LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU121919\
Data File : VU036289.D
Acq On : 19 Dec 2019 17:46
Operator : JC/MD
Sample : K6282-08
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDW4

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\SOMUTR121319WMA.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	1.372	3	10	30	rVB	3803424	3802433	90.78%	18.515%
2	1.507	45	52	71	rVB	233914	262571	6.27%	1.279%
3	1.607	74	83	100	rBV3	1482530	2564886	61.24%	12.489%
4	1.678	100	105	110	rBV	46123	42328	1.01%	0.206%
5	1.752	120	128	143	rVB	235695	265178	6.33%	1.291%
6	1.928	174	183	201	rVB2	204140	313171	7.48%	1.525%
7	2.015	201	210	223	rVB	261064	352605	8.42%	1.717%
8	2.179	250	261	268	rBV	369592	506169	12.08%	2.465%
9	2.227	268	276	298	rVB3	328328	611514	14.60%	2.978%
10	2.343	304	312	326	rVB	41058	61873	1.48%	0.301%
11	2.440	331	342	352	rVV	115220	187312	4.47%	0.912%
12	2.597	377	391	404	rBV2	196269	346150	8.26%	1.686%
13	3.012	505	520	541	rBV9	31124	103871	2.48%	0.506%
14	3.118	544	553	562	rVB4	23743	43535	1.04%	0.212%
15	3.404	622	642	660	rBV6	54912	135523	3.24%	0.660%
16	3.629	696	712	733	rVV5	62167	153694	3.67%	0.748%
17	3.742	733	747	767	rVB2	36530	85370	2.04%	0.416%
18	4.247	887	904	916	rBV4	19163	48761	1.16%	0.237%
19	4.690	1024	1042	1043	rBV	131182	220024	5.25%	1.071%
20	5.112	1158	1173	1191	rBV	168971	391994	9.36%	1.909%
21	5.771	1353	1378	1407	rBV2	330237	892569	21.31%	4.346%
22	6.292	1525	1540	1563	rBV	310175	625987	14.95%	3.048%
23	6.581	1612	1630	1663	rBV	2168396	4188545	100.00%	20.395%
24	6.732	1665	1677	1694	rVB2	206526	415185	9.91%	2.022%
25	7.600	1933	1947	1963	rBV	96706	183271	4.38%	0.892%
26	7.931	2037	2050	2065	rBV	373842	656389	15.67%	3.196%
27	8.214	2127	2138	2157	rBV2	59467	112825	2.69%	0.549%
28	8.684	2268	2284	2323	rBV	287565	863848	20.62%	4.206%
29	9.446	2502	2521	2556	rBV	444793	815512	19.47%	3.971%
30	10.783	2925	2937	2955	rVB	173718	294370	7.03%	1.433%
31	11.838	3251	3265	3281	rBV	298687	520041	12.42%	2.532%
32	12.217	3370	3383	3400	rVB	280279	469164	11.20%	2.285%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU121919\
Data File : VU036289.D
Acq On : 19 Dec 2019 17:46
Operator : JC/MD
Sample : K6282-08
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDW4

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\SOMUTR121319WMA.M
Title : TRACE VOA SOM01.0

Sum of corrected areas: 20536668

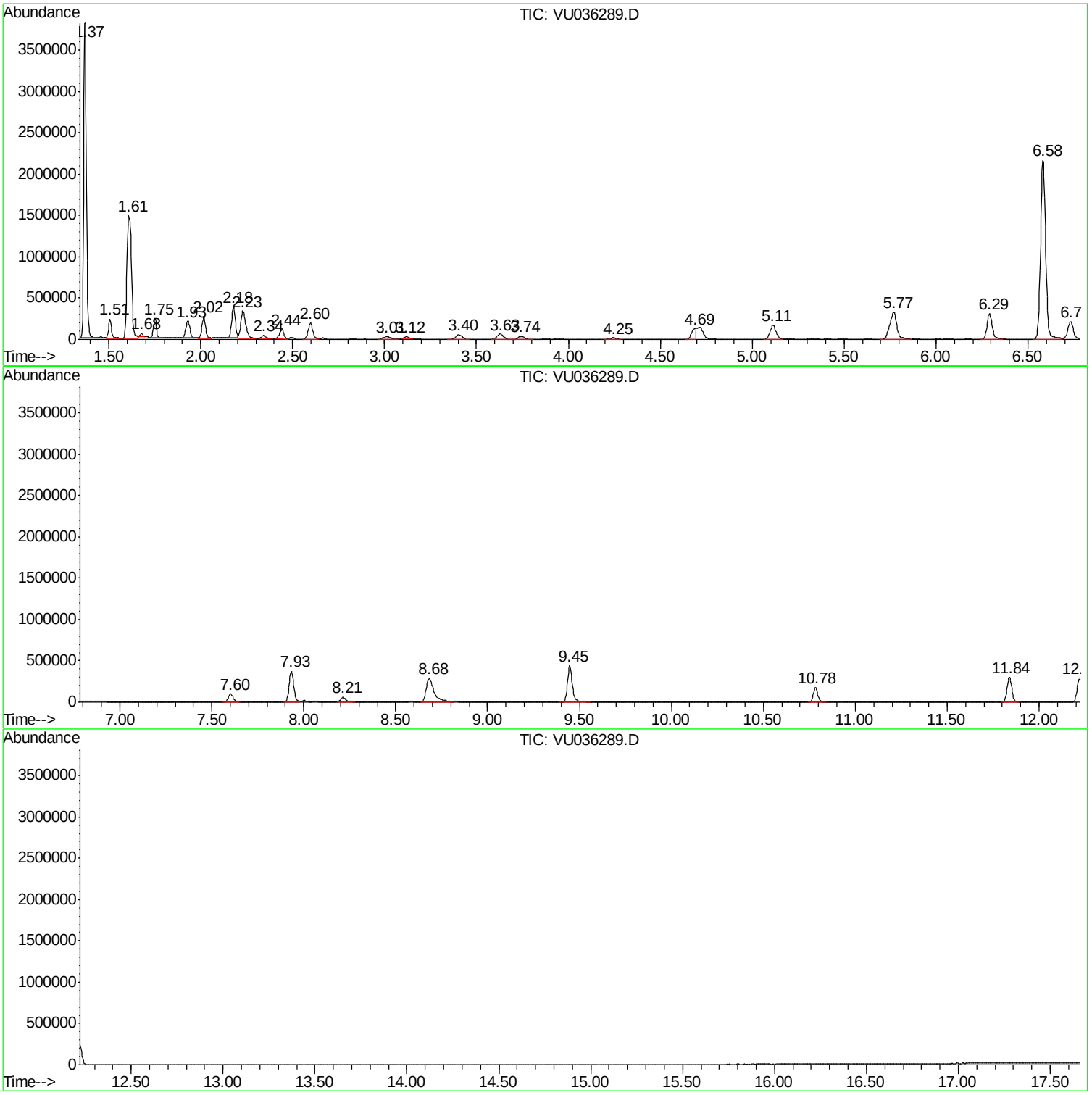
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU121919\
Data File : VU036289.D
Acq On : 19 Dec 2019 17:46
Operator : JC/MD
Sample : K6282-08
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDW4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR121319WMA.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\VU121919\
Data File : VU036289.D
Acq On : 19 Dec 2019 17:46
Operator : JC/MD
Sample : K6282-08
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDW4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR121319WMA.M
Quant Title : TRACE VOA SOM01.0

