LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX100623\
Data File : VX038122.D
Acq On : 06 Oct 2023 11:51
Operator : JC/MD
Sample : 04720-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-1041

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\82X100523W.M
Title : SW846 8260

Signal : TIC: VX038122.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.429	54	56	57	rBV	17534776	12456144	100.00%	54.654%
2	2.057	152	159	190	rVB	833169	1432691	11.50%	6.286%
3	4.227	503	515	537	rBV	607974	1608866	12.92%	7.059%
4	5.385	694	705	722	rBV	83369	243292	1.95%	1.067%
5	5.550	722	732	747	rBV2	135091	390018	3.13%	1.711%
6	5.830	768	778	790	rBV	76134	209800	1.68%	0.921%
7	5.958	790	799	808	rBV	97244	249085	2.00%	1.093%
8	6.763	921	931	946	rVB	216800	530277	4.26%	2.327%
9	7.202	994	1003	1024	rBV	284274	632088	5.07%	2.773%
10	8.647	1234	1240	1248	rBV	454166	744150	5.97%	3.265%
11	9.232	1331	1336	1355	rBV	91960	171853	1.38%	0.754%
12	10.055	1465	1471	1482	rBV	501313	698671	5.61%	3.066%
13	10.311	1507	1513	1524	rVB	433396	581329	4.67%	2.551%
14	11.079	1632	1639	1645	rBV	521152	688819	5.53%	3.022%
15	11.683	1734	1738	1746	rBV	173172	206965	1.66%	0.908%
16	12.024	1789	1794	1802	rVB	540881	725571	5.83%	3.184%
17	12.219	1817	1826	1837	rBV2	582141	1008501	8.10%	4.425%
18	12.884	1930	1935	1940	rBV	180647	212810	1.71%	0.934%

Sum of corrected areas: 22790930

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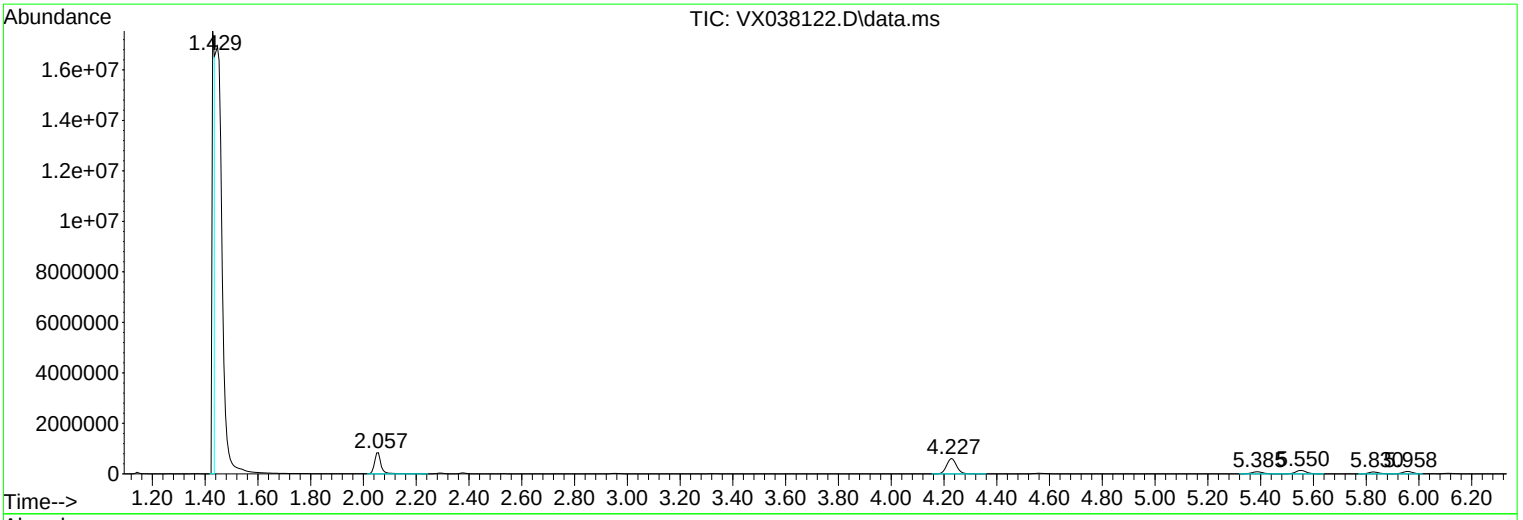
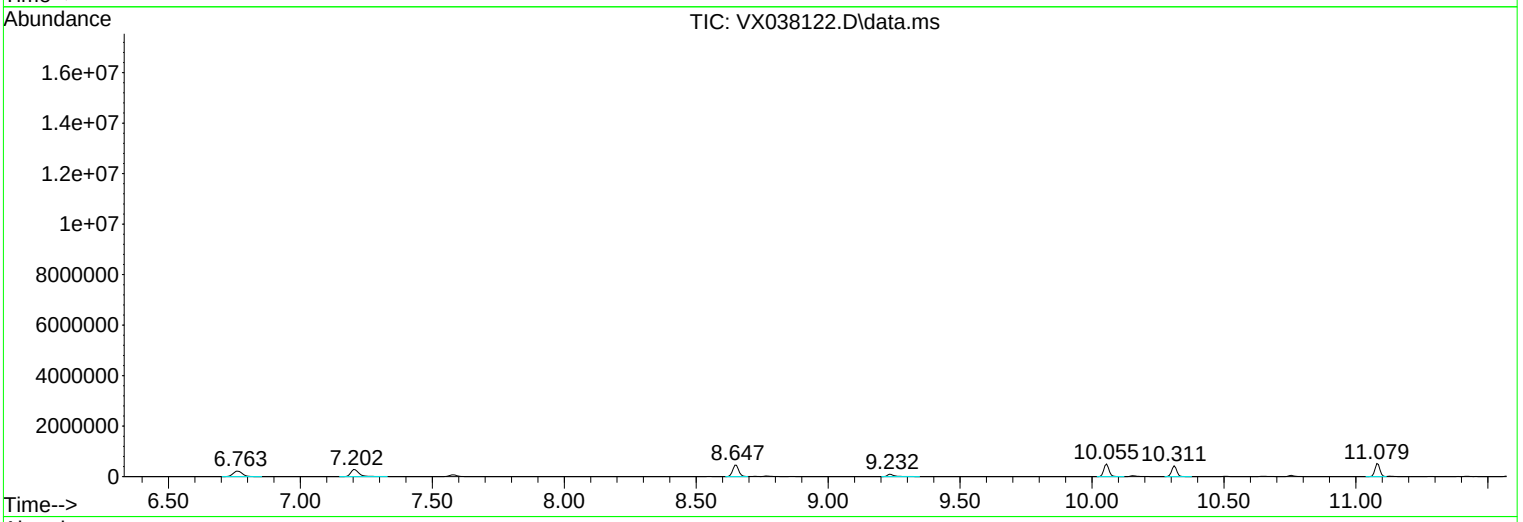
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

