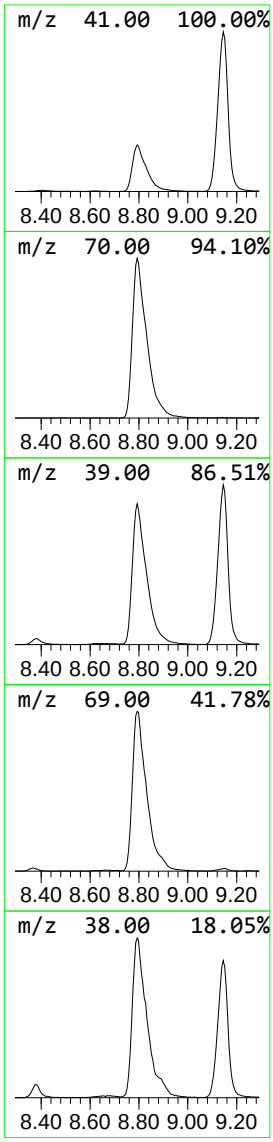
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 2-Butenal, (Z)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.792	50.00 ug/l	12616800	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, (E)-	70	C4H6O	000123-73-9	91
4	Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	90
5	2-Butenal	70	C4H6O	004170-30-3	90





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ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TRE-1614

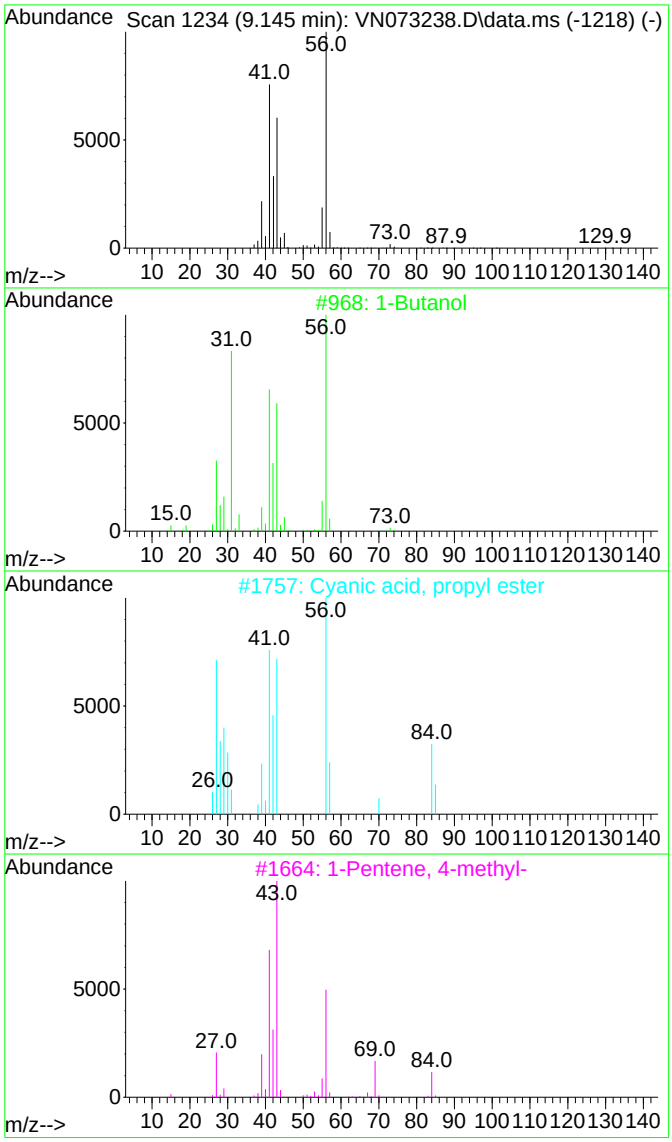
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

