LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090622\
Data File : VX031131.D
Acq On : 06 Sep 2022 16:26
Operator : JC/MD
Sample : N4489-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0045

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\82X090122W.M
Title : SW846 8260

Signal : TIC: VX031131.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.392	48	50	93	rBV3	28863170	116821170	100.00%	79.835%
2	2.166	153	177	191	rBV2	4690184	20730026	17.75%	14.167%
3	2.288	192	197	207	rVV	934531	1640154	1.40%	1.121%
4	4.233	501	516	533	rBV	1619895	4379404	3.75%	2.993%
5	6.629	895	909	914	rBV4	432408	1281014	1.10%	0.875%
6	12.219	1819	1826	1834	rBV	968499	1476080	1.26%	1.009%

Sum of corrected areas: 146327848

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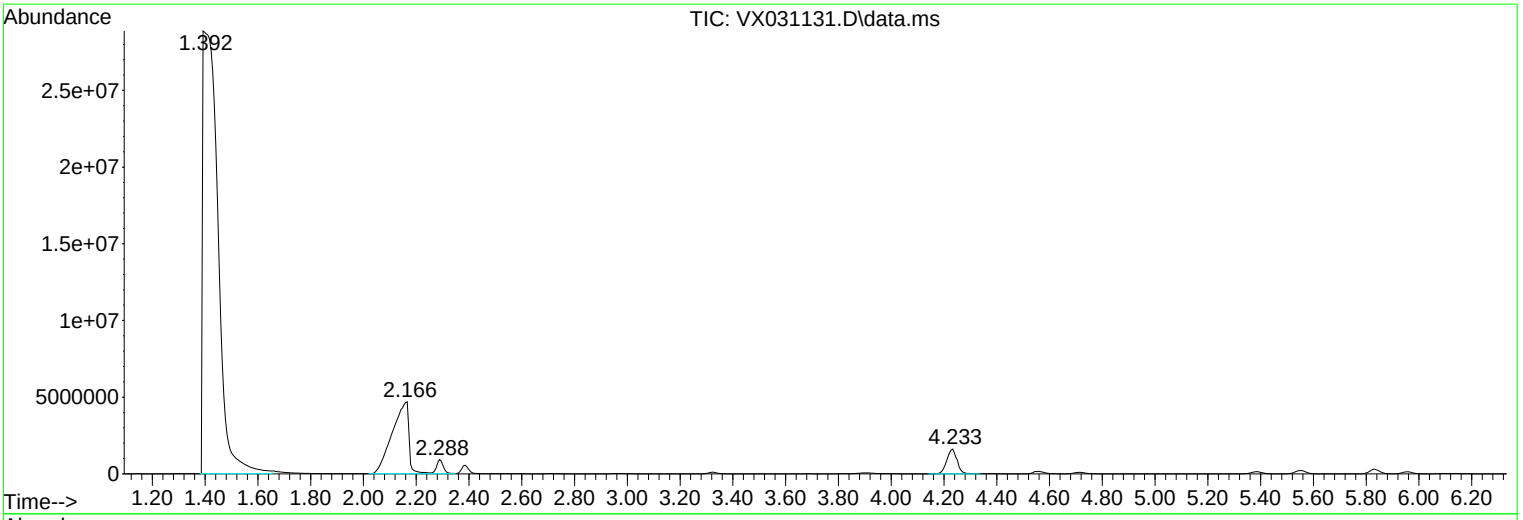
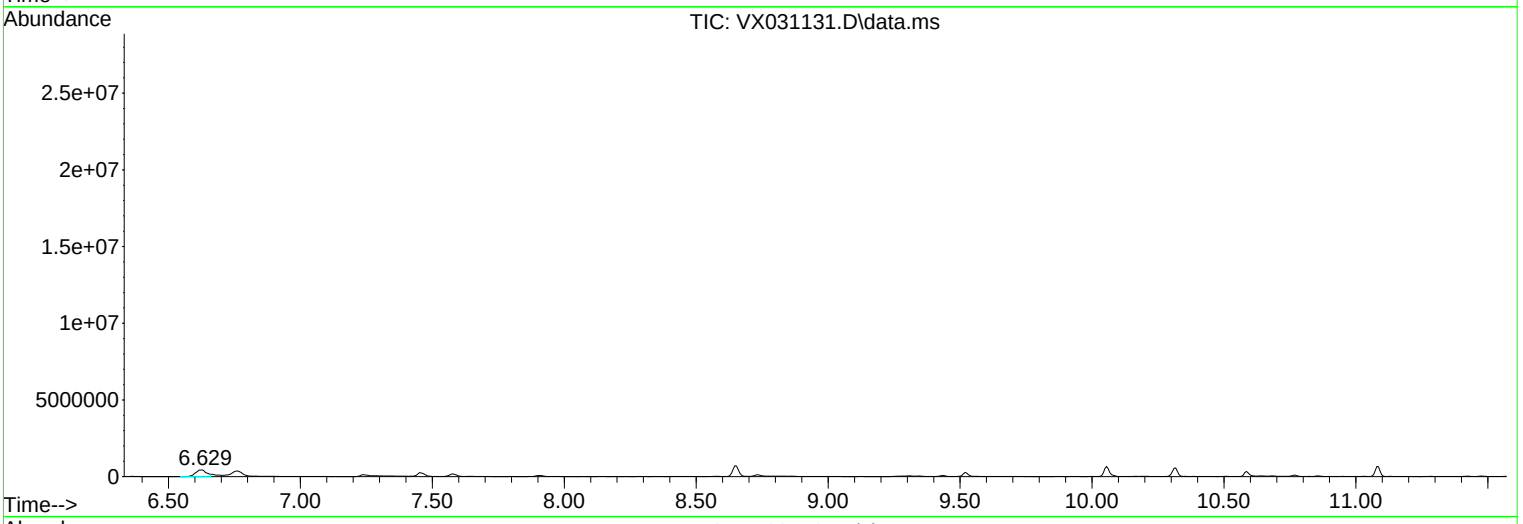
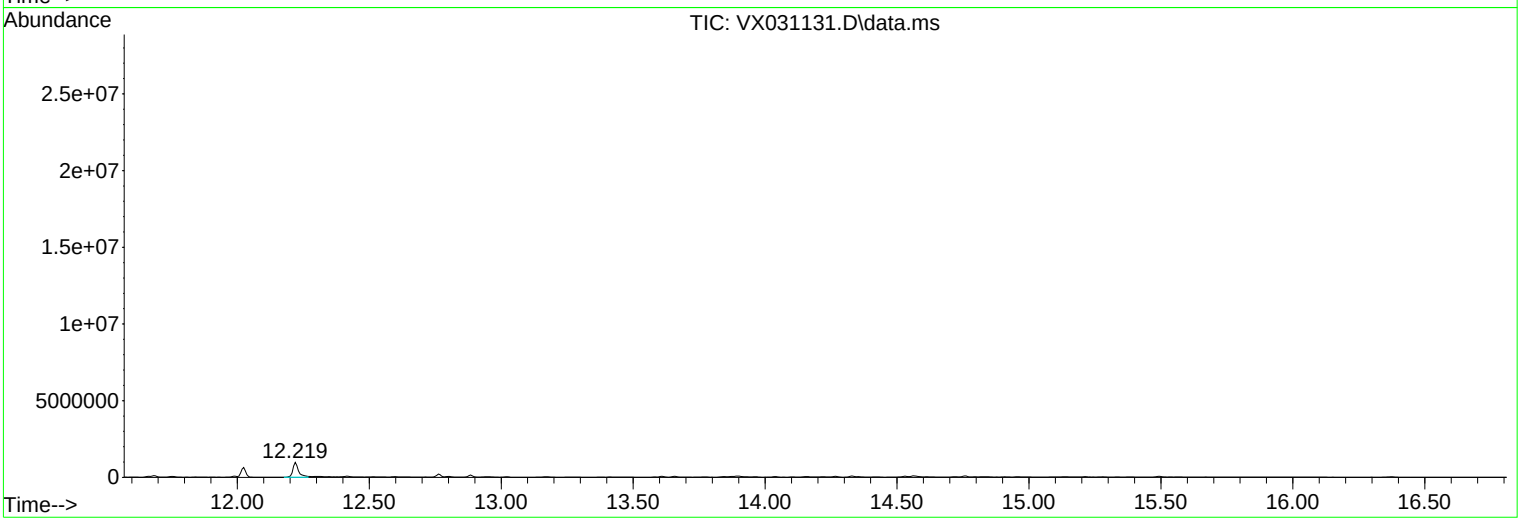
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090122W.M
Quant Title : SW846 8260