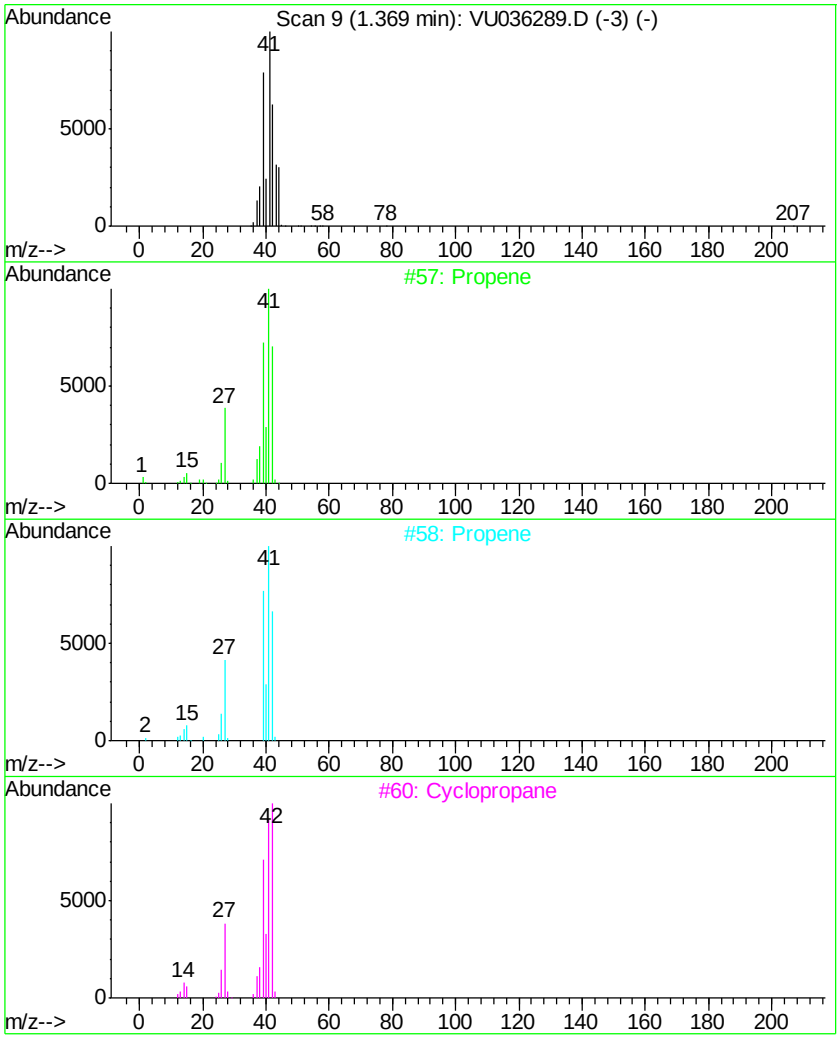
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

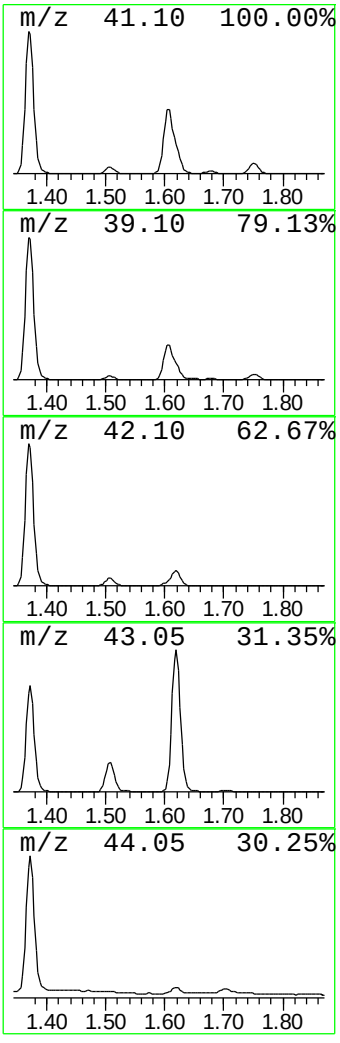
****

Peak Number 1 (DEL) Alkane: Cyclic1.37 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.37	30.37 ug/L	3802430	1,4-Difluorobenzene	6.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propene	42	C3H6	000115-07-1	90
2	Propene	42	C3H6	000115-07-1	42
3	Cyclopropane	42	C3H6	000075-19-4	9
4	Cyclopropene	40	C3H4	002781-85-3	9
5	Cyclopropane	42	C3H6	000075-19-4	7





