LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX100720\
Data File : VX018817.D
Acq On : 07 Oct 2020 17:40
Operator : JC/SP
Sample : L4240-10
Misc : 25.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : BG3S8

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.1 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\SOMXTR100220WMA.M
Title : TRACE VOA SOM01.0

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.885	275	295	326	rBV2	53856357	138367673	33.26%	17.001%
2	3.178	328	343	372	rBV3	66853754	194167743	46.67%	23.857%
3	3.580	385	409	415	rBV5	92675590	416059644	100.00%	51.120%
4	4.123	486	498	510	rBV	3385844	9928088	2.39%	1.220%
5	4.288	510	525	532	rVV	2126656	6668682	1.60%	0.819%
6	4.379	532	540	552	rVV	8269197	23389233	5.62%	2.874%
7	10.122	1473	1482	1487	rBV	5446797	7572526	1.82%	0.930%
8	12.079	1795	1803	1808	rVB	3458399	4849871	1.17%	0.596%
9	13.627	2052	2057	2063	rBV	10077039	12877773	3.10%	1.582%

Sum of corrected areas: 813881233

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX100720\
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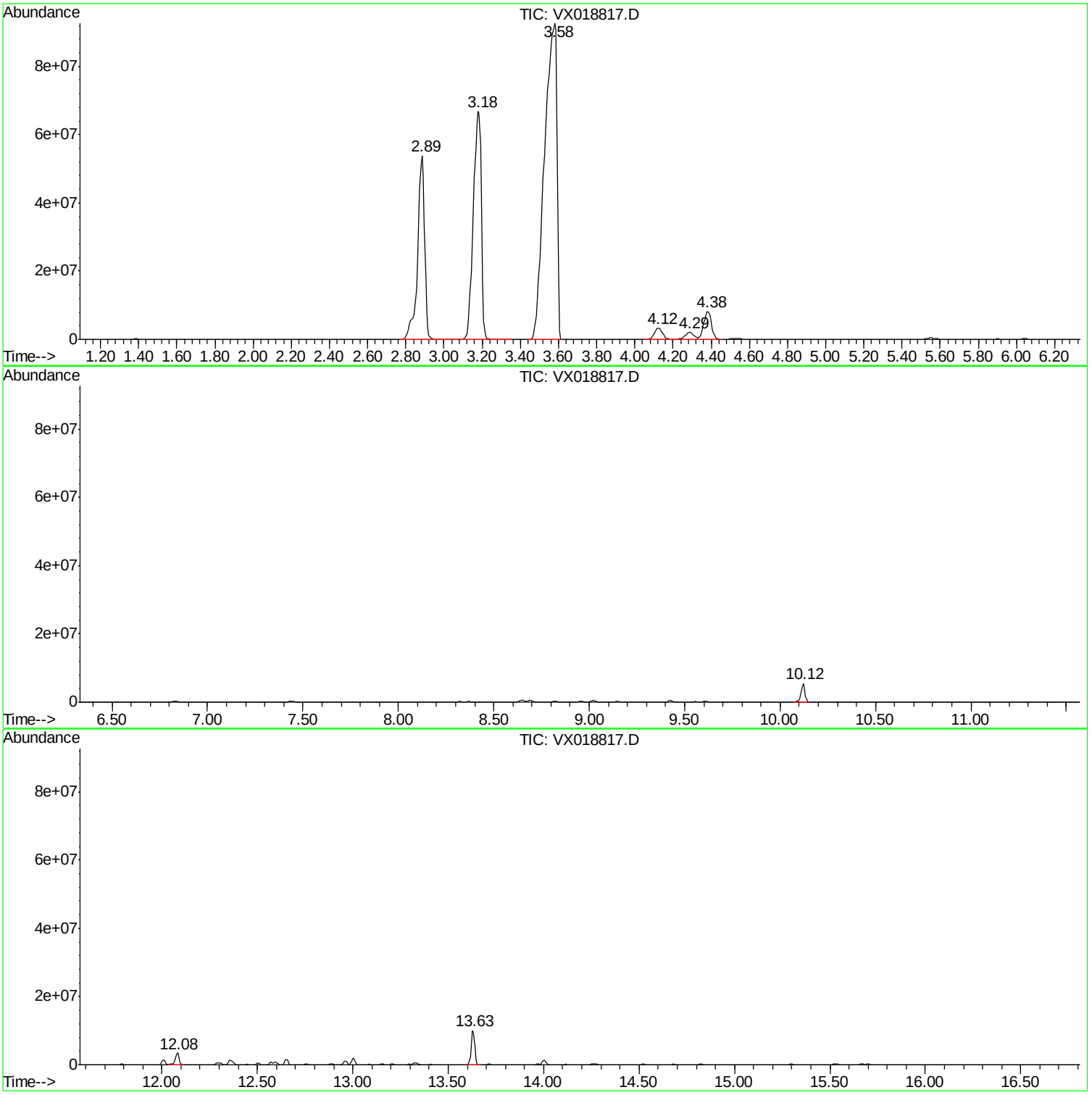
Misc : 25.0mL/MSVOA X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BG3S8

