LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090822\
Data File : VX031222.D
Acq On : 08 Sep 2022 19:24
Operator : JC/MD
Sample : N4505-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
CLI-79

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_X\Method\82X090722W.M
Title : SW846 8260

Signal : TIC: VX031222.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.447	55	59	72	rBV	1794275	2154852	1.45%	0.771%
2	2.343	188	206	207	rBV	15205686	54580583	36.73%	19.529%
3	2.422	214	219	236	rVB	8859958	11800893	7.94%	4.222%
4	4.044	446	485	489	rBV	1541297	10821353	7.28%	3.872%
5	4.257	505	520	536	rBV	1003332	2761951	1.86%	0.988%
6	9.019	1291	1301	1307	rBV	13446194	23641116	15.91%	8.459%
7	9.183	1319	1328	1333	rBV	9551912	15043431	10.12%	5.383%
8	10.317	1507	1514	1524	rVB	3772582	5289681	3.56%	1.893%
9	11.207	1646	1660	1665	rBV3	41210424	148595884	100.00%	53.168%
10	11.262	1665	1669	1673	rVB	2368883	2664940	1.79%	0.954%
11	12.049	1789	1798	1803	rBV	1497088	2129542	1.43%	0.762%

Sum of corrected areas: 279484226

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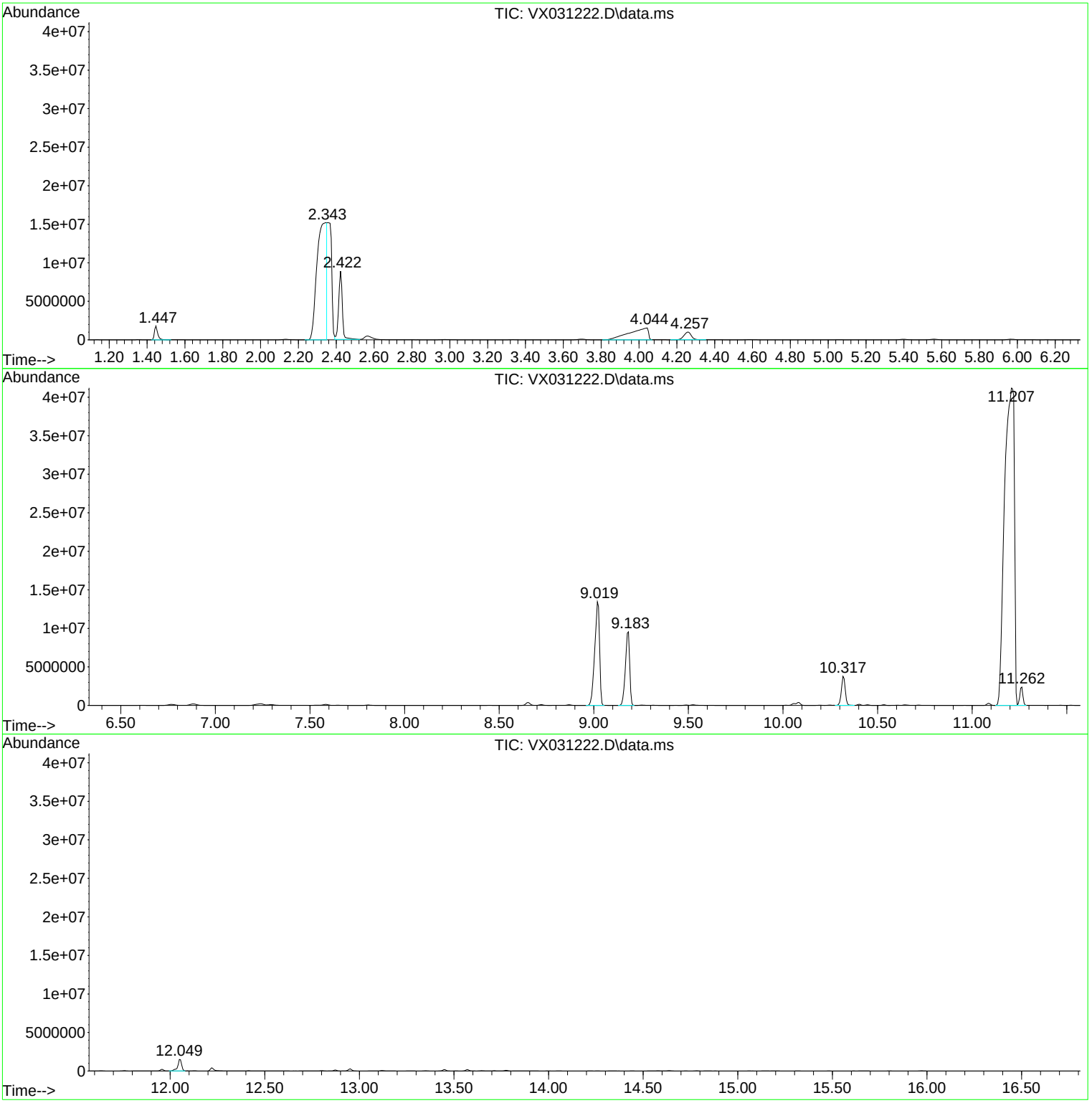
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090722W.M
Quant Title : SW846 8260