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU121919\
Data File : VU036289.D
Acq On : 19 Dec 2019 17:46
Operator : JC/MD
Sample : K6282-08
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDW4

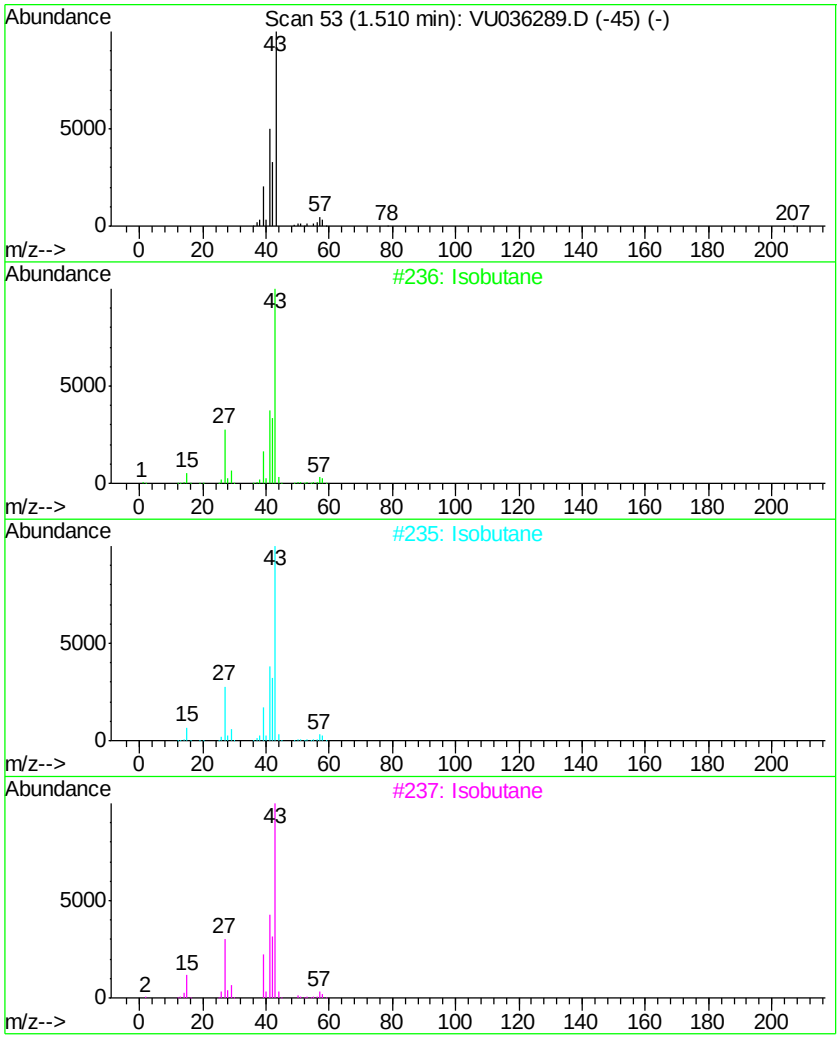
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR121319WMA.M
Quant Title : TRACE VOA SOM01.0

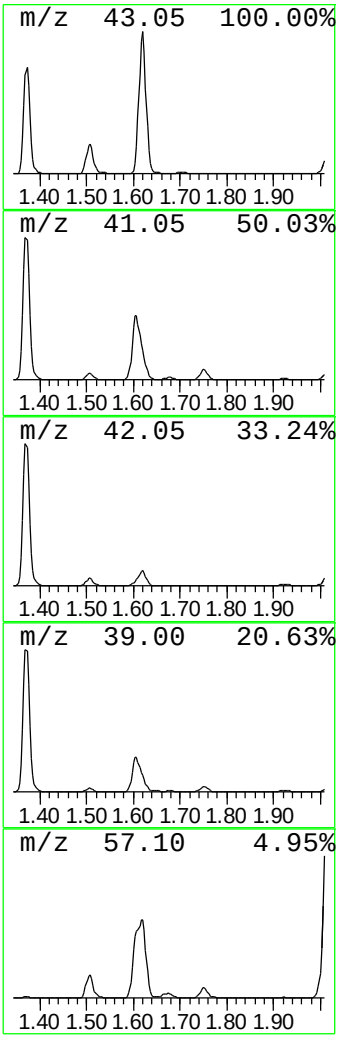
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.51	2.10 ug/L	262571	1,4-Difluorobenzene	6.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutane	58	C4H10	000075-28-5	64
2	Isobutane	58	C4H10	000075-28-5	64
3	Isobutane	58	C4H10	000075-28-5	50
4	Isobutane	58	C4H10	000075-28-5	42
5	Propane, 2-nitro-	89	C3H7NO2	000079-46-9	9





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU121919\
Data File : VU036289.D
Acq On : 19 Dec 2019 17:46
Operator : JC/MD
Sample : K6282-08
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDW4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR121319WMA.M
Quant Title : TRACE VOA SOM01.0