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\SOMXTR100220WMA.M
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Data File : VX018817.D
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Operator : JC/SP
Sample : L4240-10
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ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : BG3S8

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\SOMXTR100220WMA.M
Quant Title : TRACE VOA SOM01.0

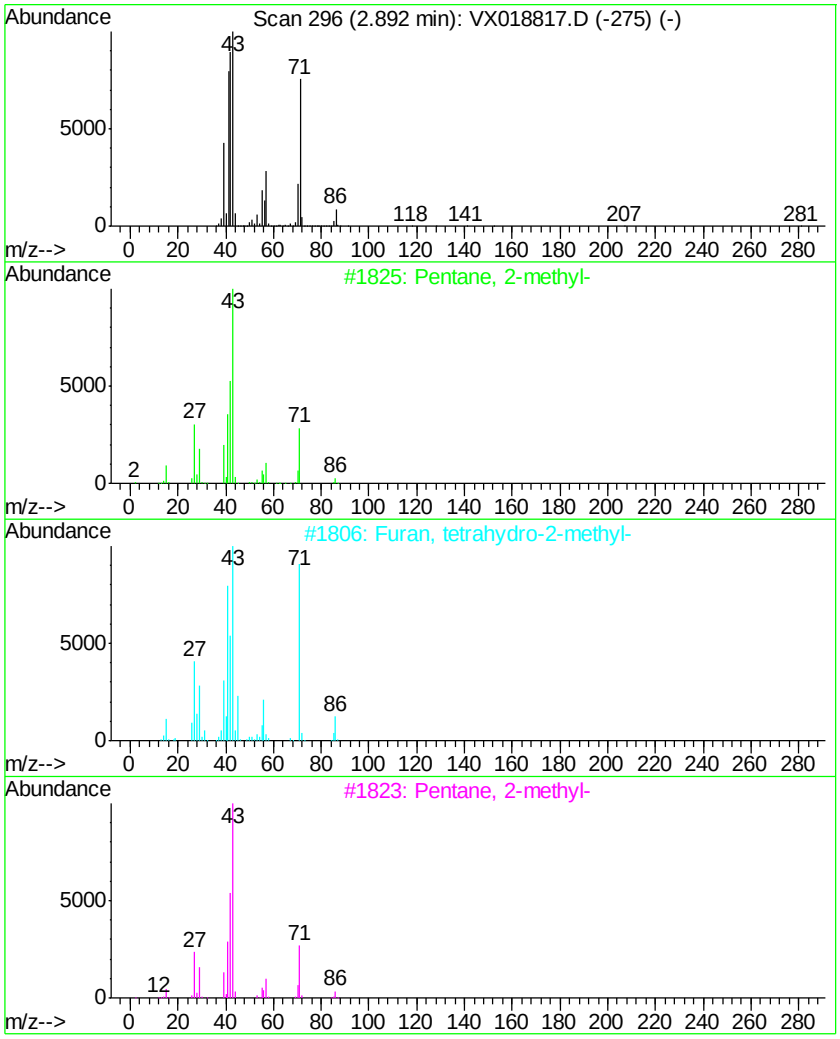
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