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



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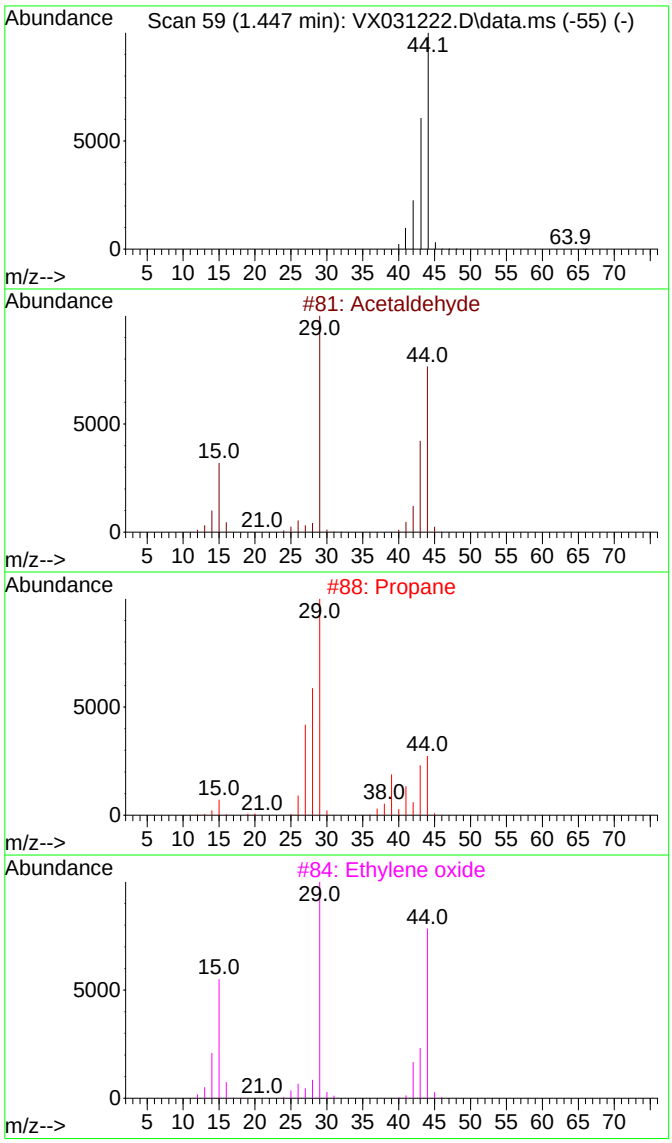
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090722W.M
Quant Title : SW846 8260

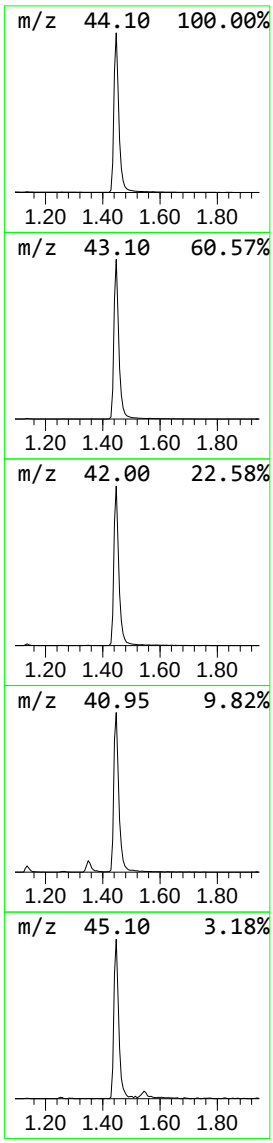
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Acetaldehyde Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.447	39.01 ug/l	2154850	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	64
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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Data File : VX031222.D
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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
CLI-79

