LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU100520\
Data File : VU040516.D
Acq On : 05 Oct 2020 17:51
Operator : SY/MD
Sample : L4240-09DL 5X
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG3S7DL

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_U\METHOD\SOMUTR092920WMA.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	3.099	517	547	568	rBV	1663948	4009080	29.34%	10.205%
2	3.379	610	634	661	rBV	4347493	9631615	70.50%	24.518%
3	3.719	720	740	765	rBV	6201039	13662683	100.00%	34.779%
4	4.318	906	926	946	rBV2	182900	501908	3.67%	1.278%
5	4.456	951	969	981	rVV3	142005	359391	2.63%	0.915%
6	4.552	982	999	1018	rVV	2330955	5556598	40.67%	14.145%
7	4.658	1018	1032	1064	rVB3	99343	342984	2.51%	0.873%
8	5.083	1150	1164	1177	rBV	74257	160886	1.18%	0.410%
9	5.408	1243	1265	1279	rBV2	219023	497184	3.64%	1.266%
10	5.742	1350	1369	1394	rVB3	145735	389421	2.85%	0.991%
11	6.263	1517	1531	1552	rBV	160170	300866	2.20%	0.766%
12	6.703	1650	1668	1681	rBV2	95867	188684	1.38%	0.480%
13	7.906	2033	2042	2057	rVB	186413	328642	2.41%	0.837%
14	8.639	2257	2270	2306	rBV	275433	516154	3.78%	1.314%
15	9.449	2500	2522	2536	rBV2	791183	1652953	12.10%	4.208%
16	11.742	3224	3235	3244	rBV	103735	167705	1.23%	0.427%
17	11.809	3244	3256	3260	rBV	249909	412747	3.02%	1.051%
18	12.189	3361	3374	3389	rVB	200328	347975	2.55%	0.886%
19	13.832	3873	3885	3900	rBV	160750	256895	1.88%	0.654%

Sum of corrected areas: 39284371

LSC Report - Integrated Chromatogram

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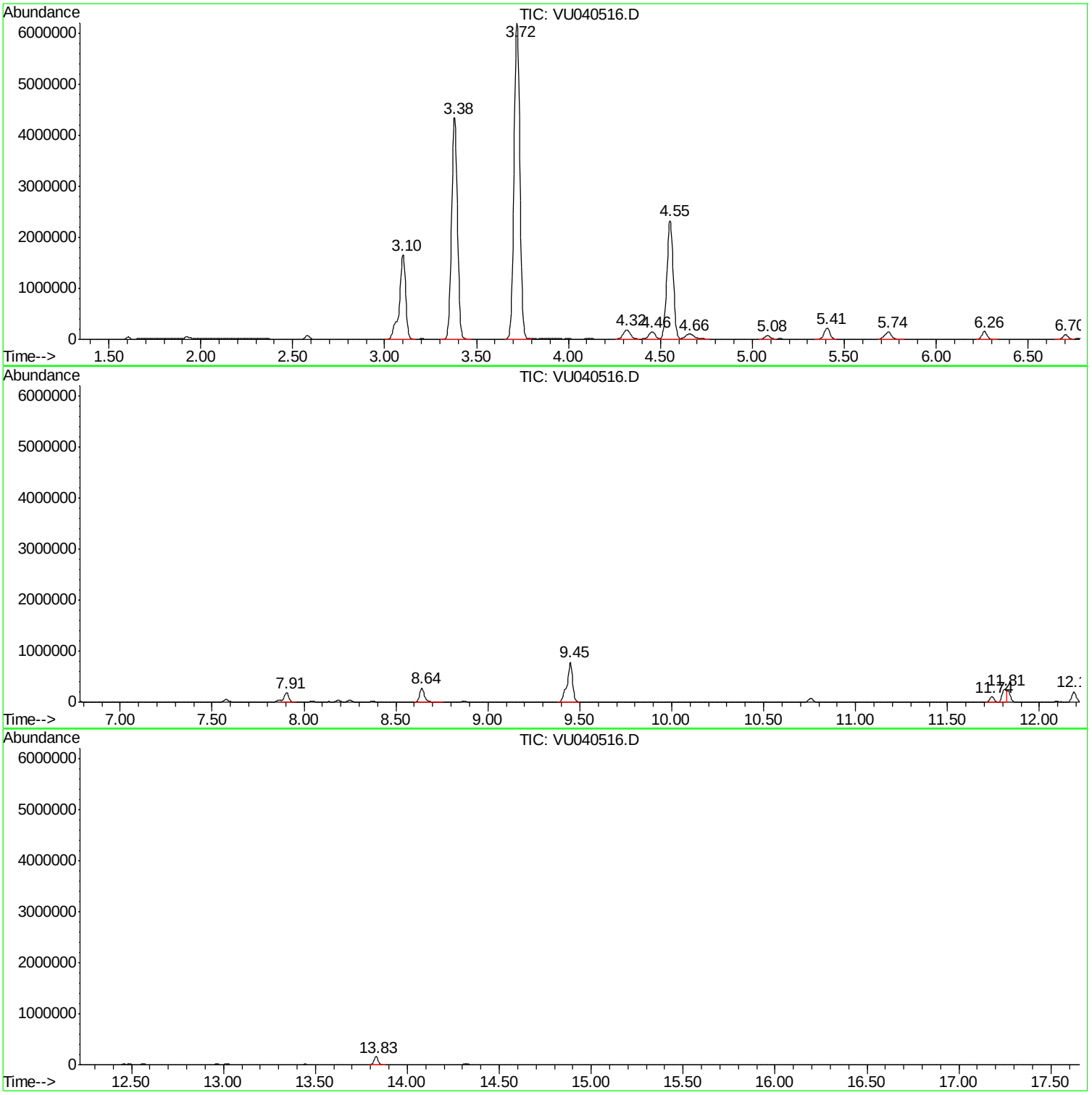
Acq On : 05 Oct 2020 17:51
Operator : SY/MD
Sample : L4240-09DL 5X
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG3S7DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR092920WMA.M
Quant Title : TRACE VOA SOM01.0