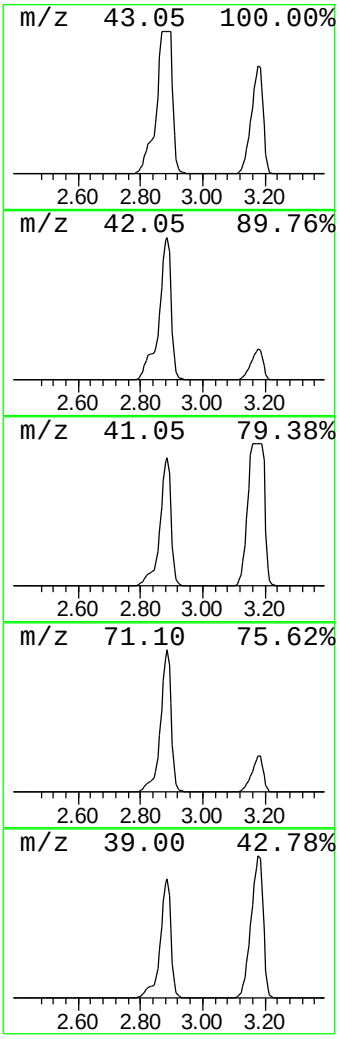
****

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.89	29.58 ug/L	138368000	1,4-Difluorobenzene	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2-methyl-	86	C6H14	000107-83-5	49
2	Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	46
3	Pentane, 2-methyl-	86	C6H14	000107-83-5	43
4	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	43
5	Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	42





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Data File : VX018817.D
Acq On : 07 Oct 2020 17:40
Operator : JC/SP
Sample : L4240-10
Misc : 25.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : BG3S8

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\SOMXTR100220WMA.M
Quant Title : TRACE VOA SOM01.0

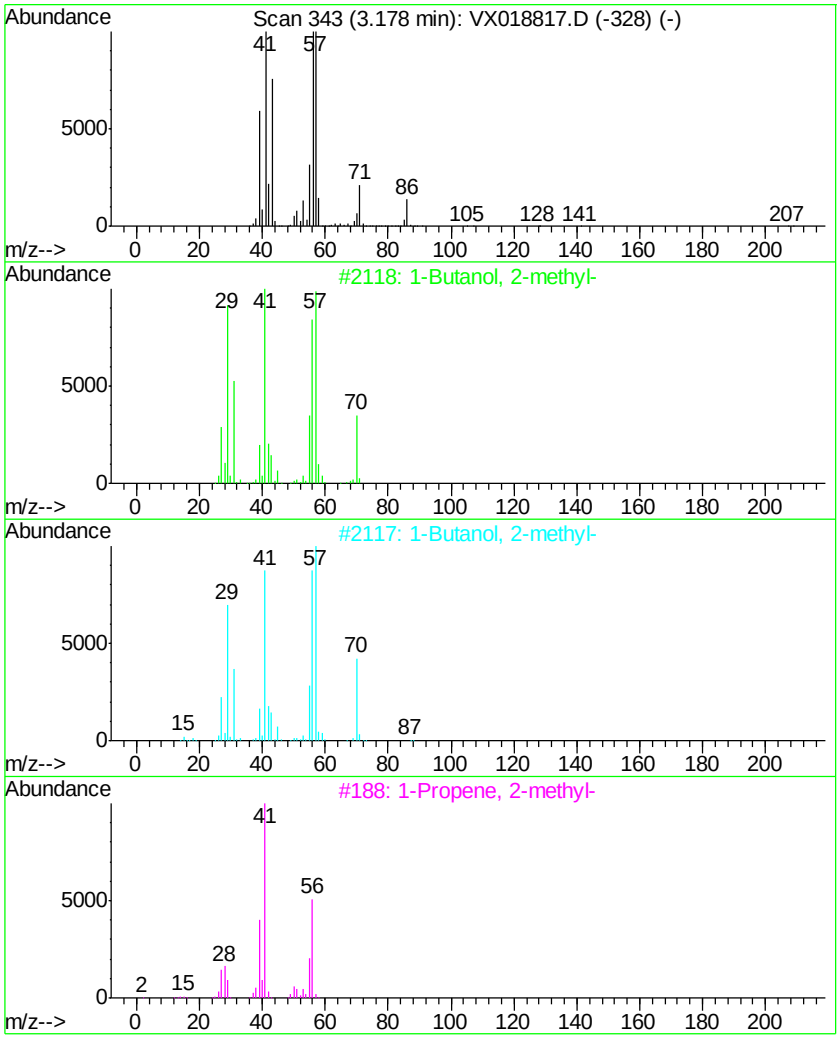
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