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090722W.M
Quant Title : SW846 8260

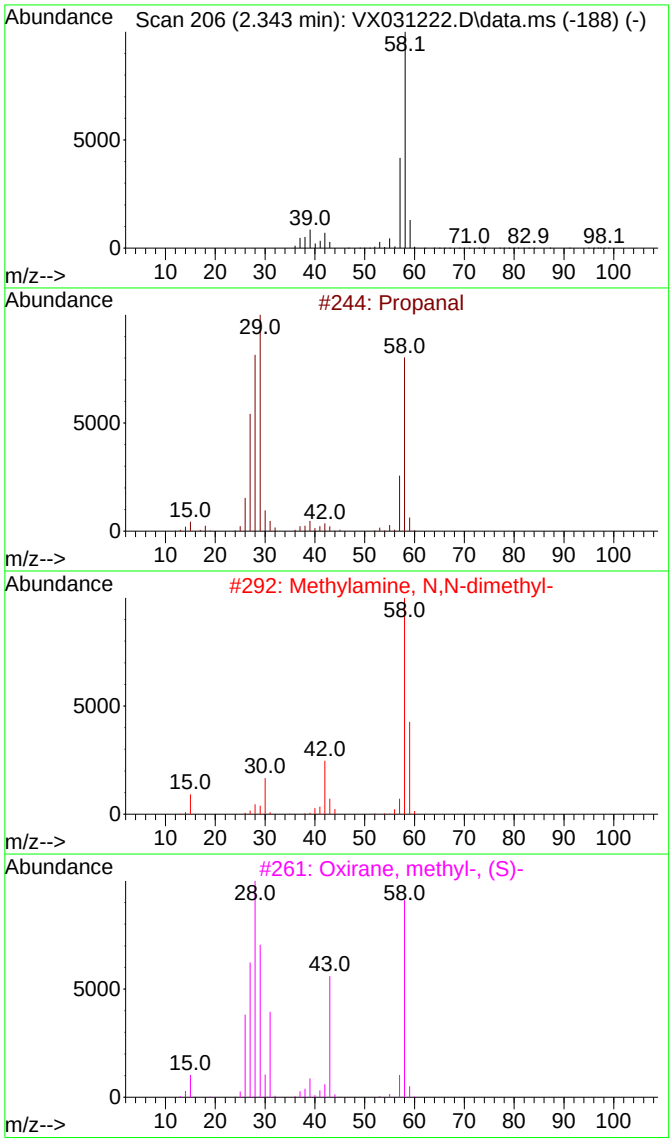
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

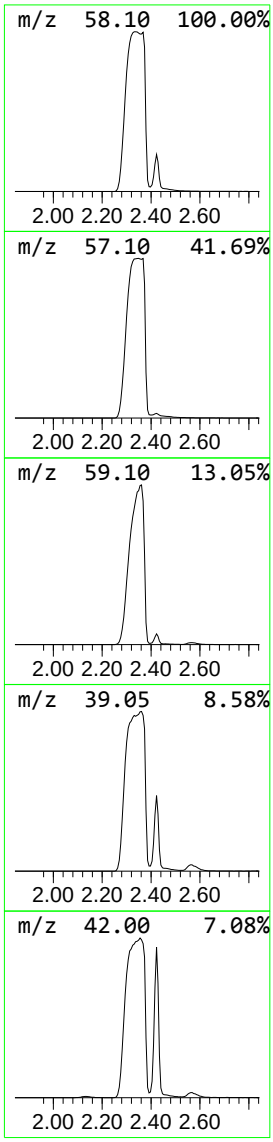
****

Peak Number 2 Propanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.343	988.08 ug/l	54580600	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal	58	C3H6O	000123-38-6	72
2	Methylamine, N,N-dimethyl-	59	C3H9N	000075-50-3	7
3	Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	4
4	Propylene oxide	58	C3H6O	000075-56-9	4
5	2-(Aminomethyl)-4-methylpentanoi...	187	C10H21NO2	1891211-54-3	4