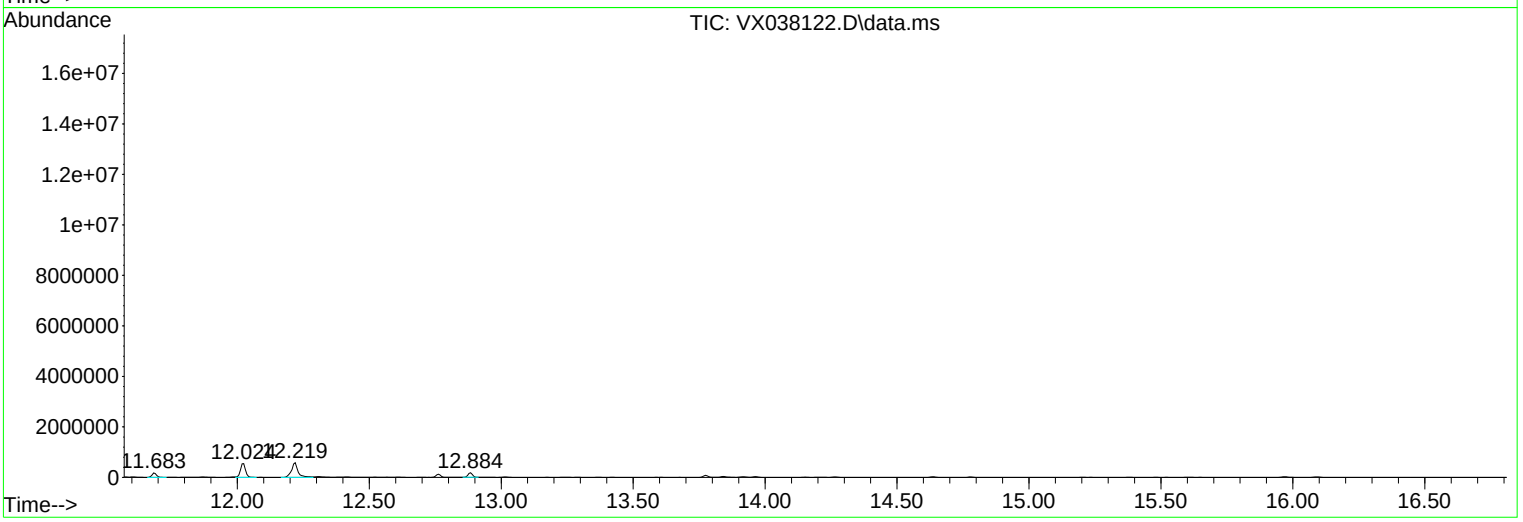
Instrument :
MSVOA_X
ClientSampleId :
ORA-1041

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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







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Data File : VX038122.D
Acq On : 06 Oct 2023 11:51
Operator : JC/MD
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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-1041