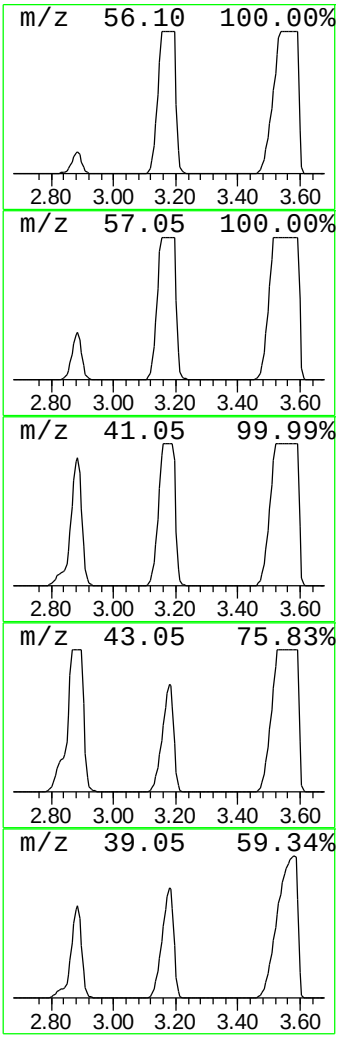
****

Peak Number 2 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.18	41.51 ug/L	194168000	1,4-Difluorobenzene	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol, 2-methyl-	88	C5H12O	000137-32-6	47
2	1-Butanol, 2-methyl-	88	C5H12O	000137-32-6	43
3	1-Propene, 2-methyl-	56	C4H8	000115-11-7	43
4	1-Hexene	84	C6H12	000592-41-6	42
5	Cyclobutane, ethyl-	84	C6H12	004806-61-5	38





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX100720\
Data File : VX018817.D
Acq On : 07 Oct 2020 17:40
Operator : JC/SP
Sample : L4240-10
Misc : 25.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : BG3S8