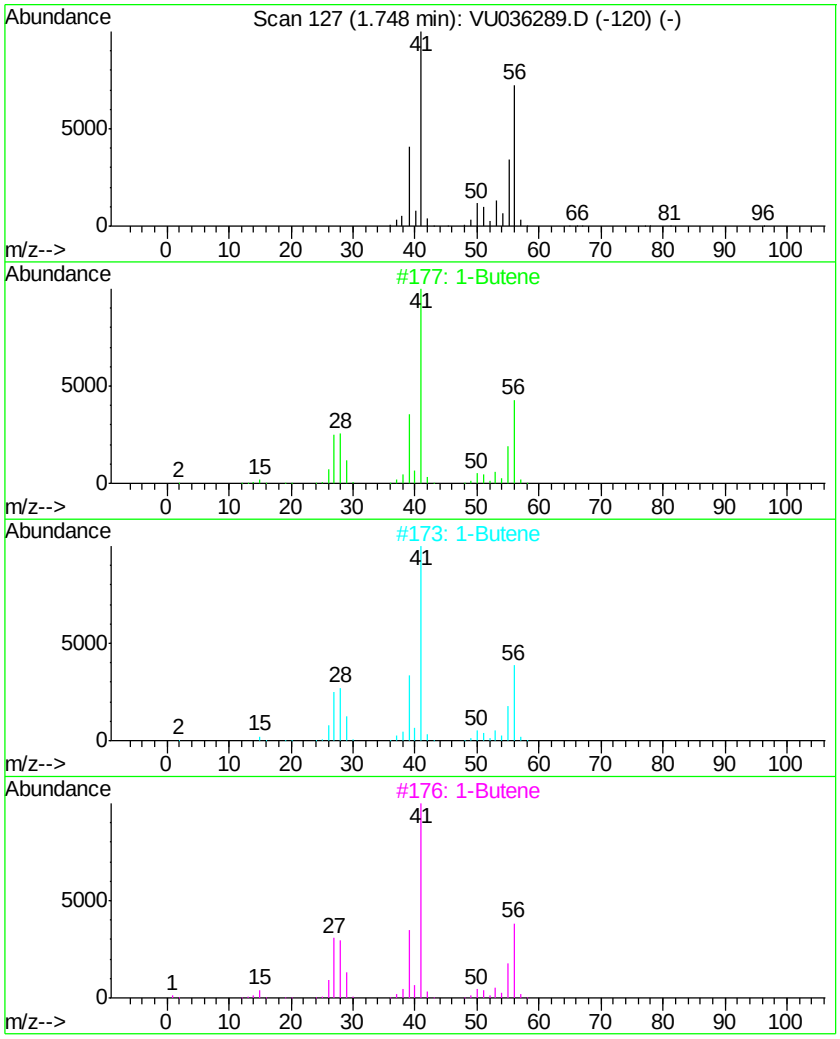
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

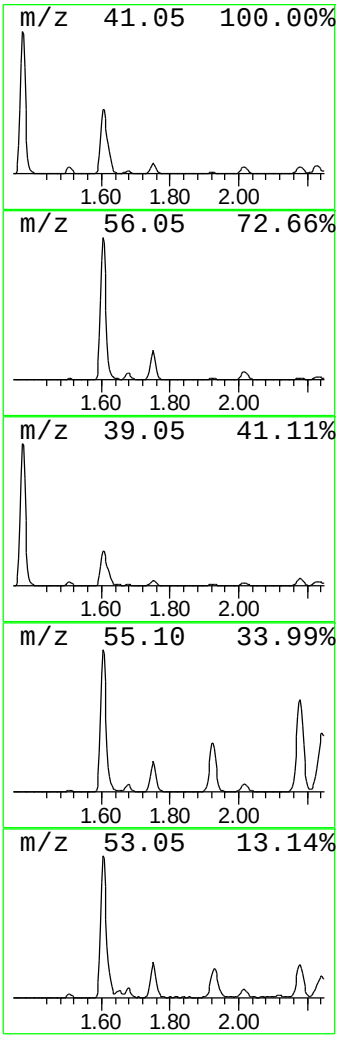
****

Peak Number 3 (DEL) Alkane: Cyclic1.75 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.75	2.12 ug/L	265178	1,4-Difluorobenzene	6.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butene	56	C4H8	000106-98-9	87
2	1-Butene	56	C4H8	000106-98-9	83
3	1-Butene	56	C4H8	000106-98-9	80
4	2-Butene, (Z)-	56	C4H8	000590-18-1	80
5	1-Propene, 2-methyl-	56	C4H8	000115-11-7	80





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU121919\
Data File : VU036289.D
Acq On : 19 Dec 2019 17:46
Operator : JC/MD
Sample : K6282-08
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDW4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR121319WMA.M
Quant Title : TRACE VOA SOM01.0

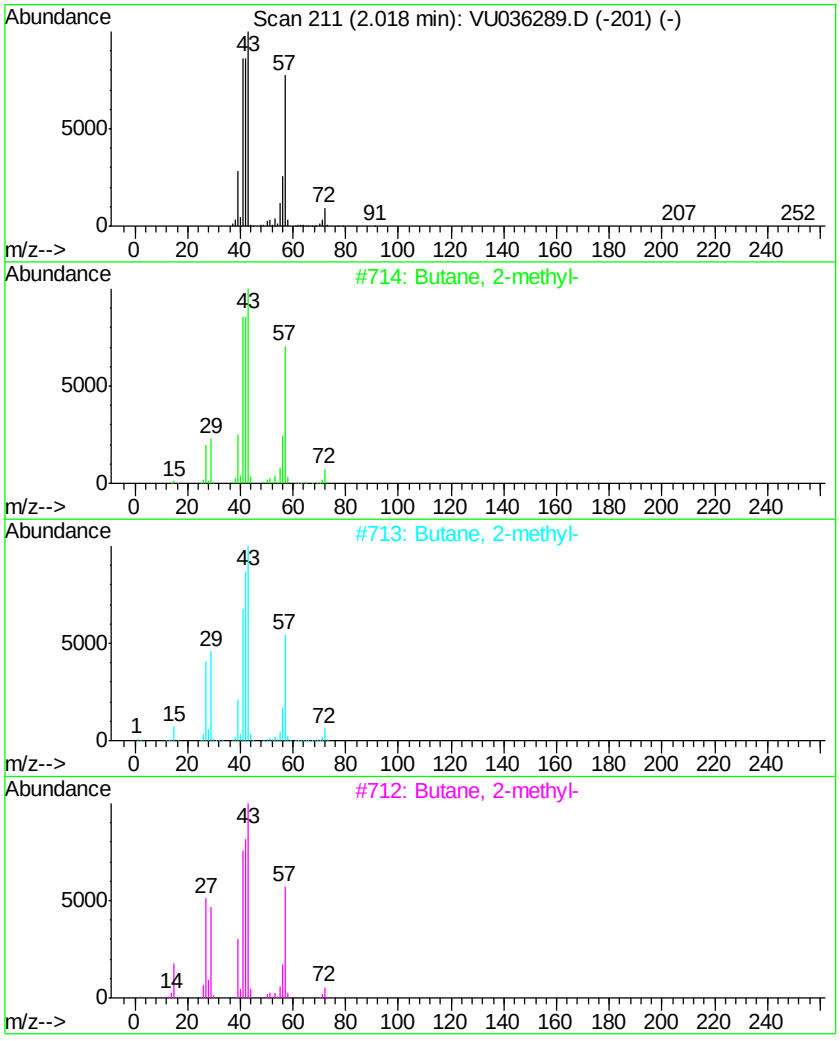
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