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







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Quant Title : SW846 8260

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

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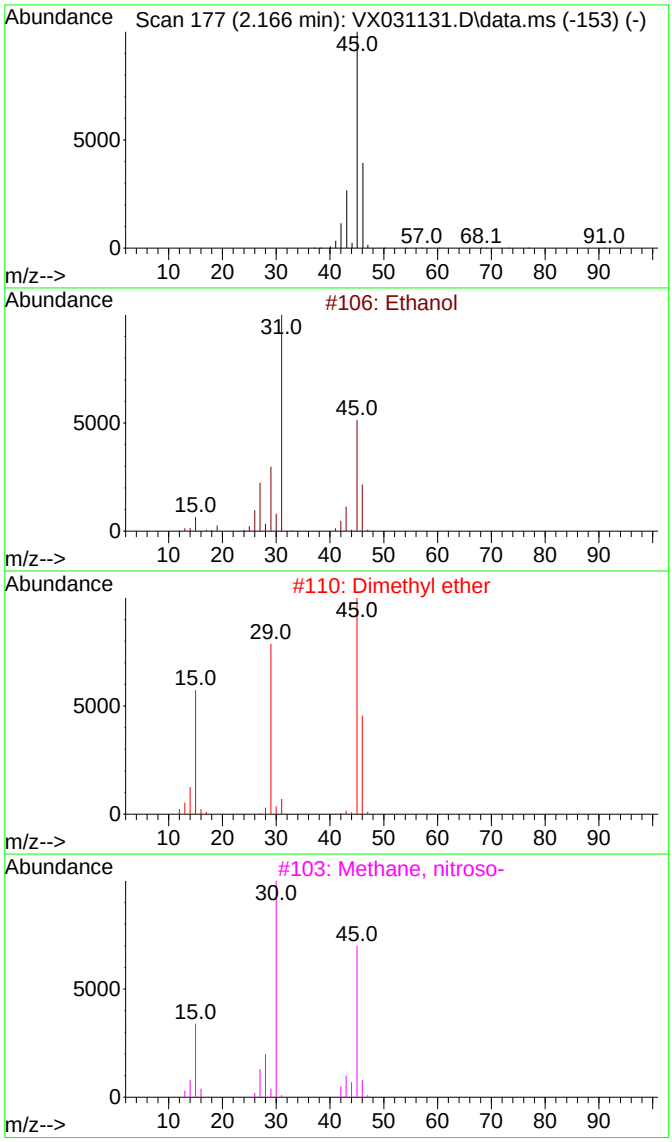
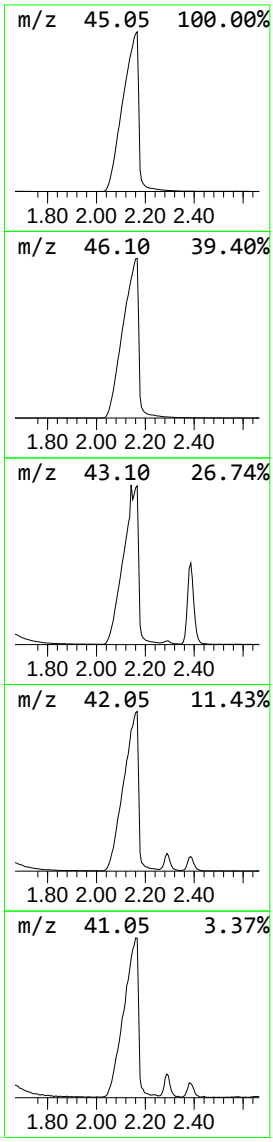
Peak Number 2 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.166	809.13 ug/l	20730000	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	64
2	Dimethyl ether	46	C2H6O	000115-10-6	9
3	Methane, nitroso-	45	CH3NO	000865-40-7	4
4	Formic acid	46	CH2O2	000064-18-6	4
5	L-Lactic acid	90	C3H6O3	000079-33-4	2