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU100520\
Data File : VU040516.D
Acq On : 05 Oct 2020 17:51
Operator : SY/MD
Sample : L4240-09DL 5X
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG3S7DL

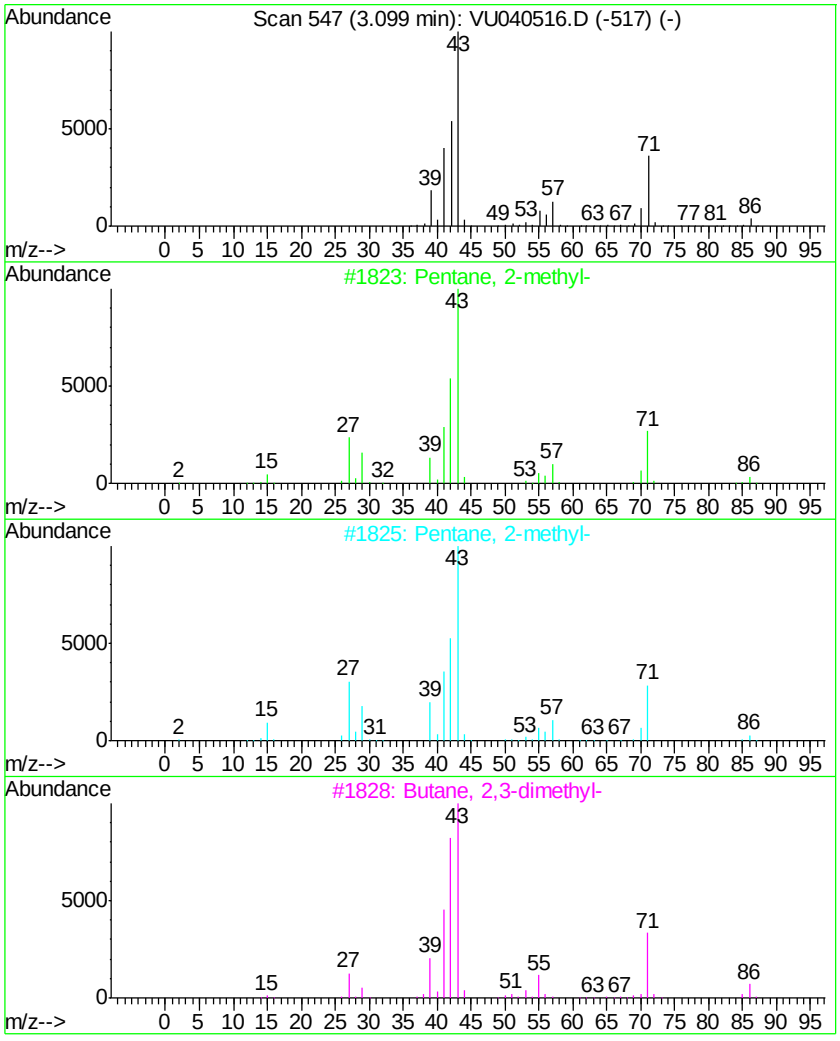
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR092920WMA.M
Quant Title : TRACE VOA SOM01.0