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

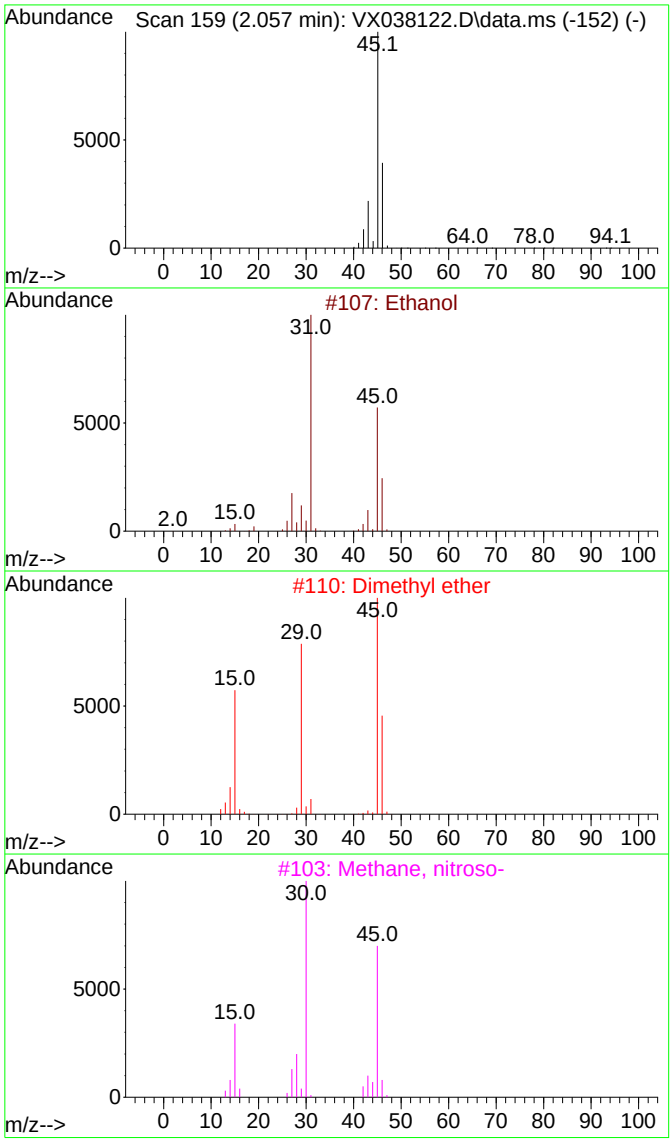
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

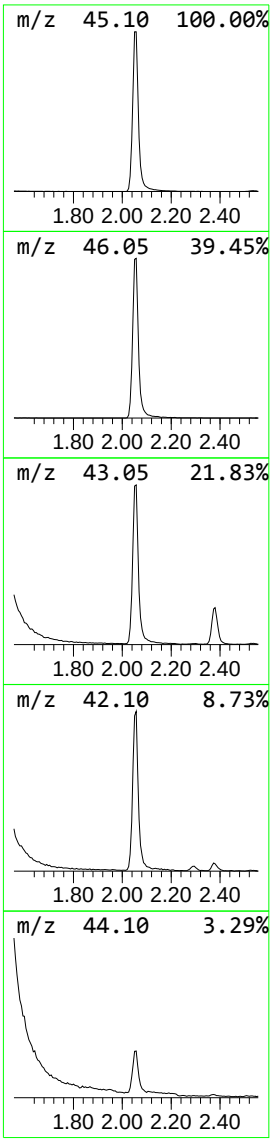
****

Peak Number 2 Ethanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.057	183.67 ug/l	1432690	Pentafluorobenzene	5.556

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	Oxalic acid	90	C2H2O4	000144-62-7	4





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Data File : VX038122.D
Acq On : 06 Oct 2023 11:51
Operator : JC/MD
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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-1041

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

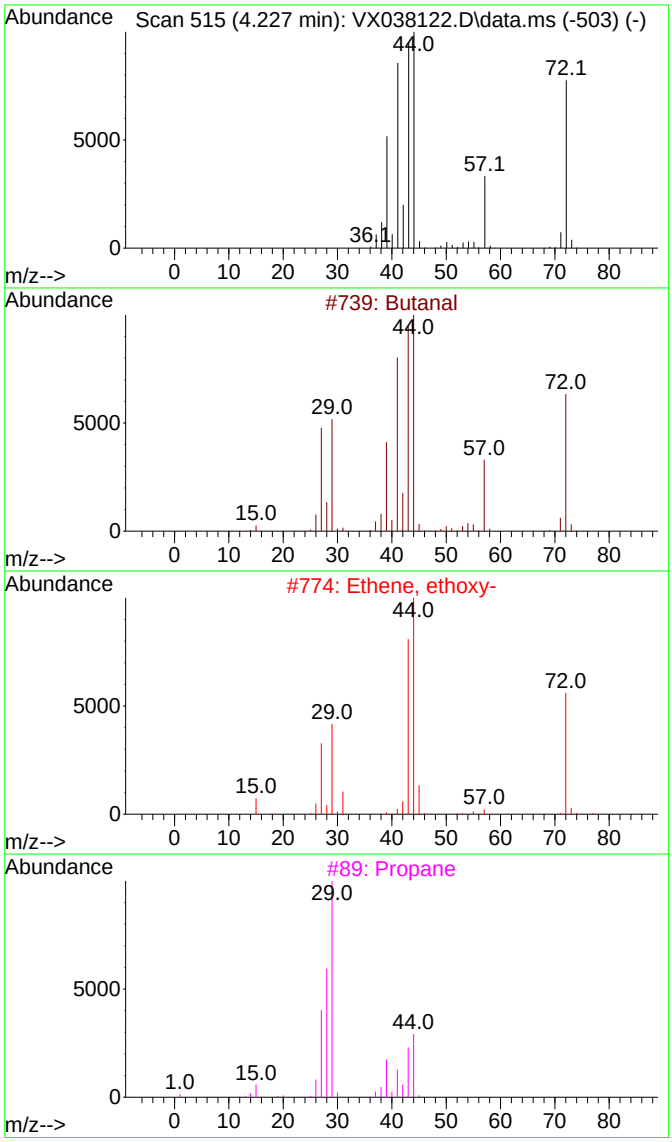
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