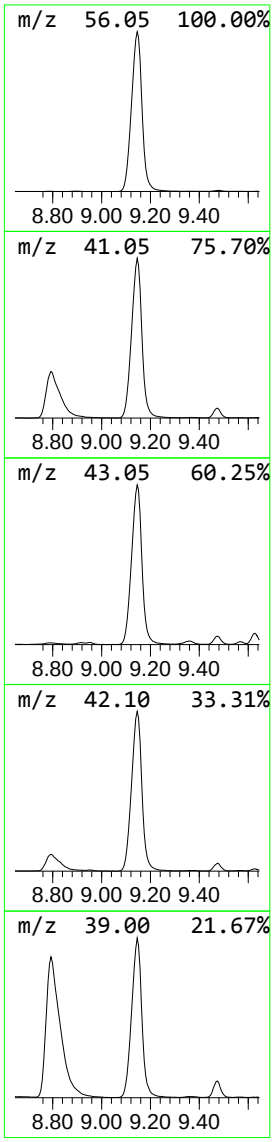
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1-Butanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.145	152.13 ug/l	38388500	1,4-Difluorobenzene	8.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	91
2	Cyanic acid, propyl ester	85	C4H7NO	001768-36-1	56
3	1-Pentene, 4-methyl-	84	C6H12	000691-37-2	40
4	1-Pentanol, 4-methyl-	102	C6H14O	000626-89-1	40
5	1-Hexanol	102	C6H14O	000111-27-3	39





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Instrument :
MSVOA_N
ClientSampleId :
TRE-1614

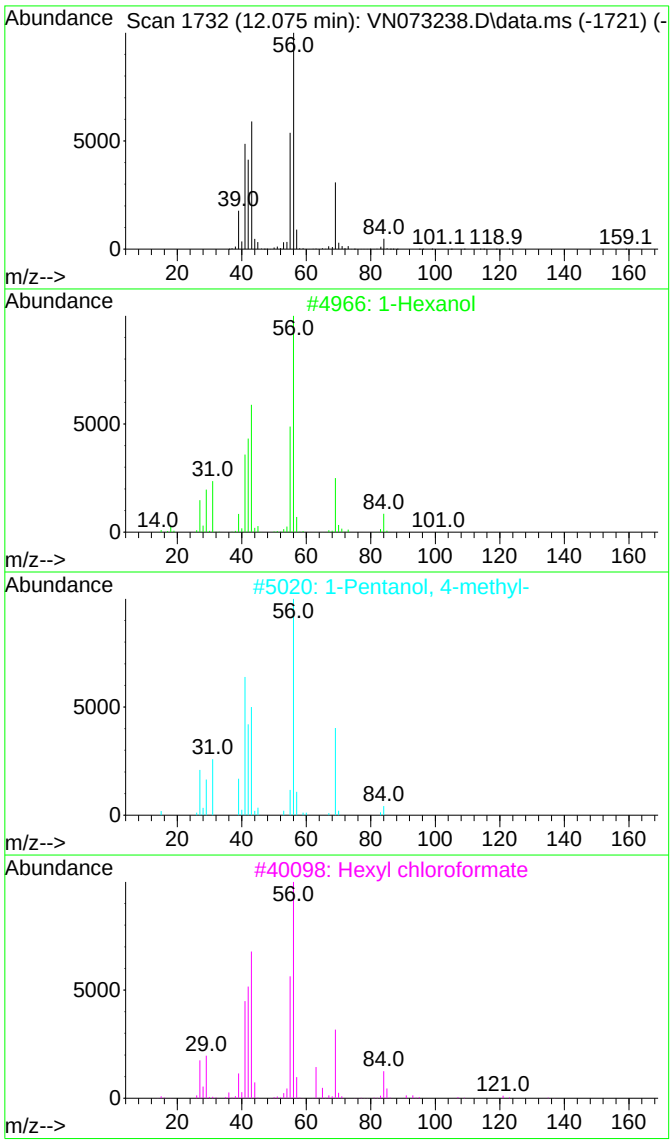
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

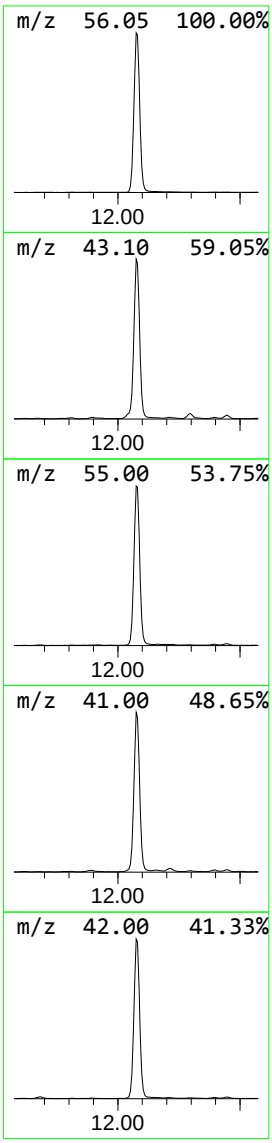
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 1-Hexanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.075	50.00 ug/l	17250900	Chlorobenzene-d5	11.681