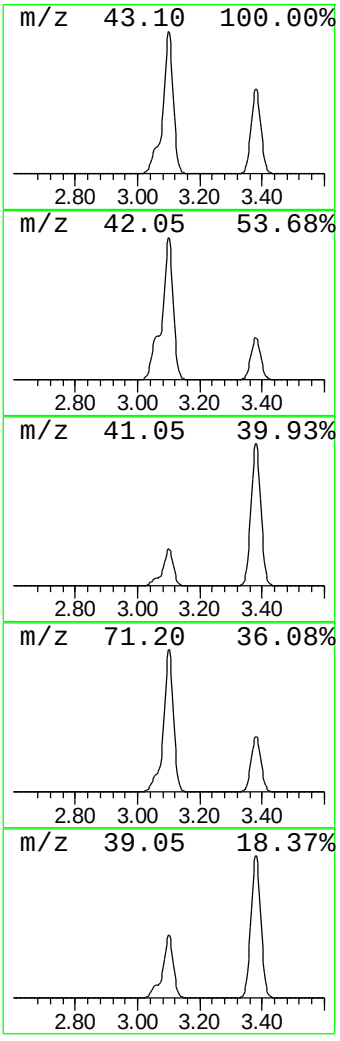
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.10	66.63 ug/L	4009080	1,4-Difluorobenzene	6.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2-methyl-	86	C6H14	000107-83-5	91
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	91
3	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	64
4	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	33
5	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	33





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU100520\
Data File : VU040516.D
Acq On : 05 Oct 2020 17:51
Operator : SY/MD
Sample : L4240-09DL 5X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG3S7DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR092920WMA.M
Quant Title : TRACE VOA SOM01.0

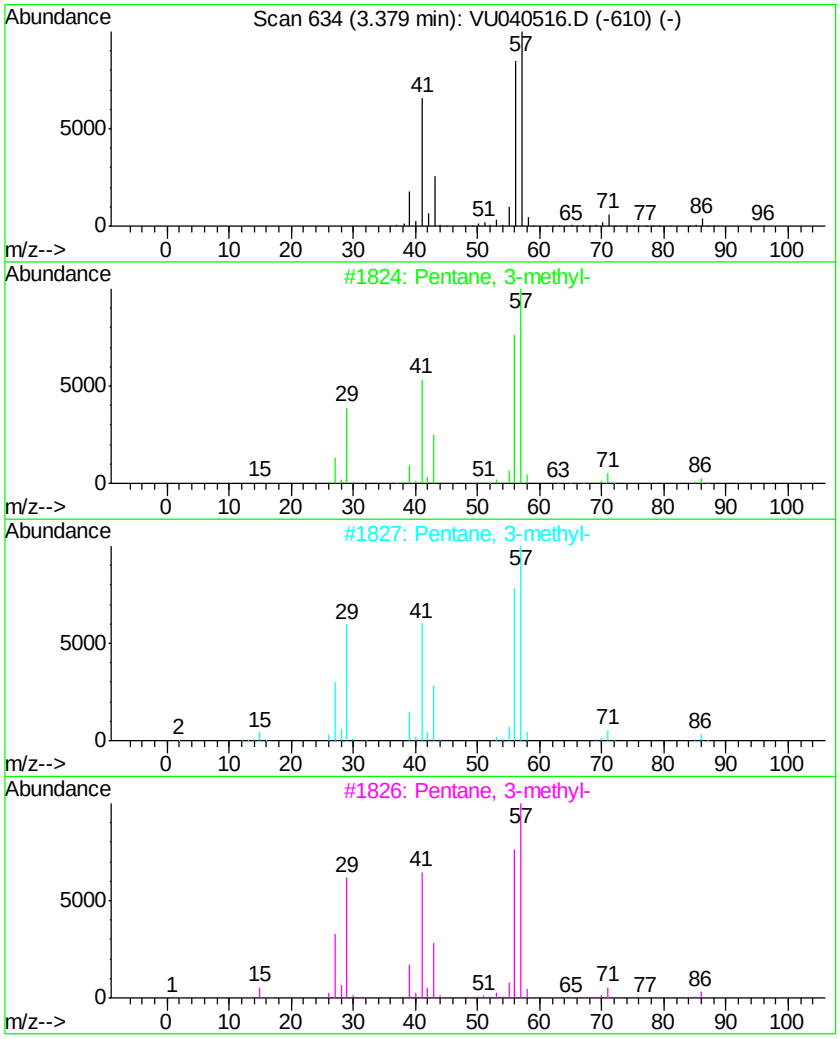
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