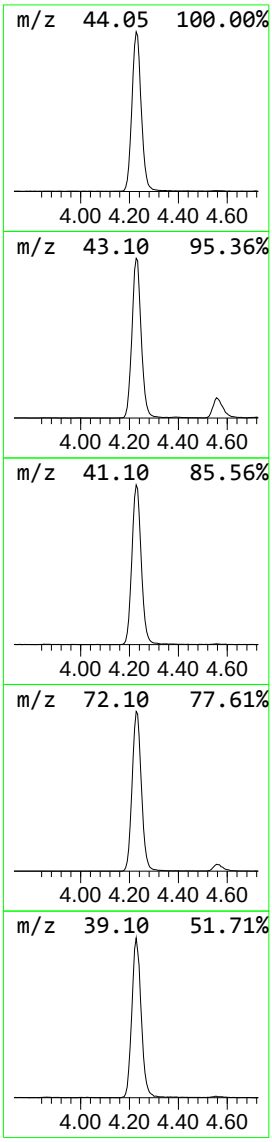
****

Peak Number 3 Butanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.227	206.26 ug/l	1608870	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	91
2	Ethene, ethoxy-	72	C4H8O	000109-92-2	52
3	Propane	44	C3H8	000074-98-6	47
4	Propanal, 2-methyl-	72	C4H8O	000078-84-2	46
5	2-Propanone, hydrazone	72	C3H8N2	005281-20-9	38





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Data File : VX038122.D
Acq On : 06 Oct 2023 11:51
Operator : JC/MD
Sample : 04720-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-1041

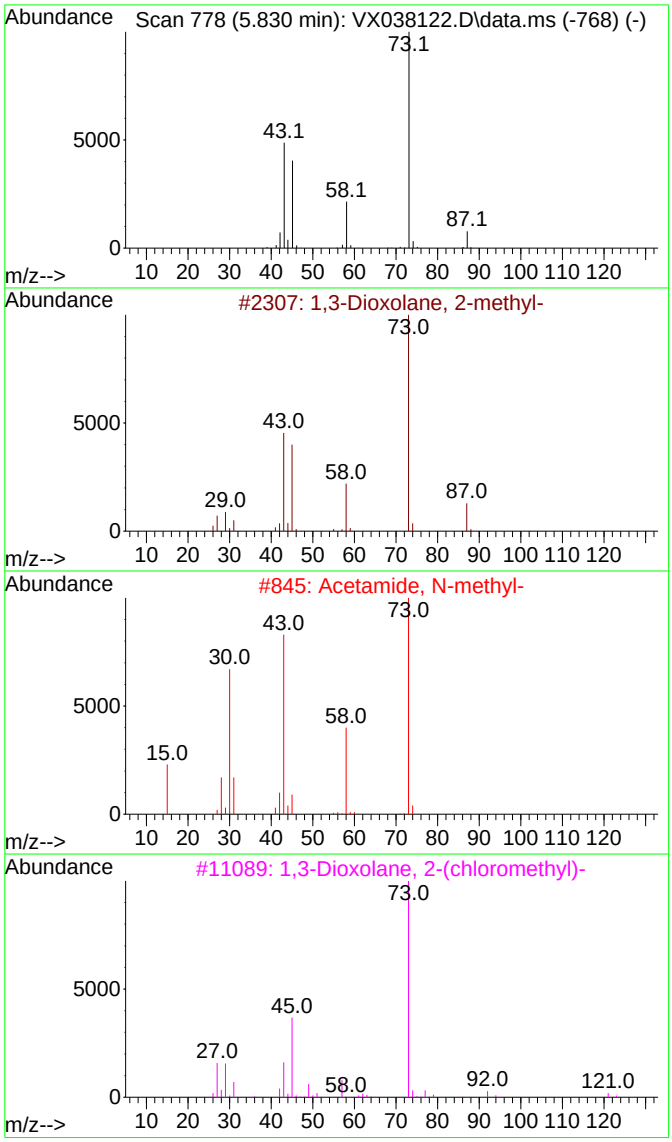
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

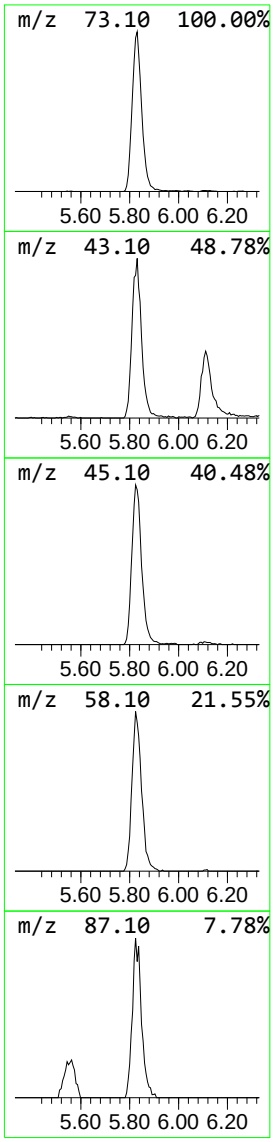
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.830	26.90 ug/l	209800	Pentafluorobenzene	5.556