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MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090122W.M
Quant Title : SW846 8260

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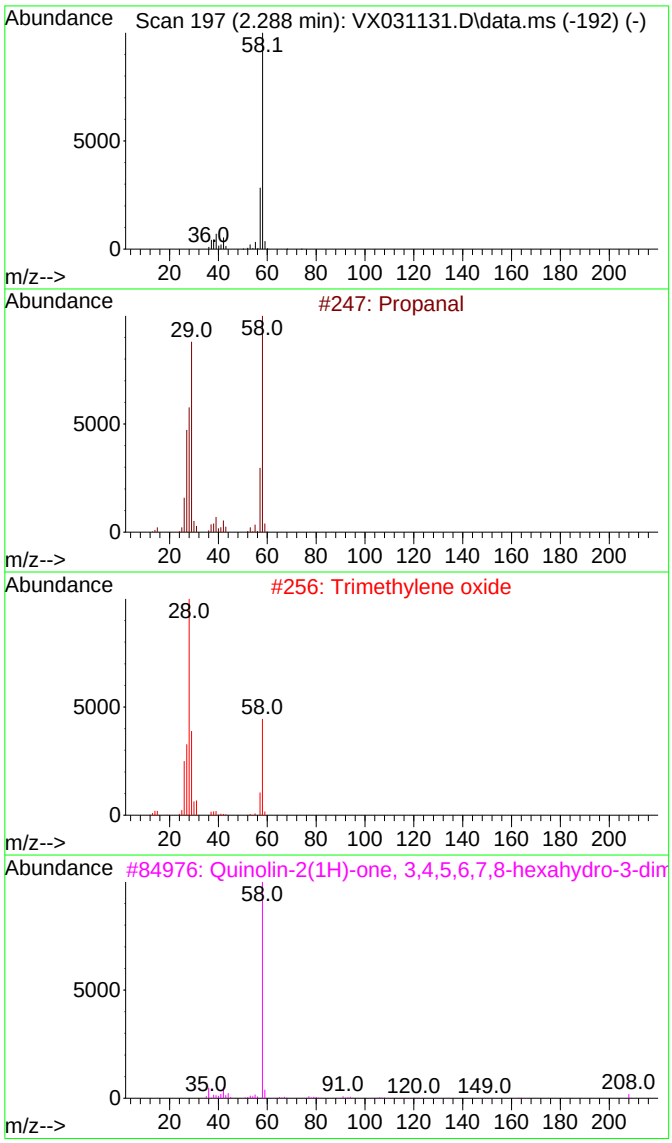
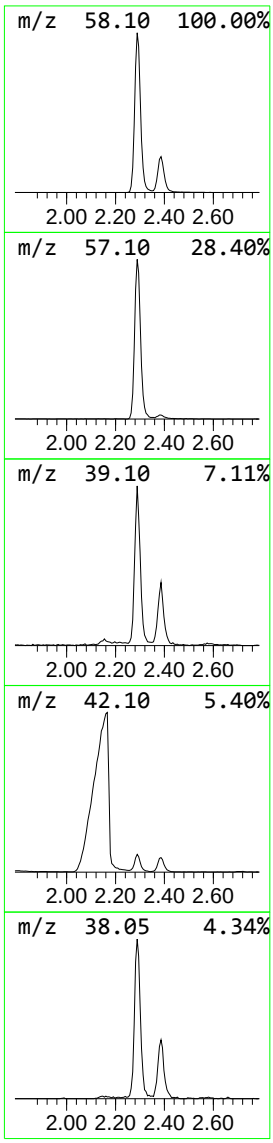
Peak Number 3 Propanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.288	64.02 ug/l	1640150	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal	58	C3H6O	000123-38-6	78
2	Trimethylene oxide	58	C3H6O	000503-30-0	56
3	Quinolin-2(1H)-one, 3,4,5,6,7,8-...	208	C12H20N2O	1000259-95-6	9
4	Borane, compd. with dimethylamin...	59	C2H10BN	000074-94-2	7
5	Propylene oxide	58	C3H6O	000075-56-9	5