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Operator : JC/MD
Sample : N4505-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
CLI-79

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090722W.M
Quant Title : SW846 8260

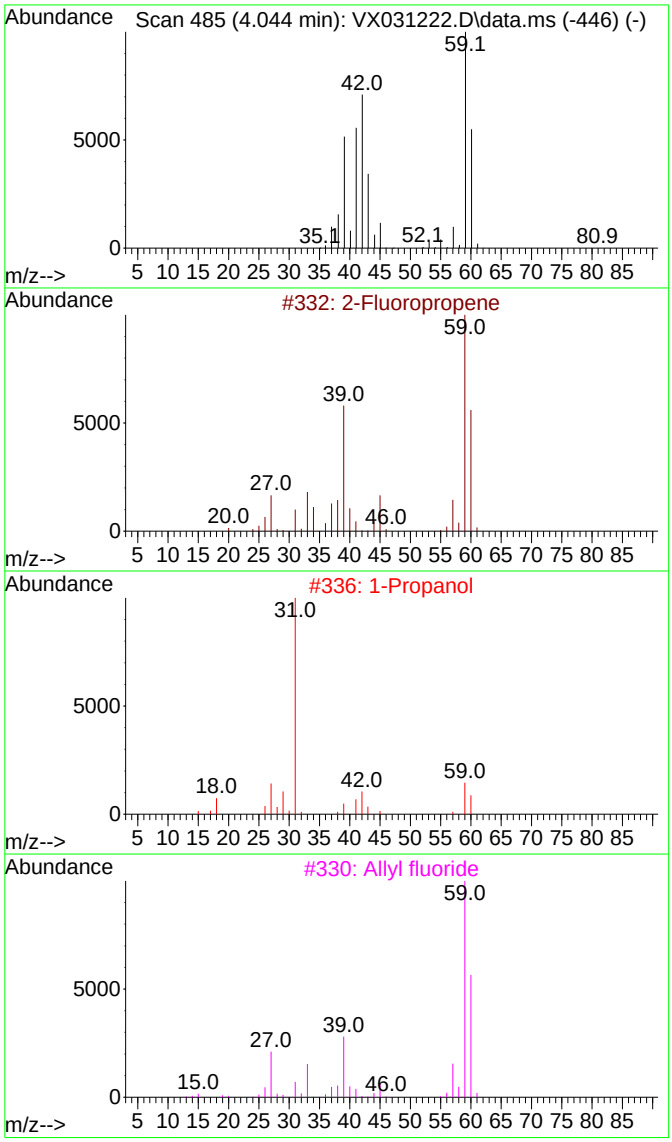
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

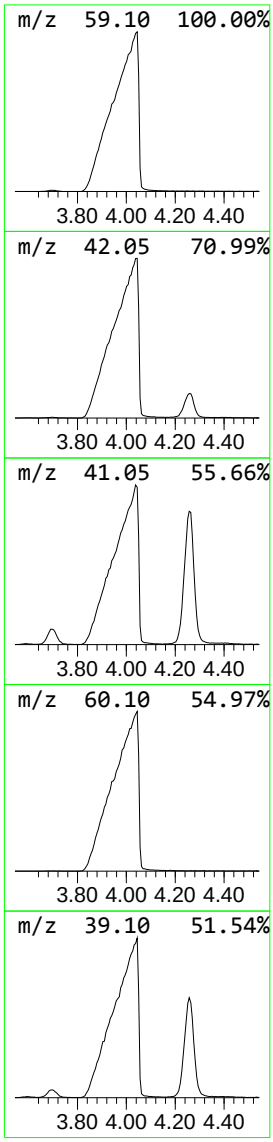
****

Peak Number 3 2-Fluoropropene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.044	195.90 ug/l	10821400	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Fluoropropene	60	C3H5F	001184-60-7	58
2	1-Propanol	60	C3H8O	000071-23-8	50
3	Allyl fluoride	60	C3H5F	000818-92-8	38
4	Cyclopropane	42	C3H6	000075-19-4	35
5	Propene	42	C3H6	000115-07-1	25