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	9
3	1,3-Dioxolane, 2-(chloromethyl)-	122	C4H7ClO2	002568-30-1	9
4	2,2'-Bi-1,3-dioxolane	146	C6H10O4	006705-89-1	9
5	2-Acetamido-N-methylacetamide	130	C5H10N2O2	007606-79-3	9





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Data File : VX038122.D
Acq On : 06 Oct 2023 11:51
Operator : JC/MD
Sample : 04720-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-1041

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

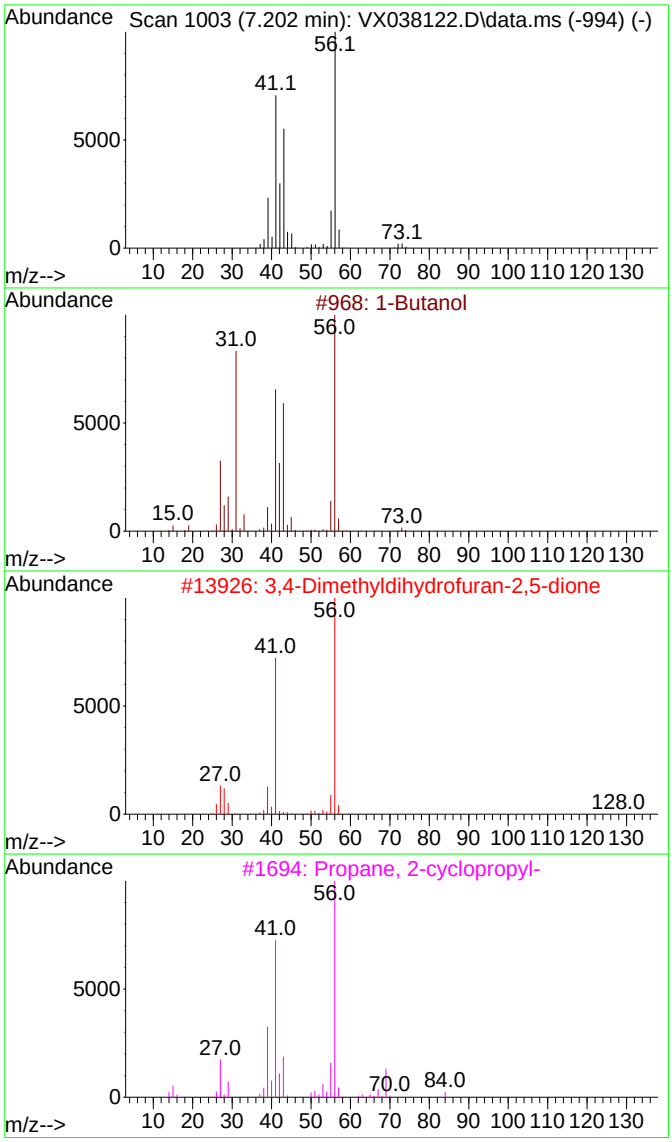
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

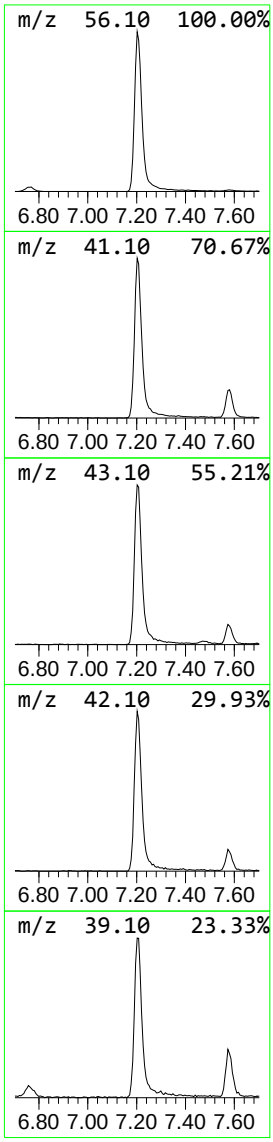
****

Peak Number 5 1-Butanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.202	59.60 ug/l	632088	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	86
2	3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	40
3	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	36
4	Formic acid, butyl ester	102	C5H10O2	000592-84-7	9
5	3-Butenoic acid, 2-amino-	101	C4H7NO2	056512-51-7	9





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Data File : VX038122.D
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Operator : JC/MD
Sample : 04720-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-1041