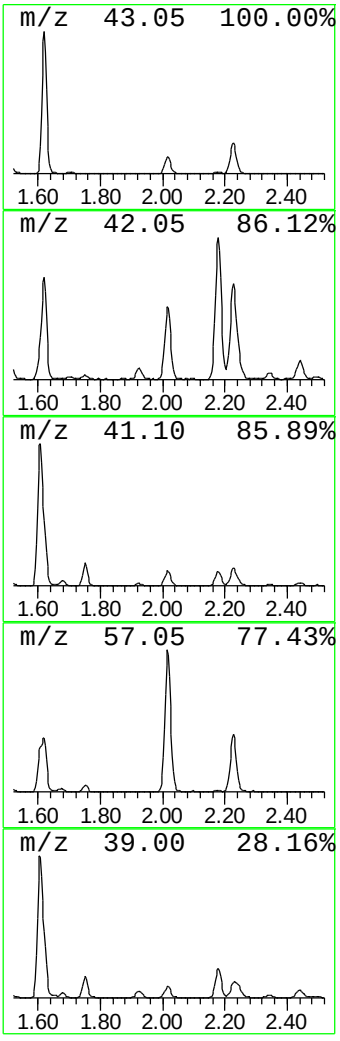
****

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.02	2.82 ug/L	352605	1,4-Difluorobenzene	6.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	91
2	Butane, 2-methyl-	72	C5H12	000078-78-4	91
3	Butane, 2-methyl-	72	C5H12	000078-78-4	86
4	Pentane	72	C5H12	000109-66-0	42
5	3-Buten-1-ol	72	C4H8O	000627-27-0	37





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU121919\
Data File : VU036289.D
Acq On : 19 Dec 2019 17:46
Operator : JC/MD
Sample : K6282-08
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDW4

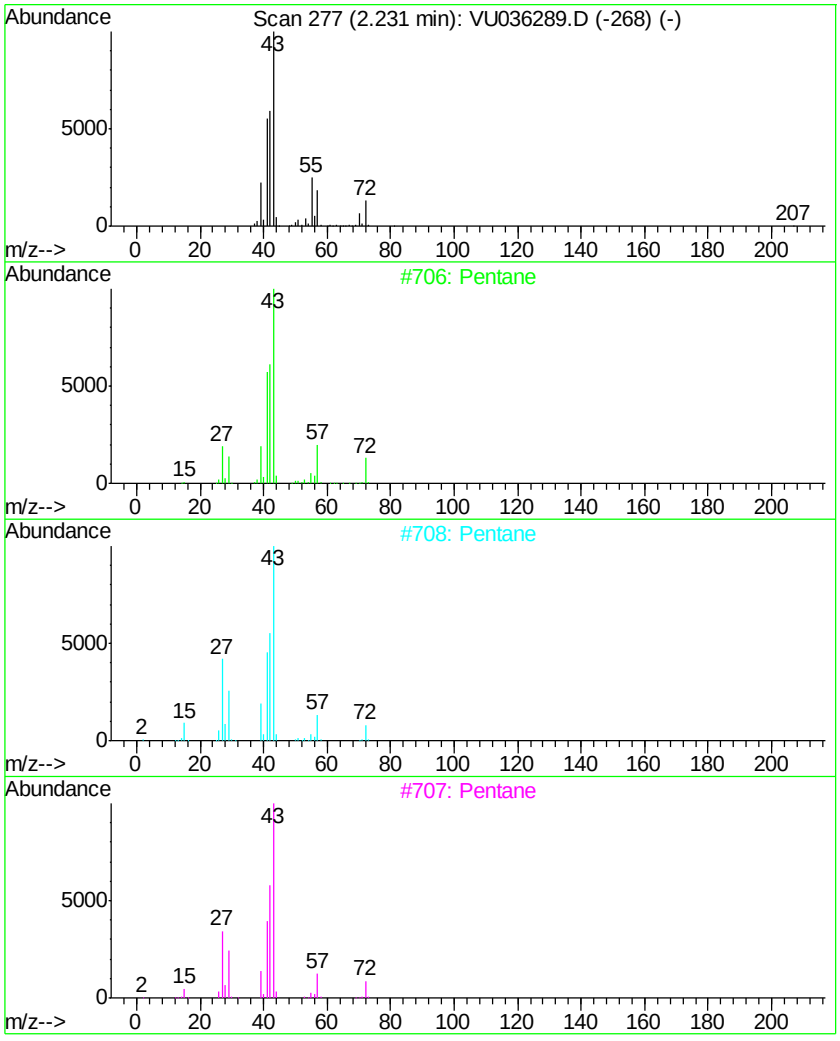
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR121319WMA.M
Quant Title : TRACE VOA SOM01.0

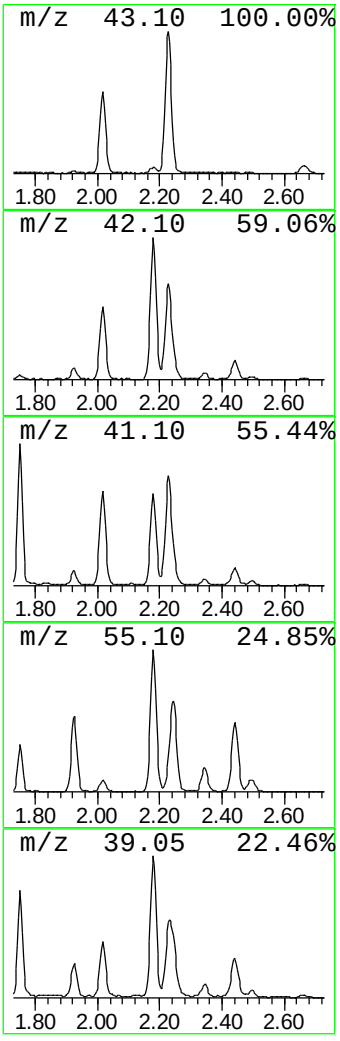
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.23	4.88 ug/L	611514	1,4-Difluorobenzene	6.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	91
2	Pentane	72	C5H12	000109-66-0	86
3	Pentane	72	C5H12	000109-66-0	86
4	Pentane	72	C5H12	000109-66-0	78
5	Oxirane, ethyl-	72	C4H8O	000106-88-7	53