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	Hexyl chloroformate	164	C7H13ClO2	006092-54-2	78
4	Formic acid, hexyl ester	130	C7H14O2	000629-33-4	72
5	Cyclopropane, propyl-	84	C6H12	002415-72-7	59





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Instrument :
MSVOA_N
ClientSampleId :
TRE-1614

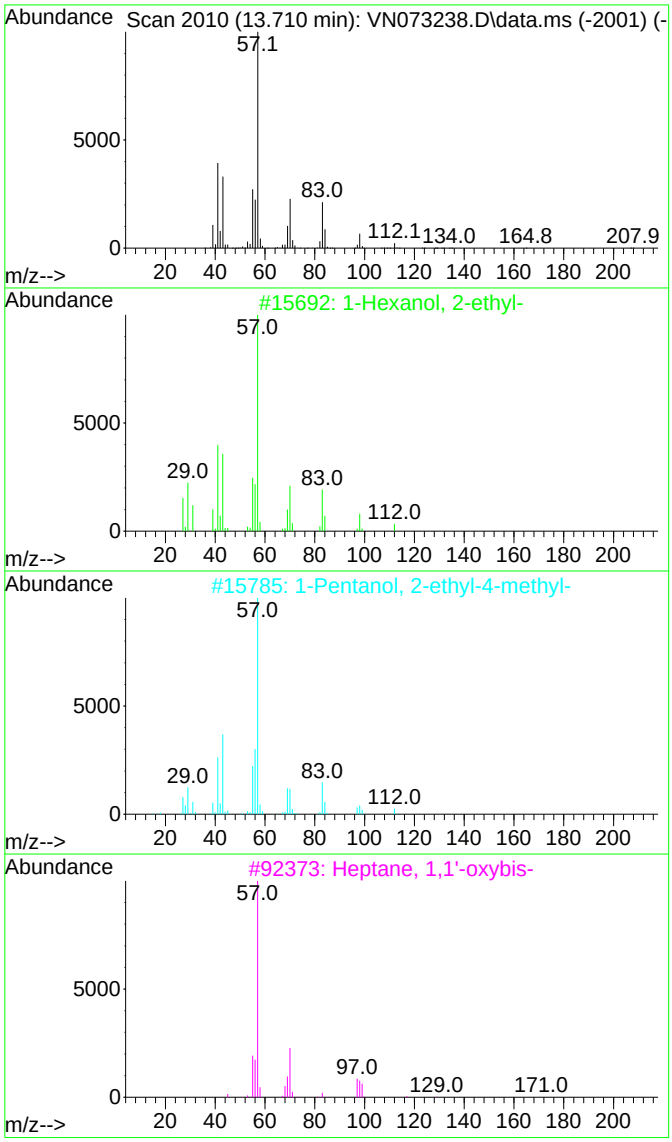
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

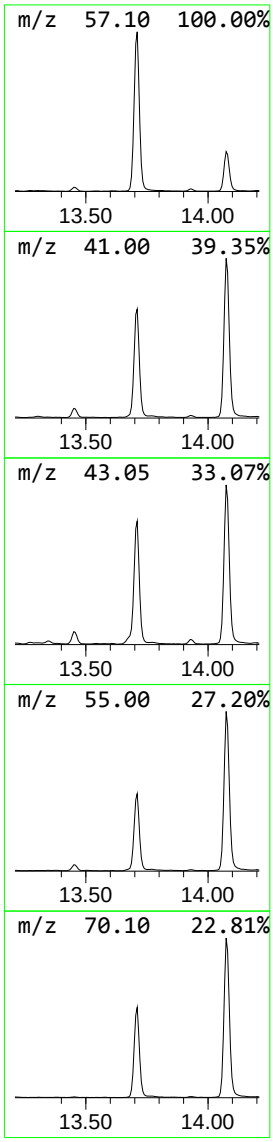
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 1-Hexanol, 2-ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.710	50.00 ug/l	16332000	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	59
3	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
4	Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	50
5	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50