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

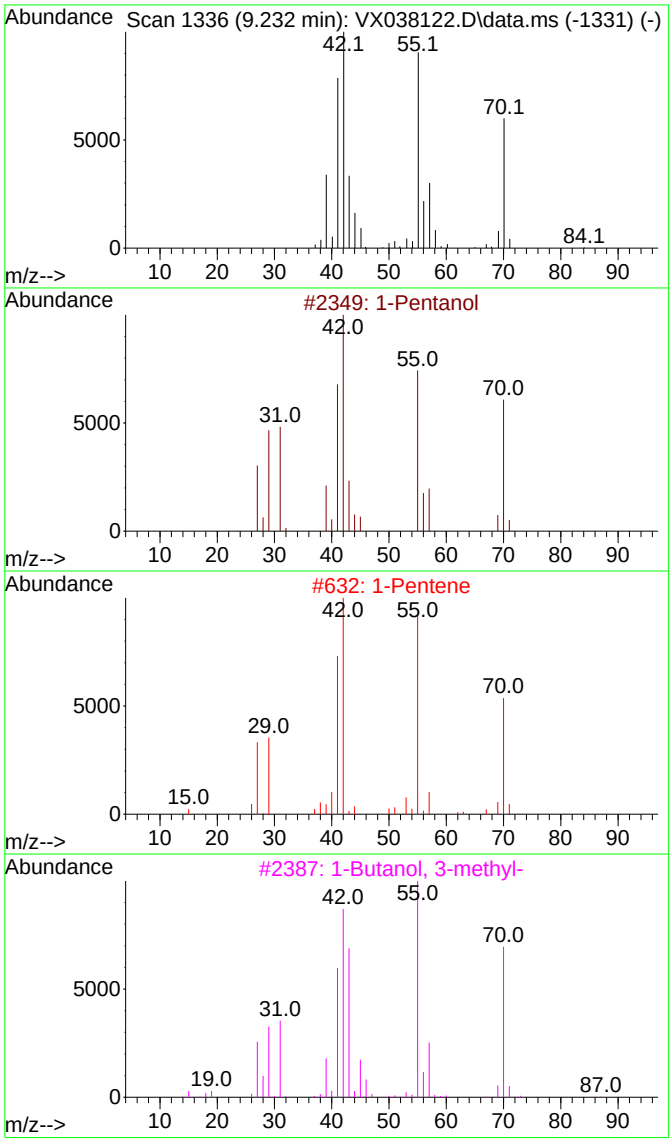
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

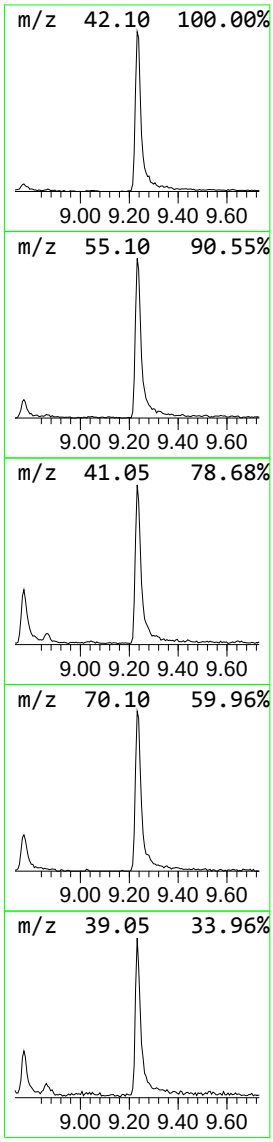
****

Peak Number 6 1-Pentanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.232	12.30 ug/l	171853	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentanol	88	C5H12O	000071-41-0	90
2	1-Pentene	70	C5H10	000109-67-1	72
3	1-Butanol, 3-methyl-	88	C5H12O	000123-51-3	59
4	Cyclopentane	70	C5H10	000287-92-3	53
5	2-Pentene	70	C5H10	000109-68-2	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX100623\
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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-1041

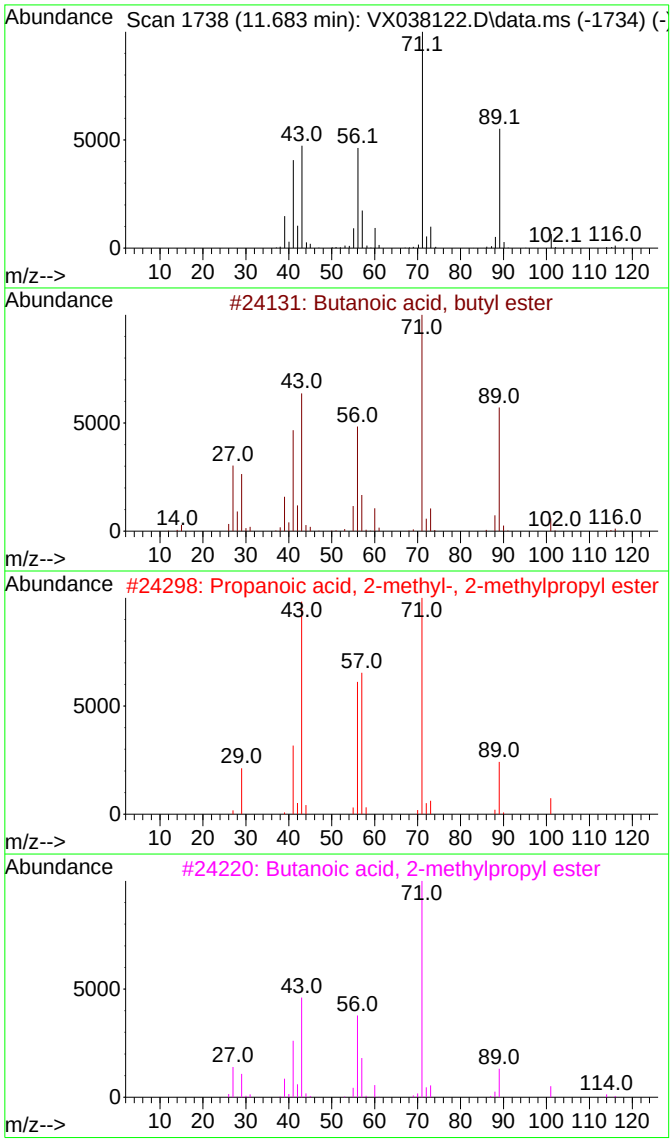
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