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Acq On : 08 Sep 2022 19:24
Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
CLI-79

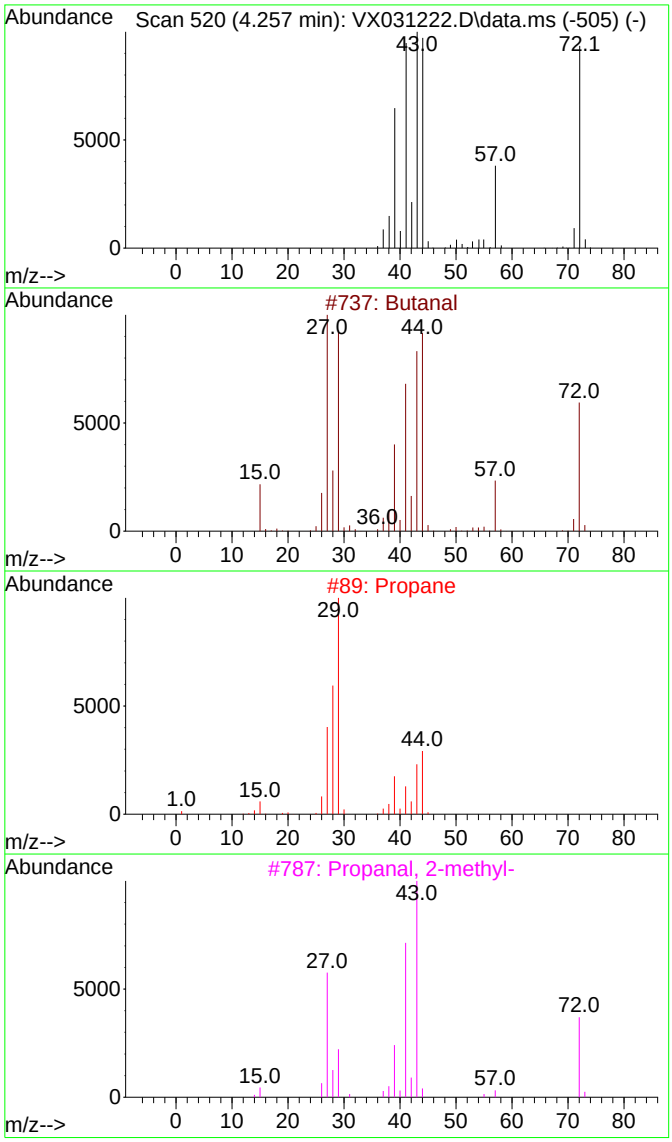
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090722W.M
Quant Title : SW846 8260

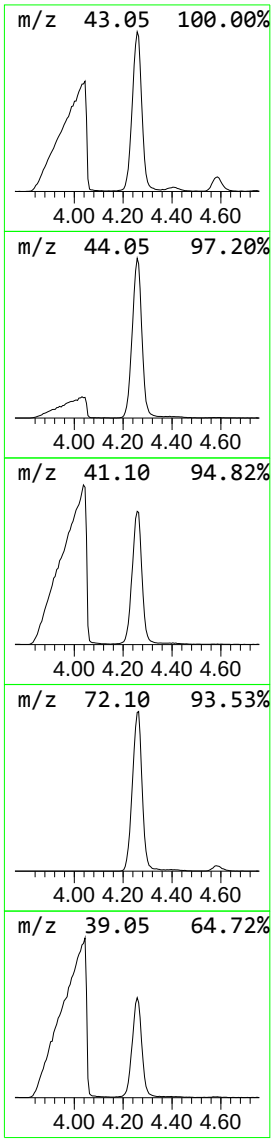
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Butanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.257	50.00 ug/l	2761950	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	91
2	Propane	44	C3H8	000074-98-6	47
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
4	2-Propanone, hydrazone	72	C3H8N2	005281-20-9	38
5	2-Propen-1-ol, 2-methyl-, acetate	114	C6H10O2	000820-71-3	33