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU121919\
Data File : VU036289.D
Acq On : 19 Dec 2019 17:46
Operator : JC/MD
Sample : K6282-08
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDW4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR121319WMA.M
Quant Title : TRACE VOA SOM01.0

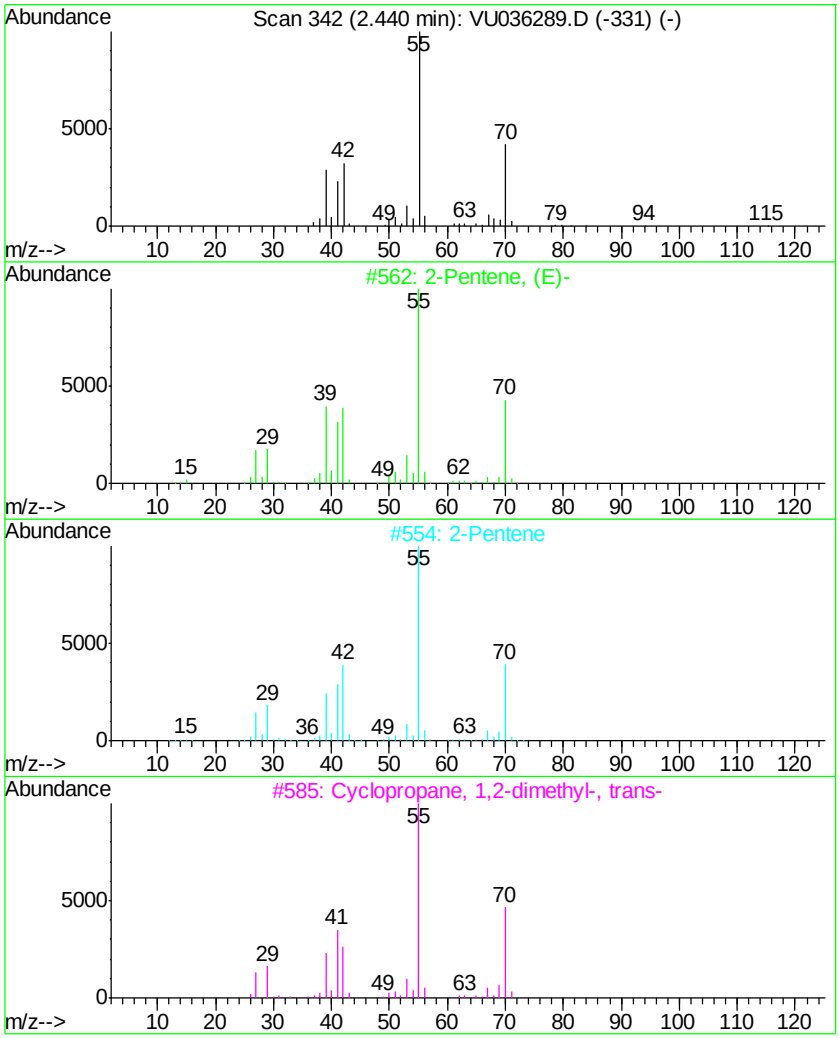
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

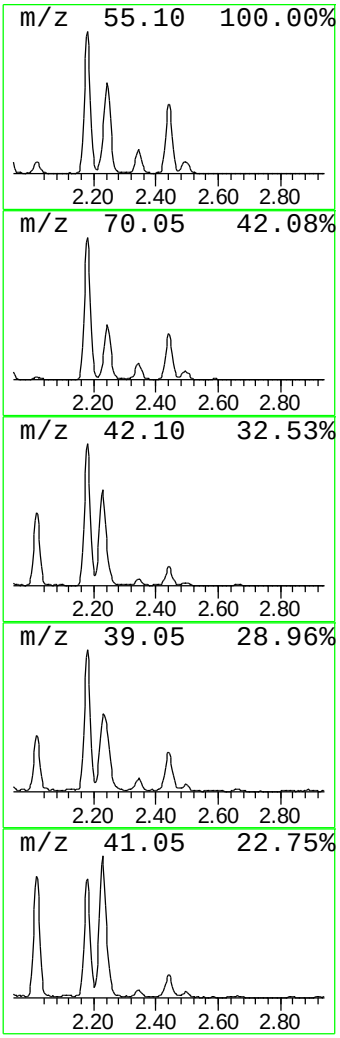
****

Peak Number 6 (DEL) Alkane: Cyclic2.44 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.44	1.50 ug/L	187312	1,4-Difluorobenzene	6.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, (E)-	70	C5H10	000646-04-8	93
2	2-Pentene	70	C5H10	000109-68-2	90
3	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	90
4	2-Methyl-1-butene	70	C5H10	000563-46-2	87
5	2-Pentene, (Z)-	70	C5H10	000627-20-3	87





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU121919\
Data File : VU036289.D
Acq On : 19 Dec 2019 17:46
Operator : JC/MD
Sample : K6282-08
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDW4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR121319WMA.M
Quant Title : TRACE VOA SOM01.0