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MSVOA_X
ClientSampleId :
ORA-0045

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090122W.M
Quant Title : SW846 8260

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

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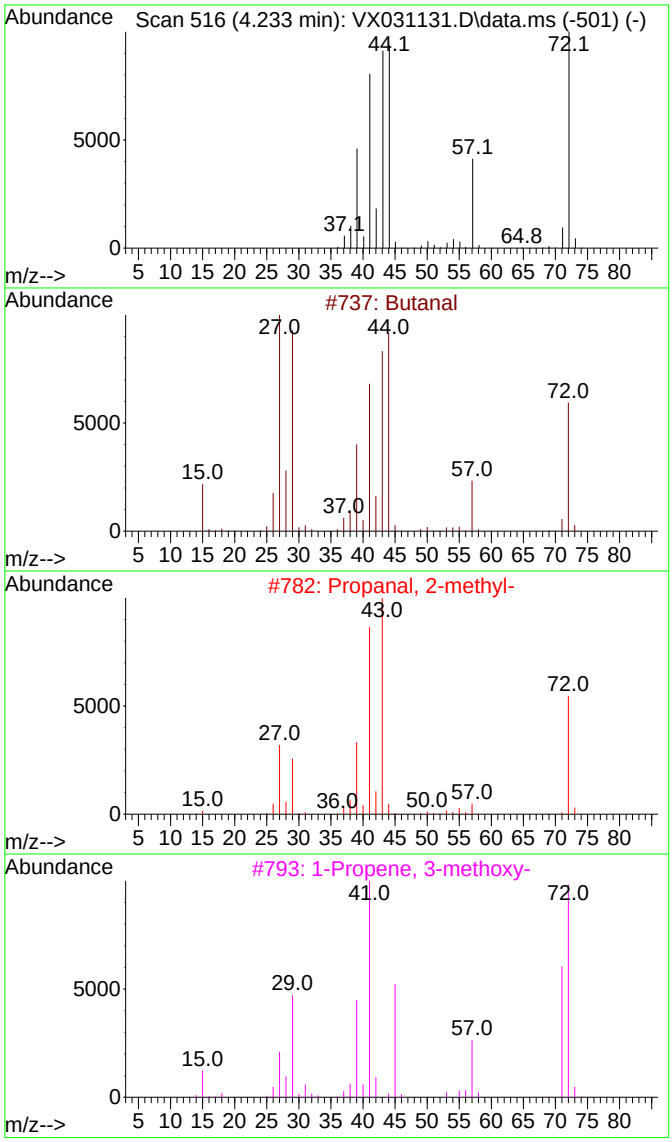
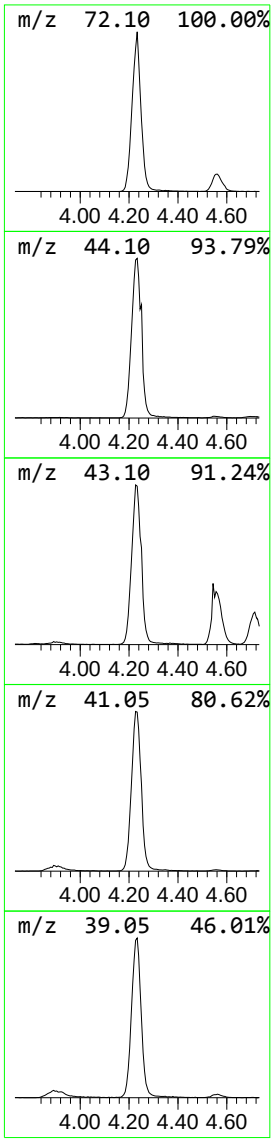
Peak Number 4 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.233	170.94 ug/l	4379400	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	91
2	Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
3	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	37
4	2-Propanone, hydrazone	72	C3H8N2	005281-20-9	35
5	Isobutylene epoxide	72	C4H8O	000558-30-5	27