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\SOMXTR100220WMA.M
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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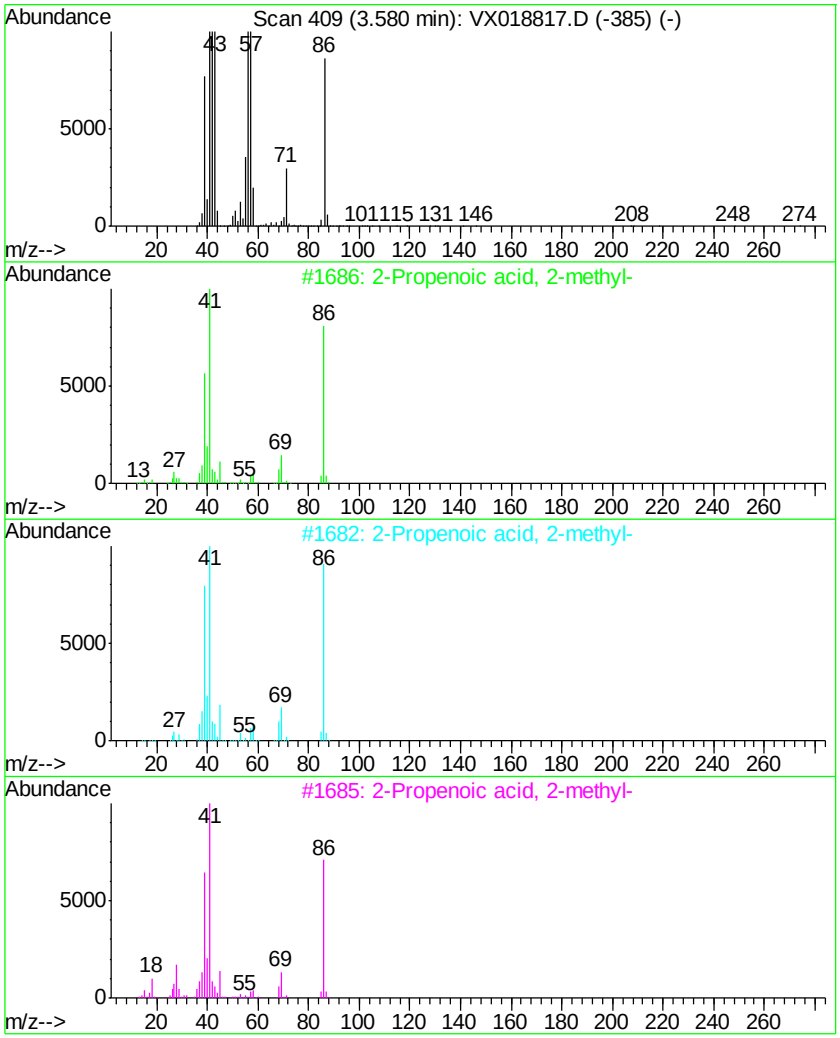
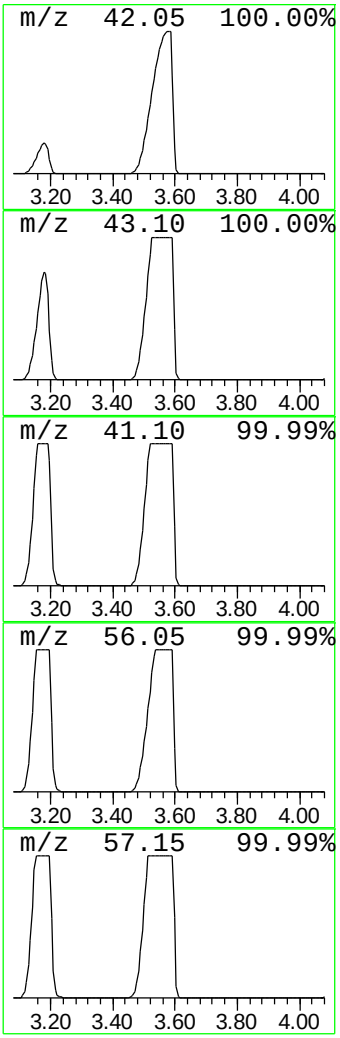
Peak Number 3 2-Propenoic acid, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.58	88.94 ug/L	416060000	1,4-Difluorobenzene	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenoic acid, 2-methyl-	86	C4H6O2	000079-41-4	50
2	2-Propenoic acid, 2-methyl-	86	C4H6O2	000079-41-4	40
3	2-Propenoic acid, 2-methyl-	86	C4H6O2	000079-41-4	38
4	2H-Pyran-2-one, tetrahydro-6,6-d...	128	C7H12O2	002610-95-9	36
5	2-Pentanol, 5-(2-propynyloxy)-	142	C8H14O2	055702-67-5	33





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX100720\
Data File : VX018817.D
Acq On : 07 Oct 2020 17:40
Operator : JC/SP
Sample : L4240-10
Misc : 25.0mL/MSVOA X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : BG3S8