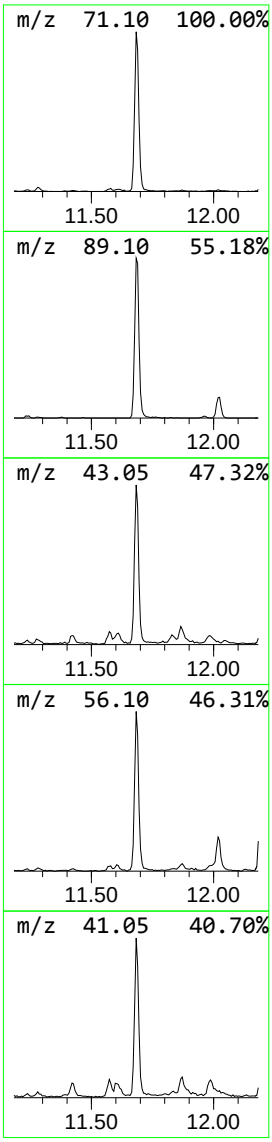
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Butanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.683	14.26 ug/l	206965	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	90
2	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	72
3	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	72
4	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	53
5	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	50





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Instrument :
MSVOA_X
ClientSampleId :
ORA-1041

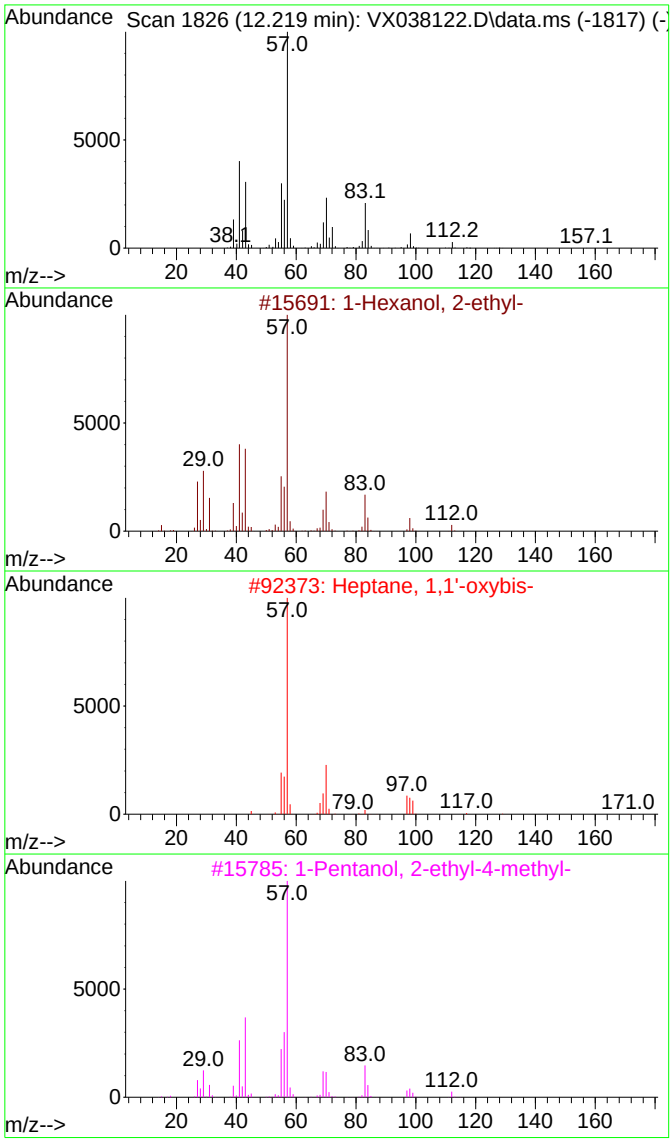
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

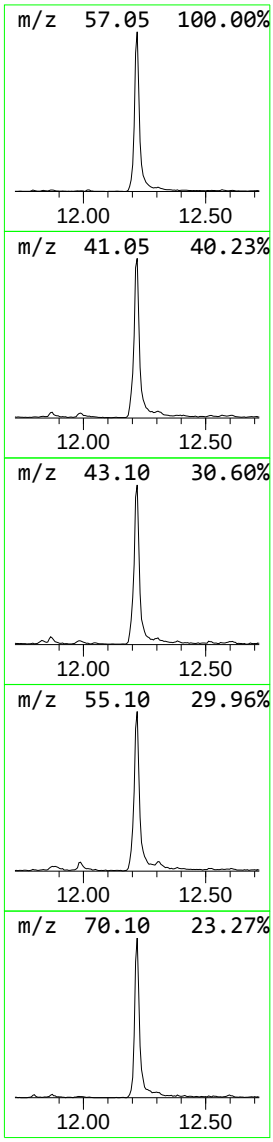
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	69.50 ug/l	1008500	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	78
2	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
3	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	50
4	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
5	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	43