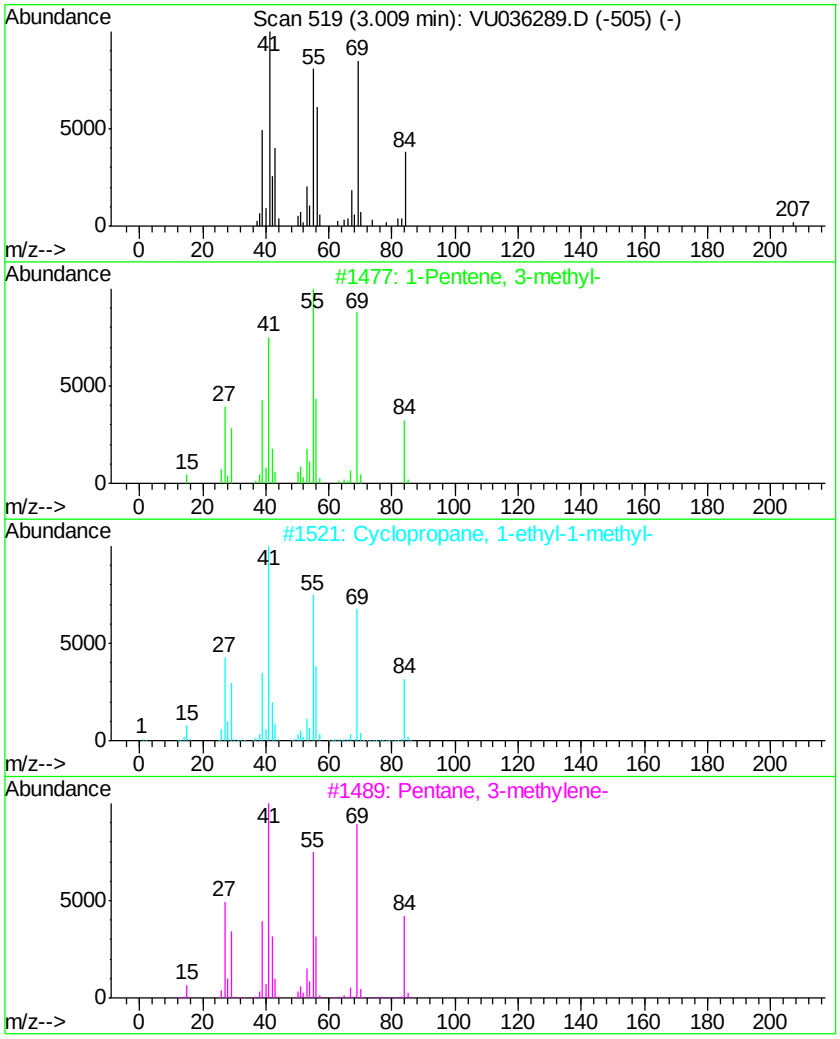
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

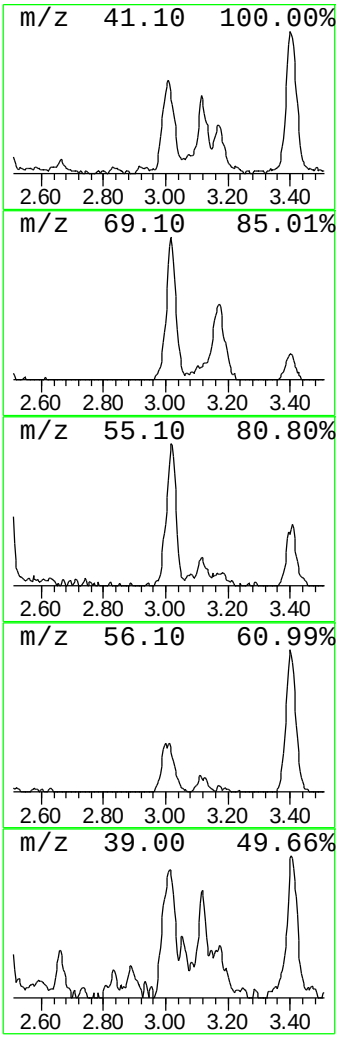
****

Peak Number 7 (DEL) Alkane: Cyclic3.01 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.01	0.83 ug/L	103871	1,4-Difluorobenzene	6.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene, 3-methyl-	84	C6H12	000760-20-3	87
2	Cyclopropane, 1-ethyl-1-methyl-	84	C6H12	053778-43-1	76
3	Pentane, 3-methylene-	84	C6H12	000760-21-4	64
4	2-Pentene, 3-methyl-, (Z)-	84	C6H12	000922-62-3	62
5	1-Pentene, 3-methyl-	84	C6H12	000760-20-3	58





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU121919\
Data File : VU036289.D
Acq On : 19 Dec 2019 17:46
Operator : JC/MD
Sample : K6282-08
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDW4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR121319WMA.M
Quant Title : TRACE VOA SOM01.0

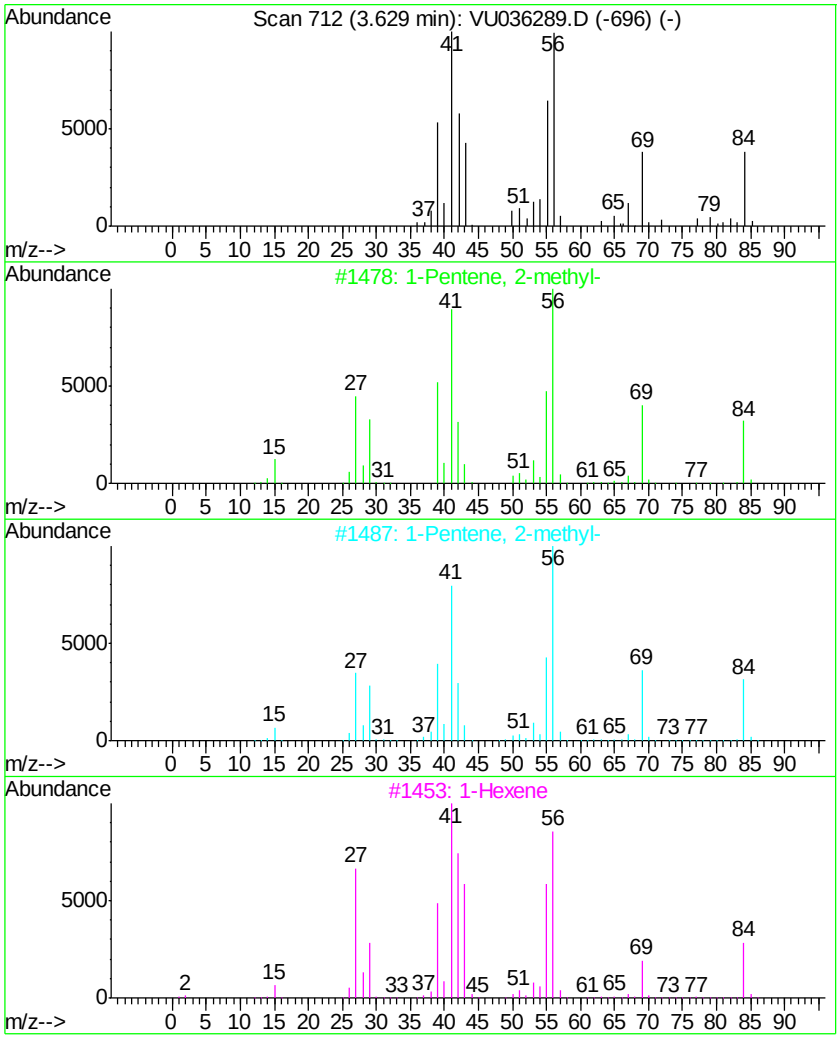
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