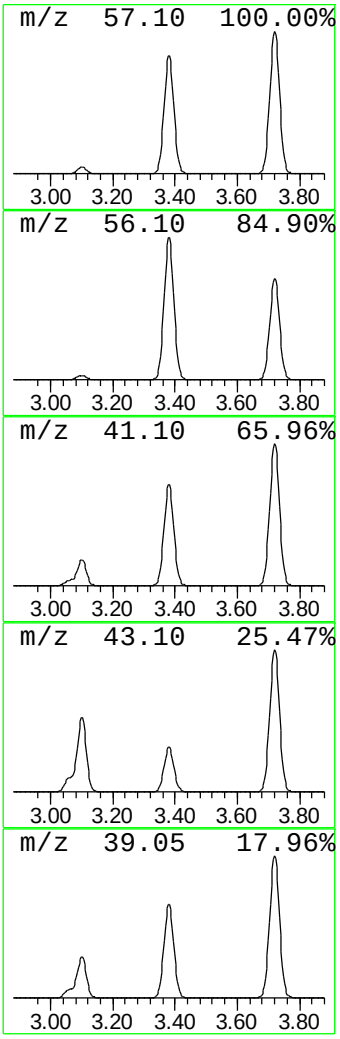
****

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.38	160.07 ug/L	9631620	1,4-Difluorobenzene	6.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2	Pentane, 3-methyl-	86	C6H14	000096-14-0	91
3	Pentane, 3-methyl-	86	C6H14	000096-14-0	91
4	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	64
5	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	64





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU100520\
Data File : VU040516.D
Acq On : 05 Oct 2020 17:51
Operator : SY/MD
Sample : L4240-09DL 5X
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG3S7DL

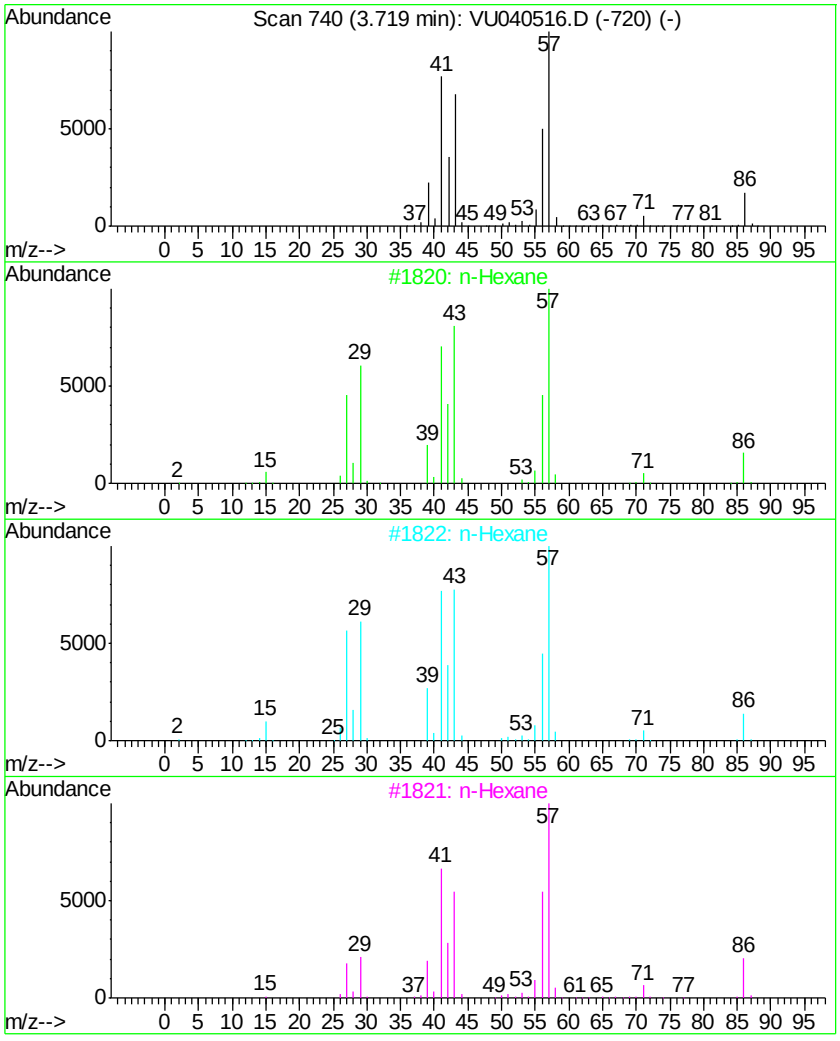
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR092920WMA.M
Quant Title : TRACE VOA SOM01.0