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Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090122W.M
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TIC Library : C:\Database\NIST20.L
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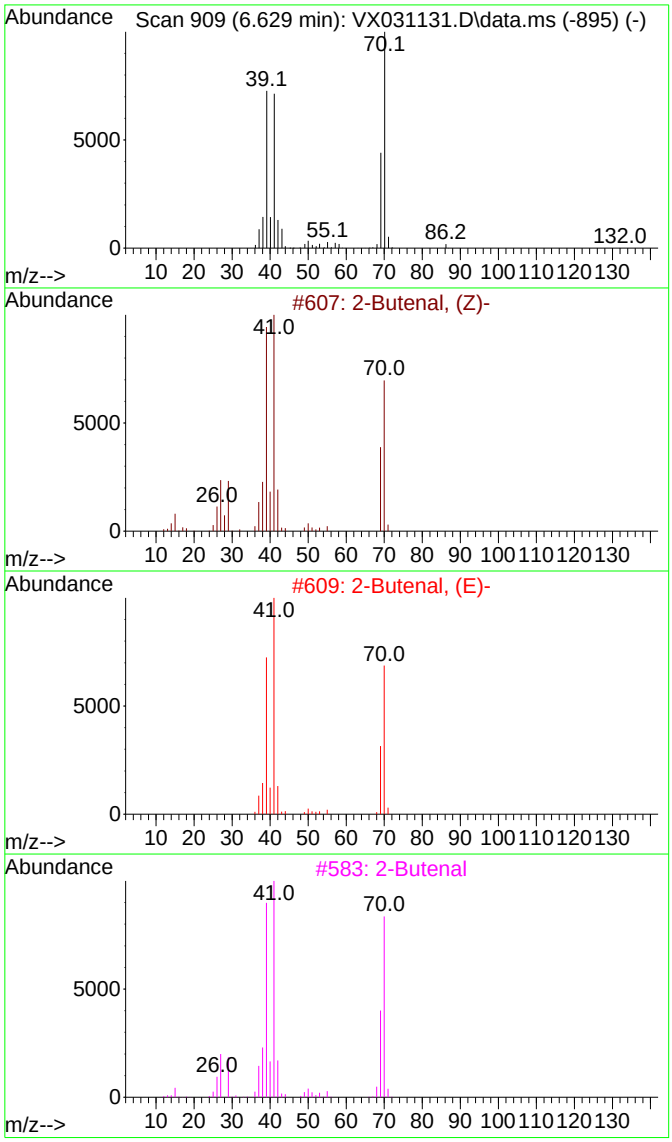
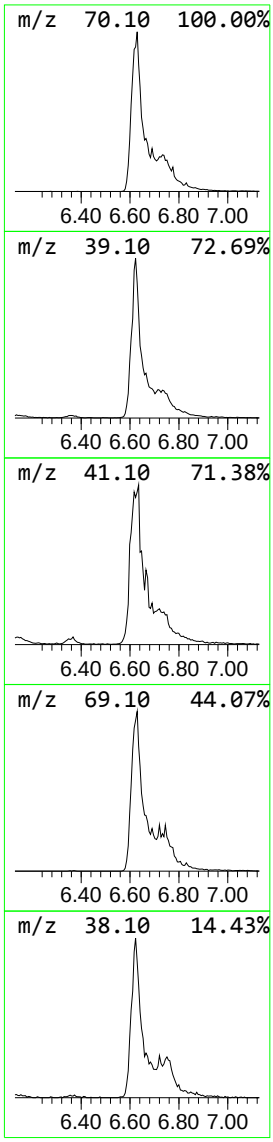
****
Peak Number 5 2-Butenal, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.629	50.00 ug/l	1281010	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenal, (Z)-	70	C4H6O	015798-64-8	91
2	2-Butenal, (E)-	70	C4H6O	000123-73-9	91
3	2-Butenal	70	C4H6O	004170-30-3	90
4	Furan, 2,3-dihydro-	70	C4H6O	001191-99-7	86
5	Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	80