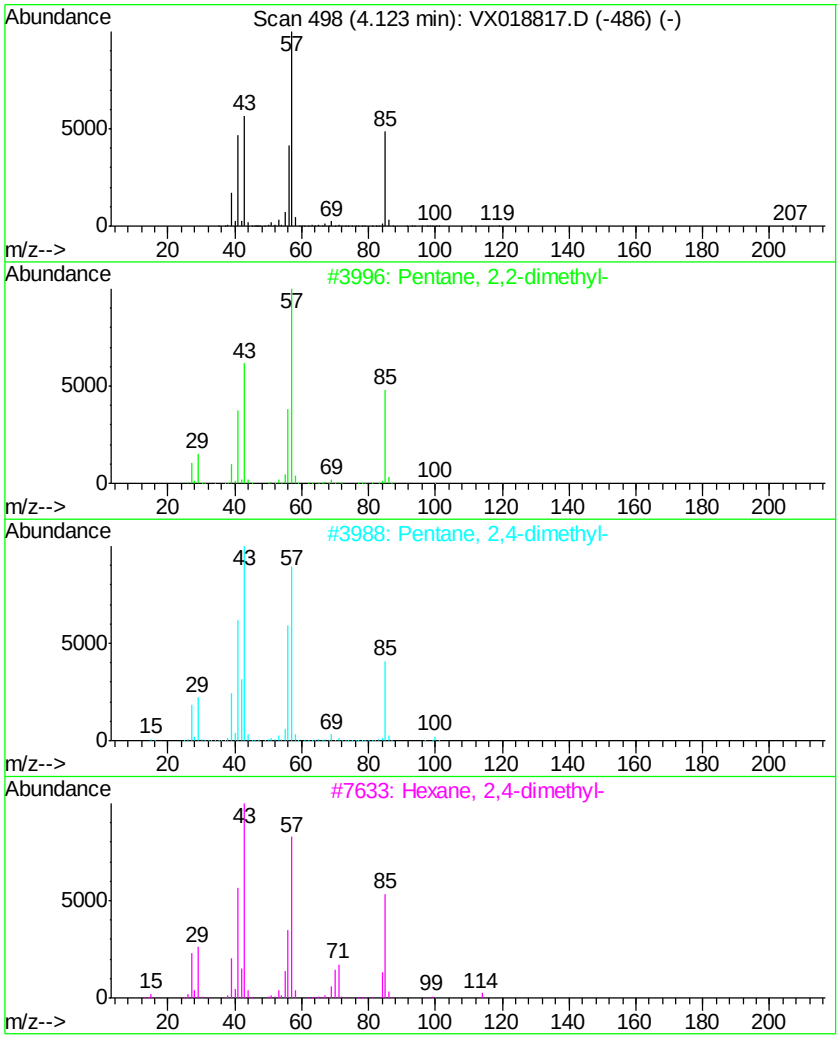
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\SOMXTR100220WMA.M
Quant Title : TRACE VOA SOM01.0

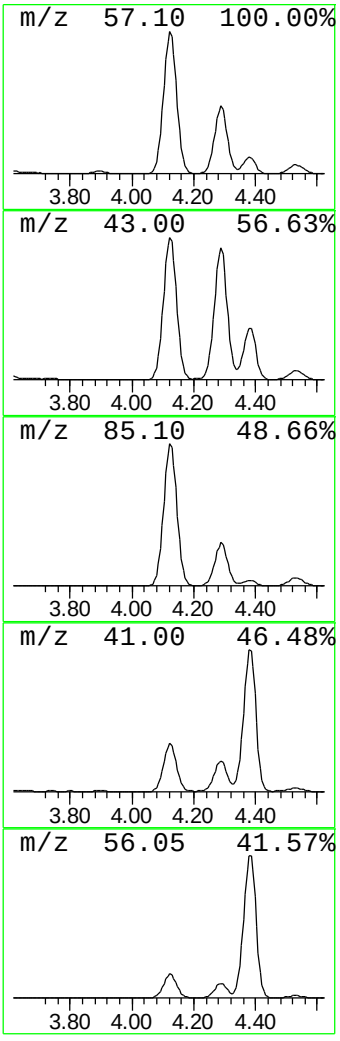
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.12	2.12 ug/L	9928090	1,4-Difluorobenzene	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	83
2	Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	72
3	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	72
4	Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	64
5	Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	64





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Operator : JC/SP
Sample : L4240-10
Misc : 25.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : BG3S8