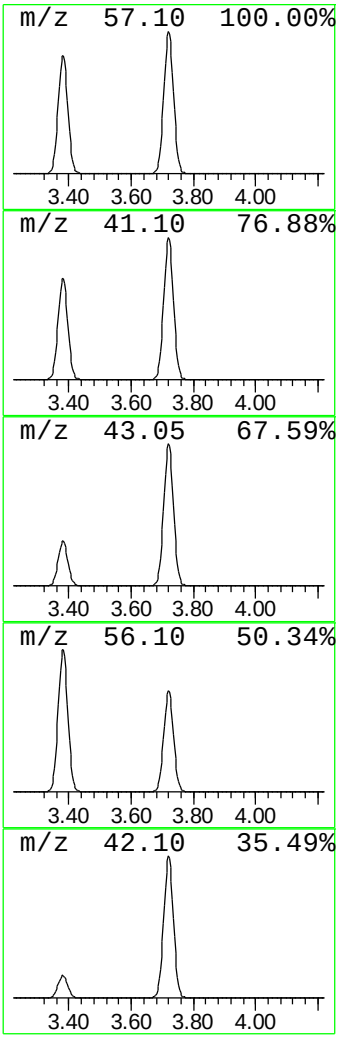
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.72	227.06 ug/L	13662700	1,4-Difluorobenzene	6.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexane	86	C6H14	000110-54-3	91
2	n-Hexane	86	C6H14	000110-54-3	91
3	n-Hexane	86	C6H14	000110-54-3	91
4	Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	40
5	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	38





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU100520\
Data File : VU040516.D
Acq On : 05 Oct 2020 17:51
Operator : SY/MD
Sample : L4240-09DL 5X
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG3S7DL