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Operator : JC/MD
Sample : N4505-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
CLI-79

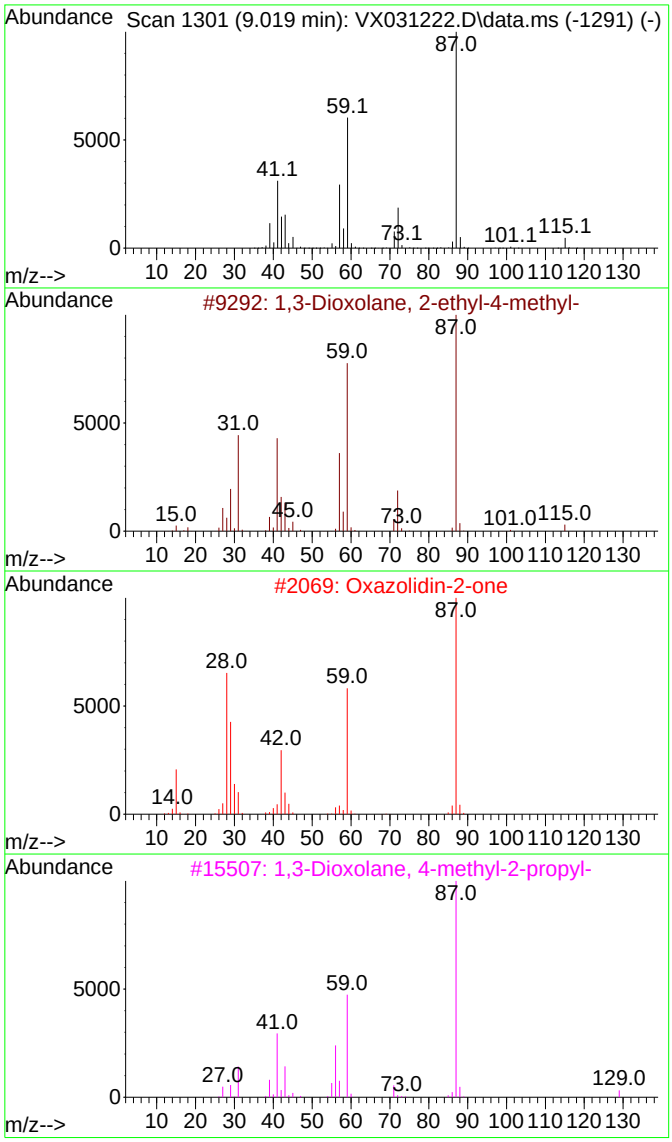
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090722W.M
Quant Title : SW846 8260

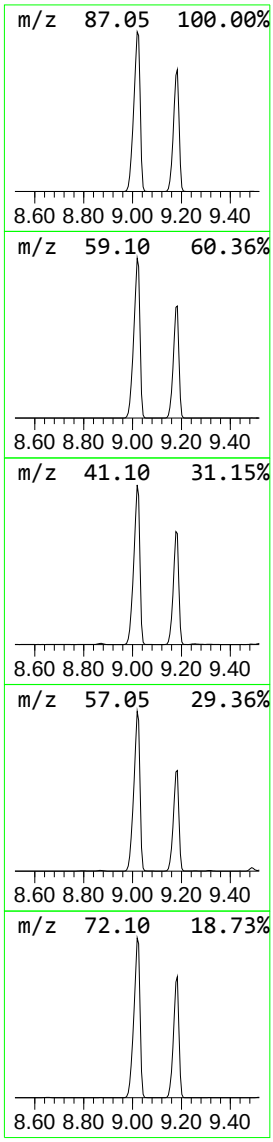
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1,3-Dioxolane, 2-ethyl-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.019	223.46 ug/l	23641100	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	90
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	2-Propanone, O-methyloxime	87	C4H9NO	003376-35-0	52
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	50





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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
CLI-79