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Instrument :
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ClientSampleId :
ORA-1041

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

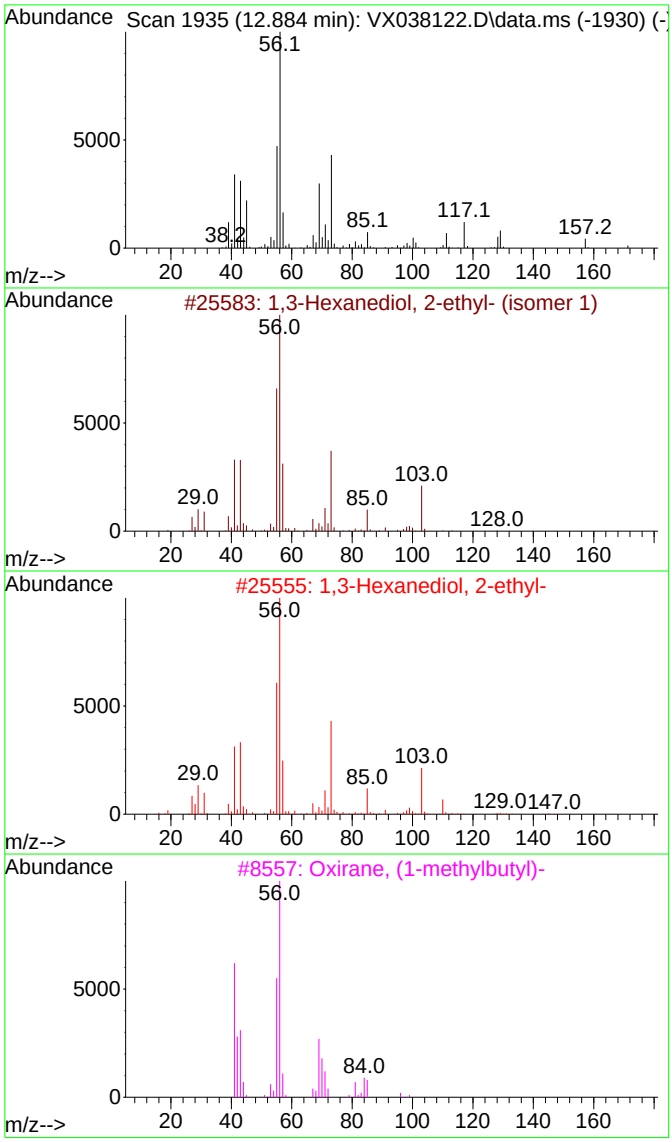
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

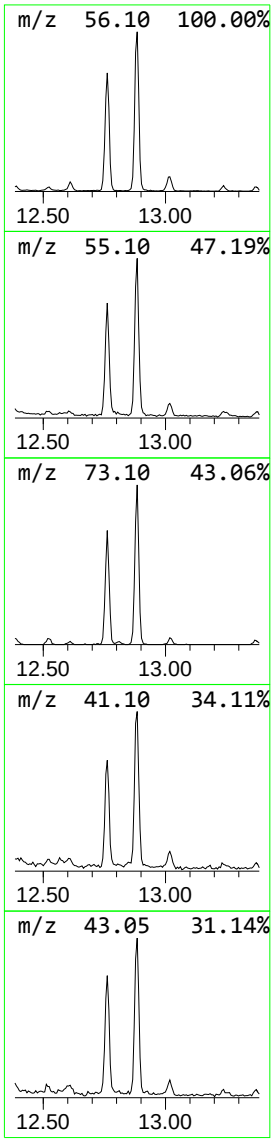
****

Peak Number 9 unknown12.884 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.884	14.66 ug/l	212810	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Hexanediol, 2-ethyl- (isomer 1)	146	C8H18O2	1000484-18-2	47
2	1,3-Hexanediol, 2-ethyl-	146	C8H18O2	000094-96-2	47
3	Oxirane, (1-methylbutyl)-	114	C7H14O	053229-39-3	43
4	Furan, tetrahydro-2,5-dimethyl-	100	C6H12O	001003-38-9	42
5	Neopentyl glycol	104	C5H12O2	000126-30-7	40





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
Ethanol	2.057	183.7	ug/l	1432690	1	5.556	390018	50.0
Butanal	4.227	206.3	ug/l	1608870	1	5.556	390018	50.0
1,3-Dioxolane, ...	5.830	26.9	ug/l	209800	1	5.556	390018	50.0
1-Butanol	7.202	59.6	ug/l	632088	2	6.763	530277	50.0
1-Pentanol	9.232	12.3	ug/l	171853	3	10.055	698671	50.0
Butanoic acid, ...	11.683	14.3	ug/l	206965	4	12.024	725571	50.0
1-Hexanol, 2-et...	12.219	69.5	ug/l	1008500	4	12.024	725571	50.0
unknown12.884	12.884	14.7	ug/l	212810	4	12.024	725571	50.0