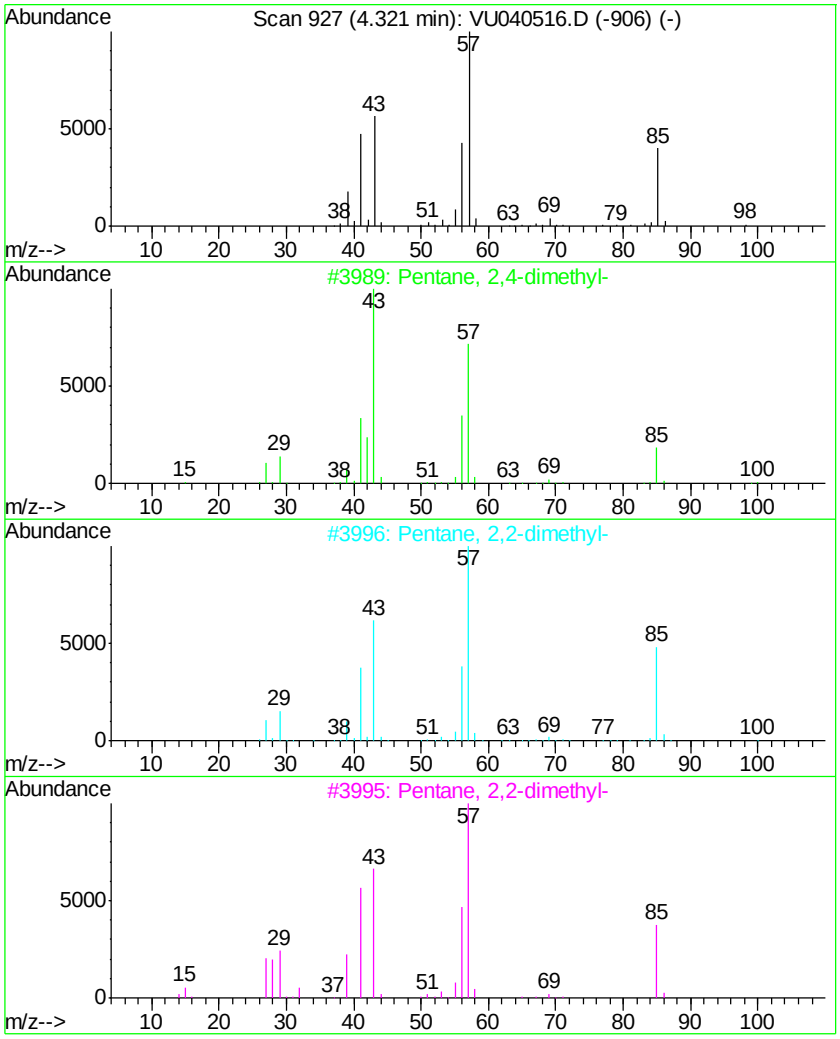
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR092920WMA.M
Quant Title : TRACE VOA SOM01.0

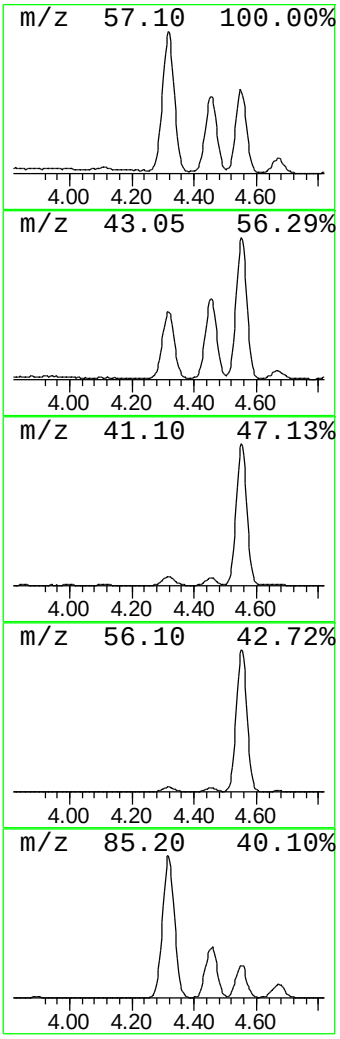
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.32	8.34 ug/L	501908	1,4-Difluorobenzene	6.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	83
2	Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	83
3	Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	83
4	Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	78
5	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	78





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU100520\
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Acq On : 05 Oct 2020 17:51
Operator : SY/MD
Sample : L4240-09DL 5X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG3S7DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR092920WMA.M
Quant Title : TRACE VOA SOM01.0