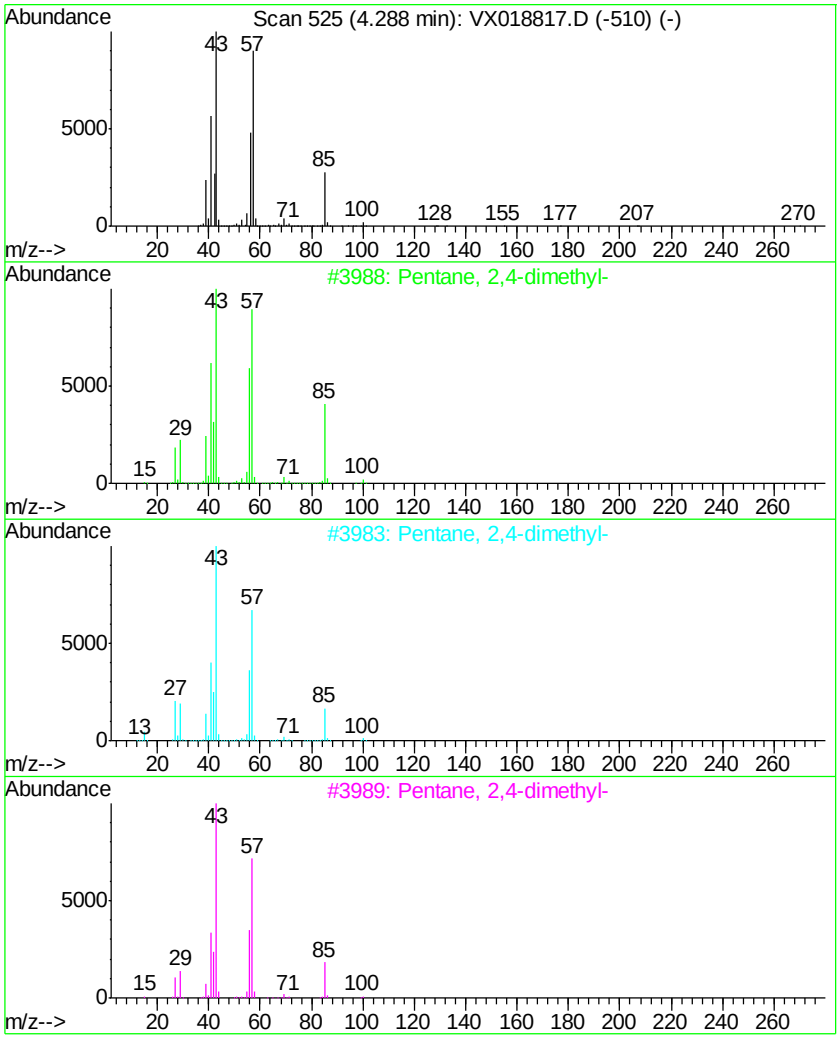
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\SOMXTR100220WMA.M
Quant Title : TRACE VOA SOM01.0

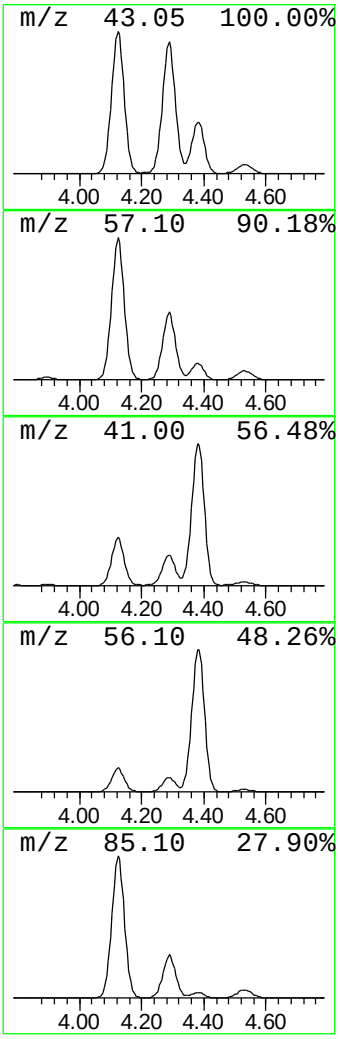
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.29	1.43 ug/L	6668680	1,4-Difluorobenzene	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	91
2	Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	91
3	Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	90
4	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	64
5	Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	59





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Acq On : 07 Oct 2020 17:40
Operator : JC/SP
Sample : L4240-10
Misc : 25.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : BG3S8

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\SOMXTR100220WMA.M
Quant Title : TRACE VOA SOM01.0