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

TIC Library : C:\Database\NIST20.L
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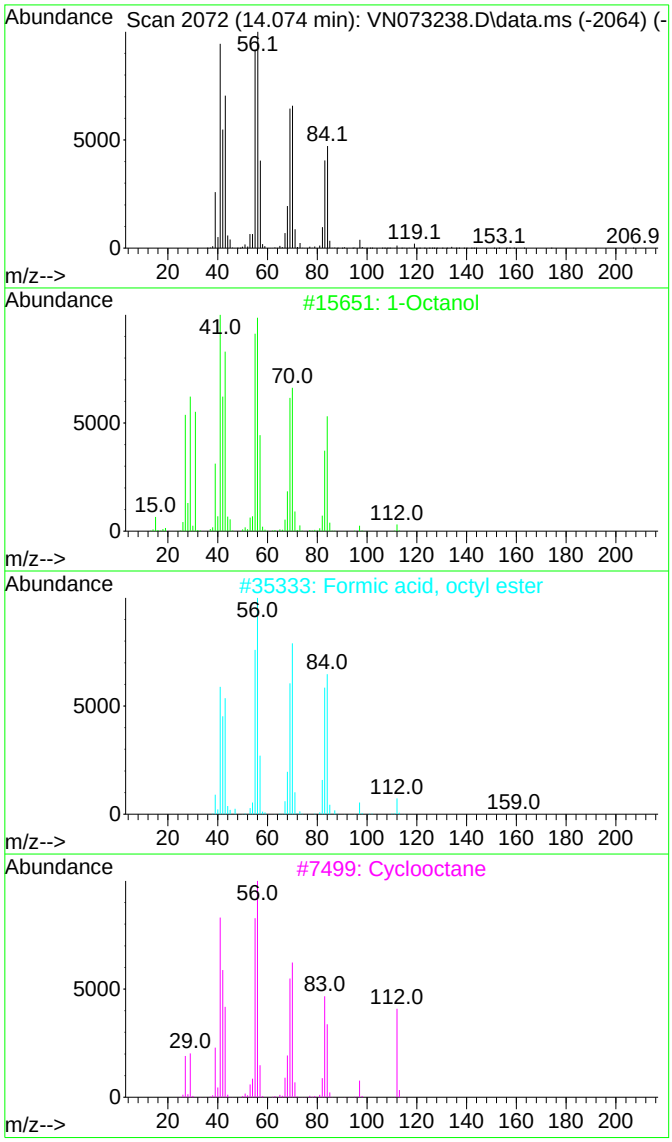
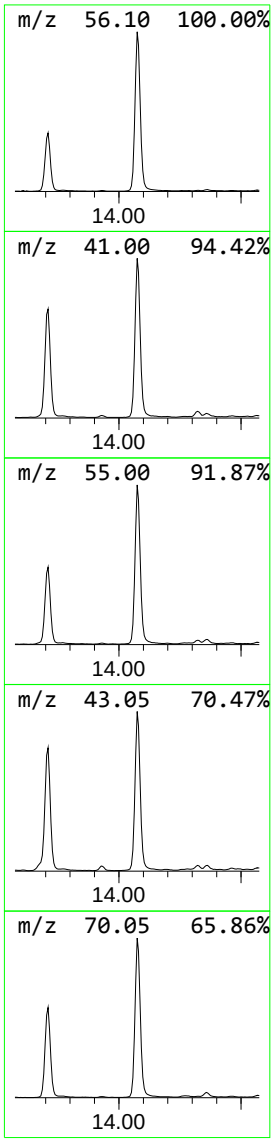
****
Peak Number 10 1-Octanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.075	70.28 ug/l	22956300	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	Cyclooctane	112	C8H16	000292-64-8	78
4	Cyclopropane, pentyl-	112	C8H16	002511-91-3	78
5	Cyclobutane, 1,2-diethyl-, cis-	112	C8H16	061141-50-2	64





Tentatively Identified Compound (LSC) summary

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Quant Title : SW846 8260

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Propanol, 2-m...	5.469	91.7	ug/l	27127000	1	8.004	14789200	50.0
Butanal	6.993	114.9	ug/l	33990300	1	8.004	14789200	50.0
1,3-Dioxolane, ...	8.192	50.0	ug/l	14789200	1	8.004	14789200	50.0
2-Butenal, (Z)-	8.792	50.0	ug/l	12616800	2	8.898	12616800	50.0
1-Butanol	9.145	152.1	ug/l	38388500	2	8.898	12616800	50.0
1-Hexanol	12.075	50.0	ug/l	17250900	3	11.681	17250900	50.0
1-Hexanol, 2-et...	13.710	50.0	ug/l	16332000	4	13.610	16332000	50.0
1-Octanol	14.075	70.3	ug/l	22956300	4	13.610	16332000	50.0