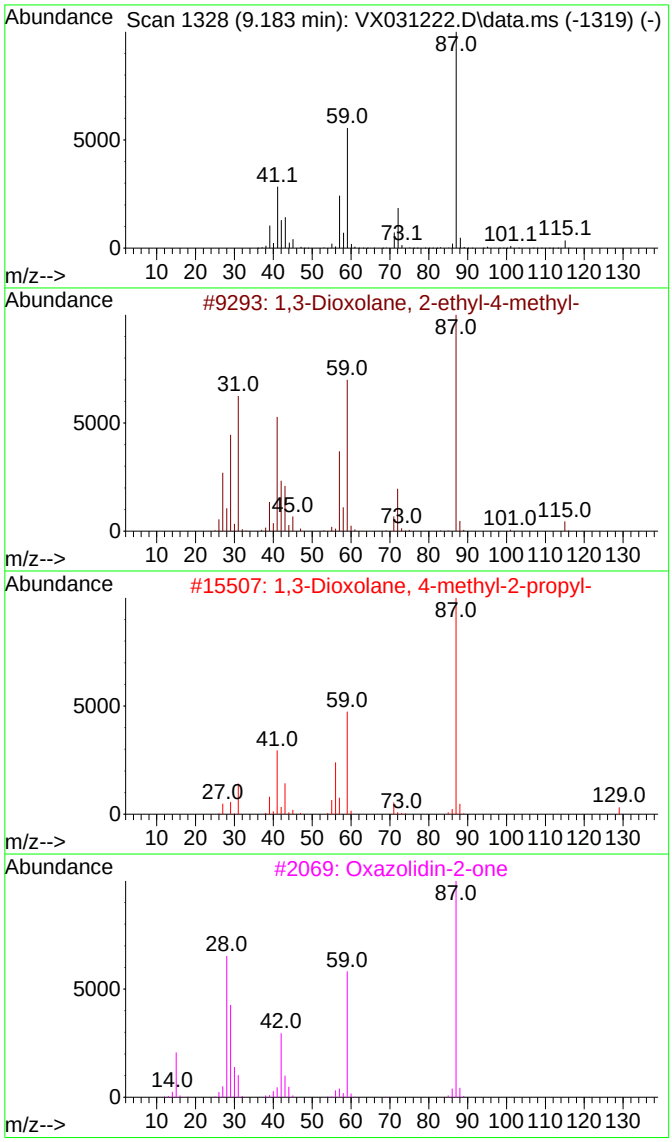
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090722W.M
Quant Title : SW846 8260

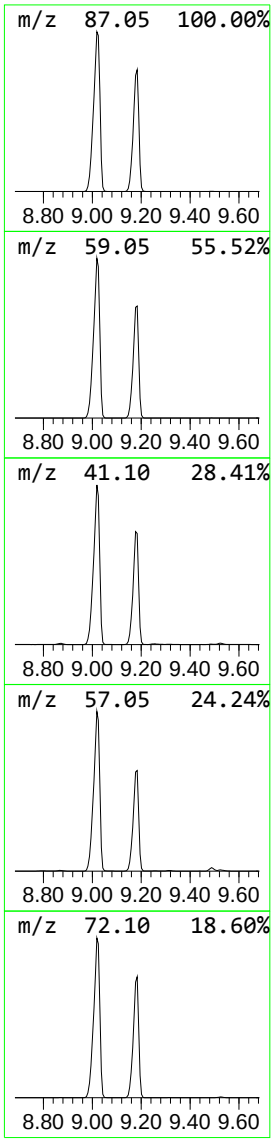
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1,3-Dioxolane, 4-methyl-2-p... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.183	142.20 ug/l	15043400	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	91
2	1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	72
3	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	56
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	53
5	2-Propanone, O-methyloxime	87	C4H9NO	003376-35-0	52