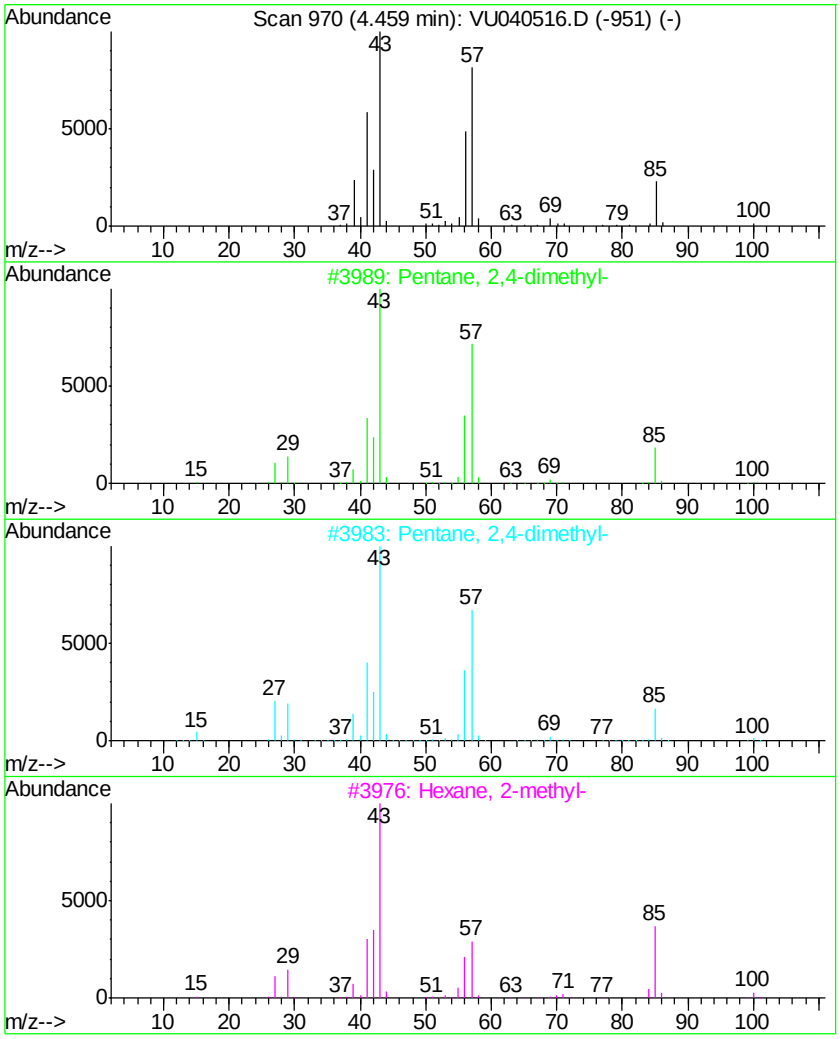
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

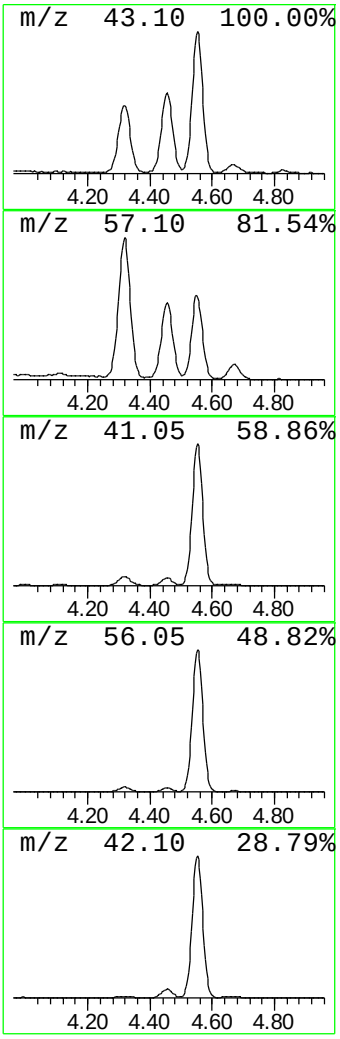
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.46	5.97 ug/L	359391	1,4-Difluorobenzene	6.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	80
2	Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	74
3	Hexane, 2-methyl-	100	C7H16	000591-76-4	72
4	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	59
5	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	59





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Acq On : 05 Oct 2020 17:51
Operator : SY/MD
Sample : L4240-09DL 5X
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ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG3S7DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR092920WMA.M
Quant Title : TRACE VOA SOM01.0