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Quant Title : SW846 8260

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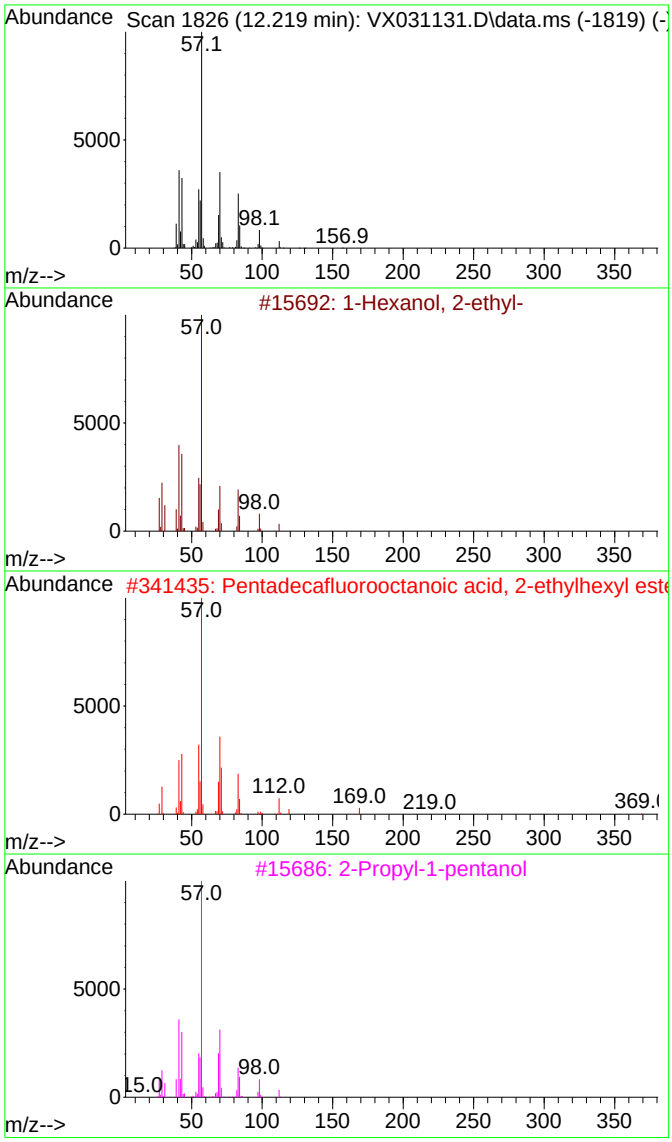
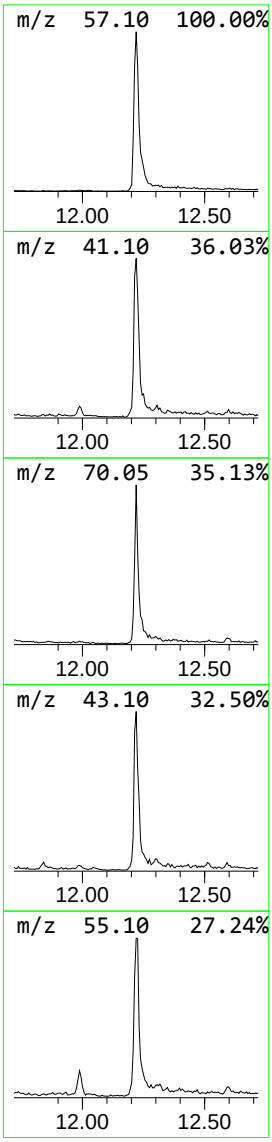
****
Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	50.00 ug/l	1476080	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	64
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	64
4	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
5	Bicyclo[3.1.0]hexan-2-ol	98	C6H10O	1000194-18-6	43





Tentatively Identified Compound (LSC) summary

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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090122W.M
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
Ethanol	2.166	809.1	ug/l	20730000	1	5.550	1281010	50.0
Propanal	2.288	64.0	ug/l	1640150	1	5.550	1281010	50.0
Butanal	4.233	170.9	ug/l	4379400	1	5.550	1281010	50.0
2-Butenal, (Z)-	6.629	50.0	ug/l	1281010	2	6.763	1281010	50.0
1-Hexanol, 2-et...	12.219	50.0	ug/l	1476080	4	12.024	1476080	50.0