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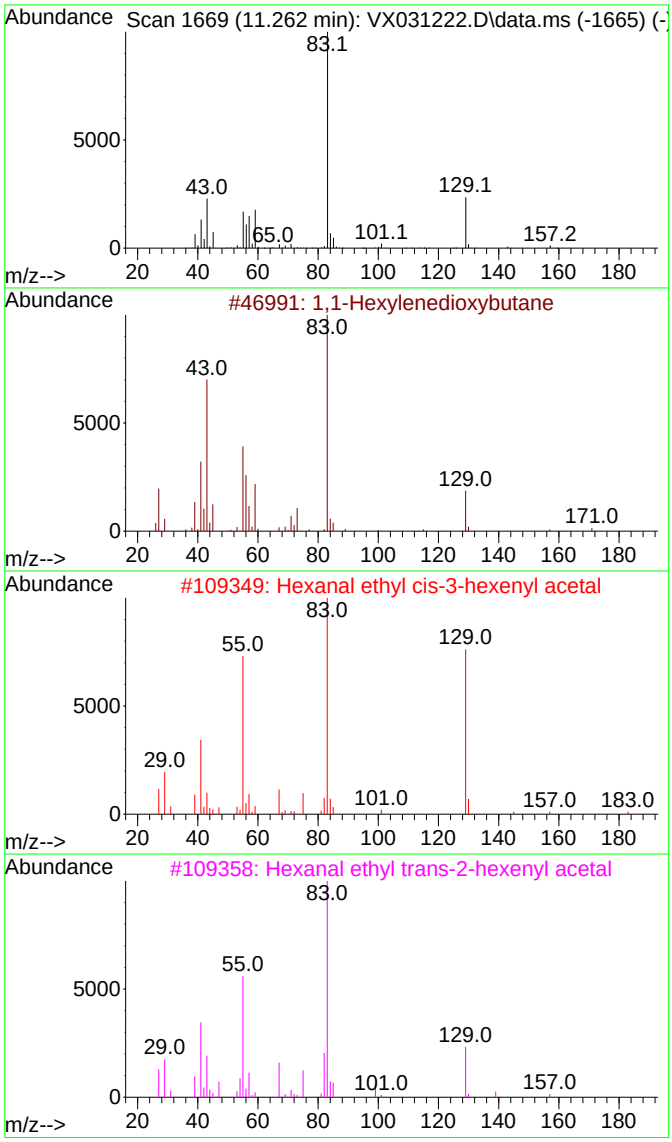
Quant Title : SW846 8260

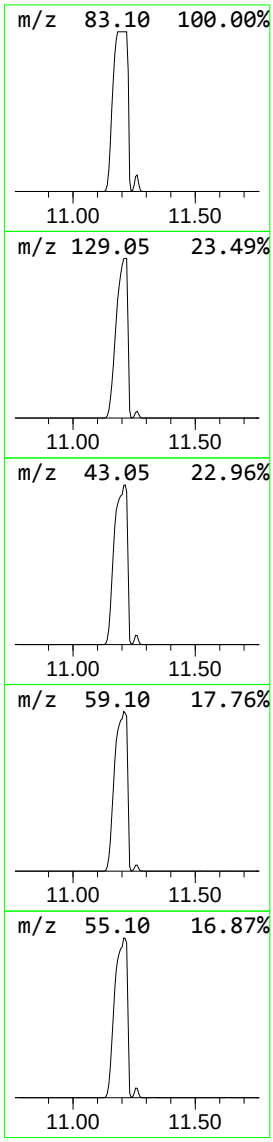
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1,1-Hexylenedioxybutane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.262	62.57 ug/l	2664940	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1-Hexylenedioxybutane	172	C10H20O2	1000249-77-4	78
2	Hexanal ethyl cis-3-hexenyl acetal	228	C14H28O2	1000431-42-9	64
3	Hexanal ethyl trans-2-hexenyl ac...	228	C14H28O2	1000431-42-6	56
4	.alpha.-Amino-2,5-dihydro-5-meth...	157	C7H11NO3	018455-25-9	53
5	5-Cyano-1,2,3-thiadiazole	111	C3HN3S	057352-02-0	45





Tentatively Identified Compound (LSC) summary

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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Acetaldehyde	1.447	39.0	ug/l	2154850	1	5.556	2761950	50.0
Propanal	2.343	988.1	ug/l	54580600	1	5.556	2761950	50.0
2-Fluoropropene	4.044	195.9	ug/l	10821400	1	5.556	2761950	50.0
Butanal	4.257	50.0	ug/l	2761950	1	5.556	2761950	50.0
1,3-Dioxolane, ...	9.019	223.5	ug/l	23641100	3	10.055	5289680	50.0
1,3-Dioxolane, ...	9.183	142.2	ug/l	15043400	3	10.055	5289680	50.0
1,1-Hexylenedio...	11.262	62.6	ug/l	2664940	4	12.024	2129540	50.0