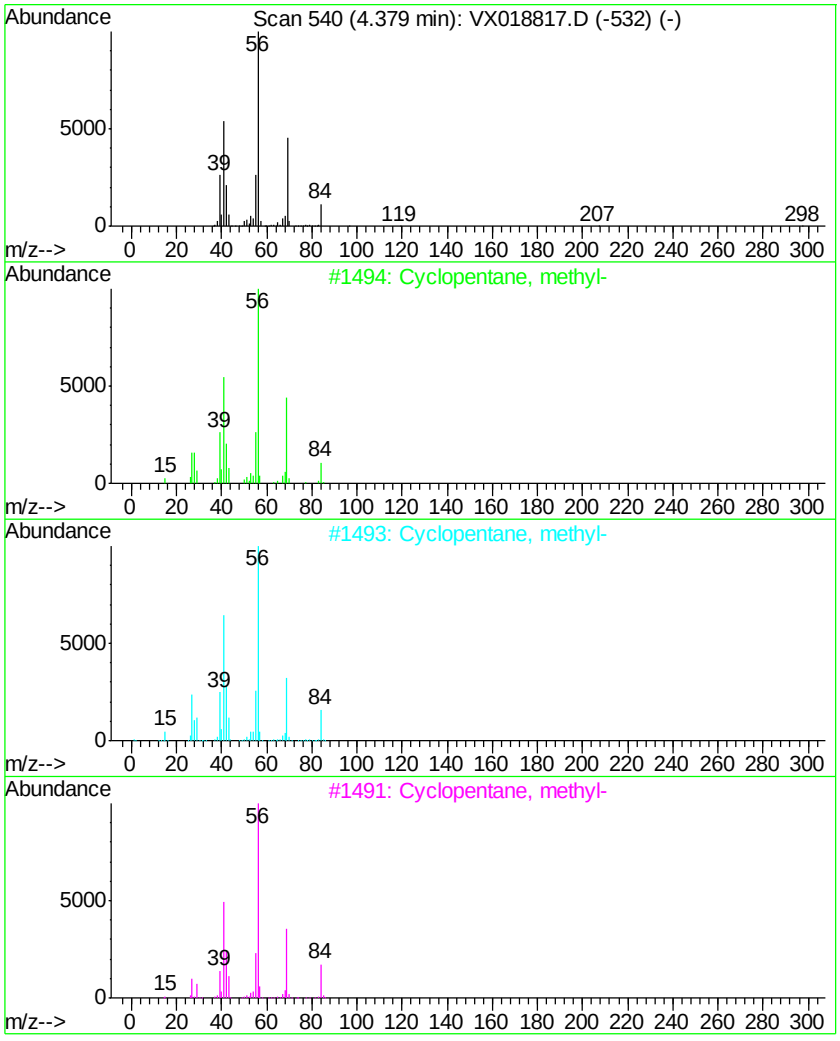
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

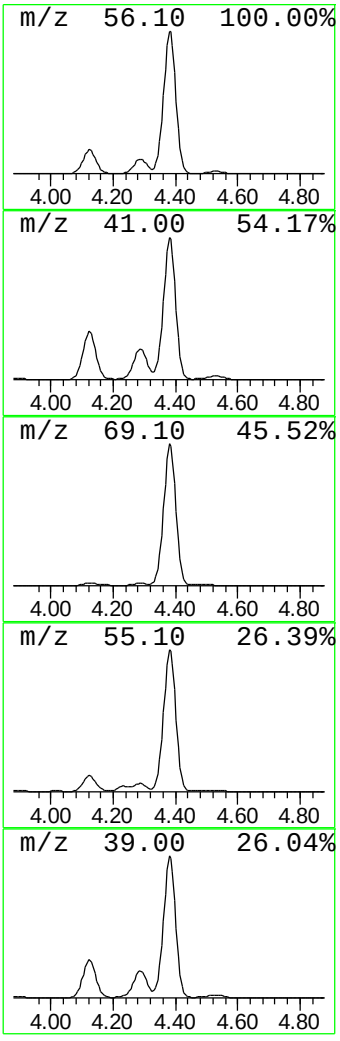
****

Peak Number 6 (DEL) Alkane: Cyclic4.38 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.38	5.00 ug/L	23389200	1,4-Difluorobenzene	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
3	Cyclopentane, methyl-	84	C6H12	000096-37-7	86
4	Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
5	Cyclobutane, ethyl-	84	C6H12	004806-61-5	53





Tentatively Identified Compound (LSC) summary

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Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
(DEL) Alkane: Str...	2.89	29.6	ug/L	138368000	1	6.83	23389200	5.0
unknown-01	3.18	41.5	ug/L	194168000	1	6.83	23389200	5.0
2-Propenoic acid,...	3.58	88.9	ug/L	416060000	1	6.83	23389200	5.0
(DEL) Alkane: Str...	4.12	2.1	ug/L	9928090	1	6.83	23389200	5.0
(DEL) Alkane: Str...	4.29	1.4	ug/L	6668680	1	6.83	23389200	5.0
(DEL) Alkane: Cyc...	4.38	5.0	ug/L	23389200	1	6.83	23389200	5.0