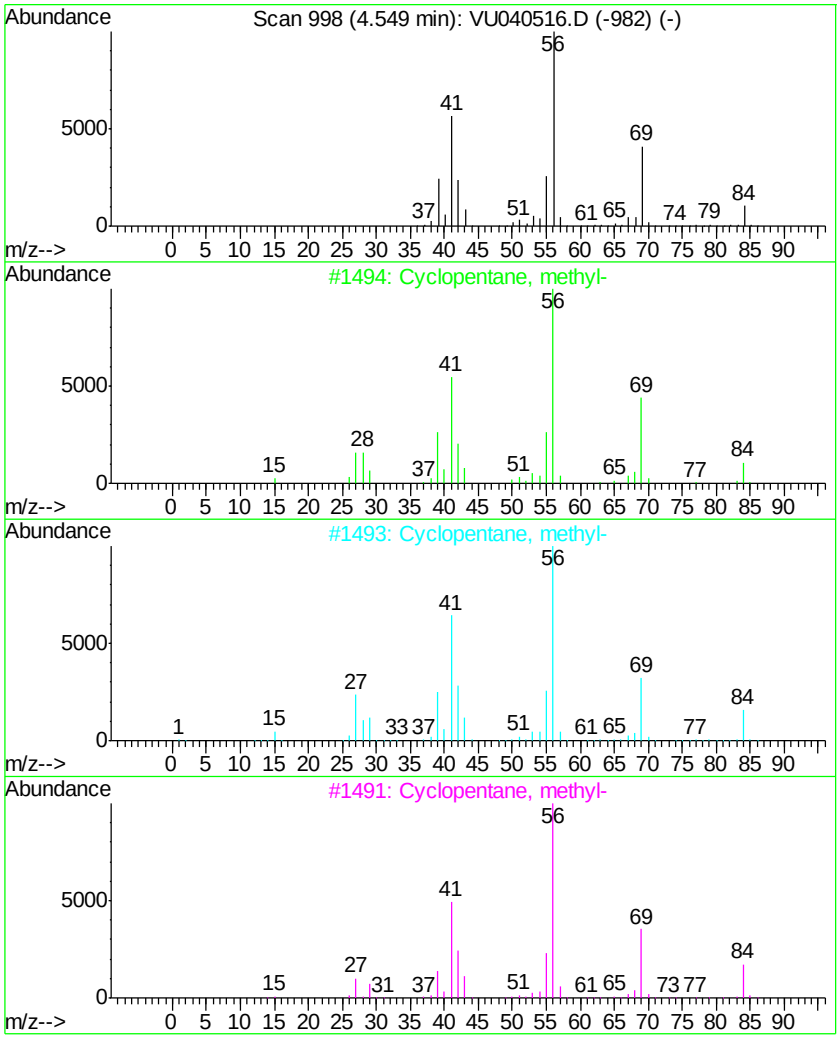
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

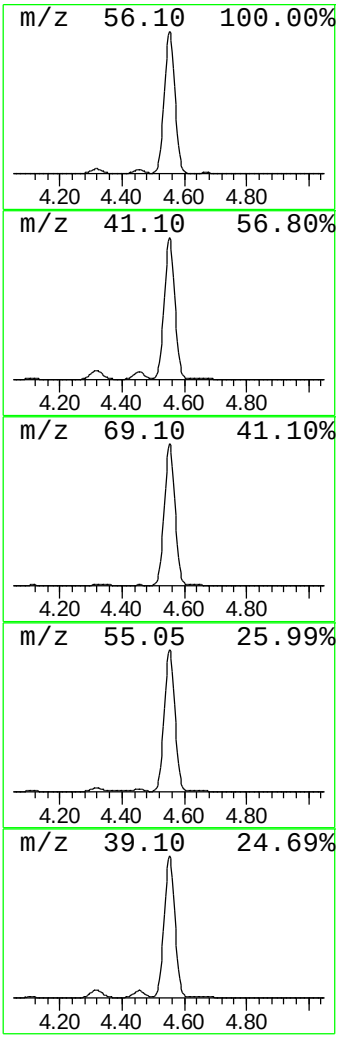
****

Peak Number 6 (DEL) Alkane: Cyclic4.55 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.55	92.34 ug/L	5556600	1,4-Difluorobenzene	6.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
3	Cyclopentane, methyl-	84	C6H12	000096-37-7	78
4	Cyclohexane	84	C6H12	000110-82-7	78
5	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72





Tentatively Identified Compound (LSC) summary

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Data File : VU040516.D
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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...	3.10	66.6	ug/L	4009080	1	6.26	300866	5.0
(DEL) Alkane: Str...	3.38	160.1	ug/L	9631620	1	6.26	300866	5.0
(DEL) Alkane: Str...	3.72	227.1	ug/L	13662700	1	6.26	300866	5.0
(DEL) Alkane: Str...	4.32	8.3	ug/L	501908	1	6.26	300866	5.0
(DEL) Alkane: Str...	4.46	6.0	ug/L	359391	1	6.26	300866	5.0
(DEL) Alkane: Cyc...	4.55	92.3	ug/L	5556600	1	6.26	300866	5.0