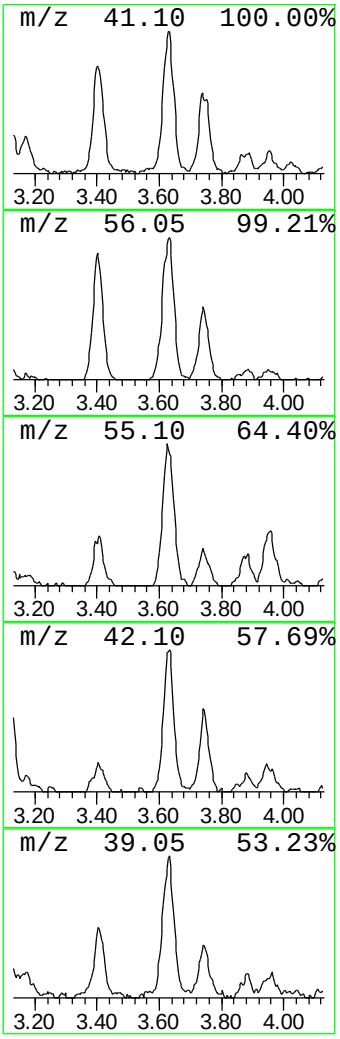
****

Peak Number 8 (DEL) Alkane: Cyclic3.63 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.63	1.23 ug/L	153694	1,4-Difluorobenzene	6.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	87
2	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	74
3	1-Hexene	84	C6H12	000592-41-6	64
4	3-Hexene, (Z)-	84	C6H12	007642-09-3	62
5	3-Hexene, (E)-	84	C6H12	013269-52-8	62





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU121919\
Data File : VU036289.D
Acq On : 19 Dec 2019 17:46
Operator : JC/MD
Sample : K6282-08
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDW4

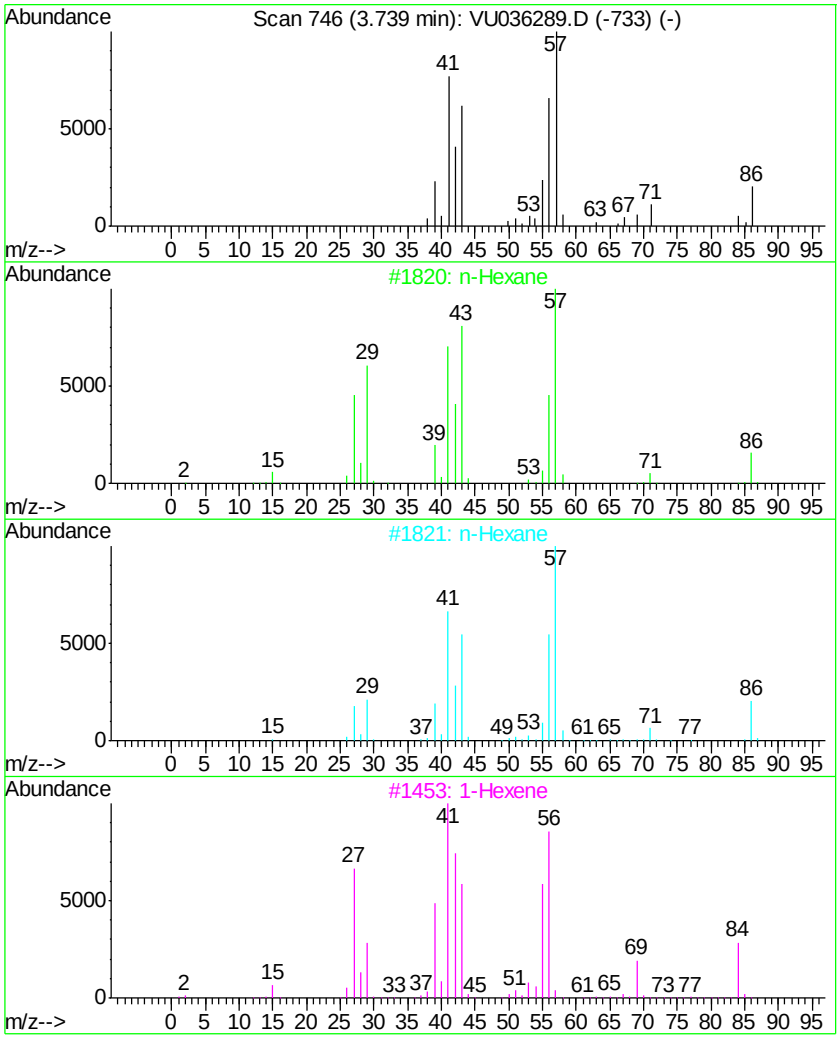
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR121319WMA.M
Quant Title : TRACE VOA SOM01.0

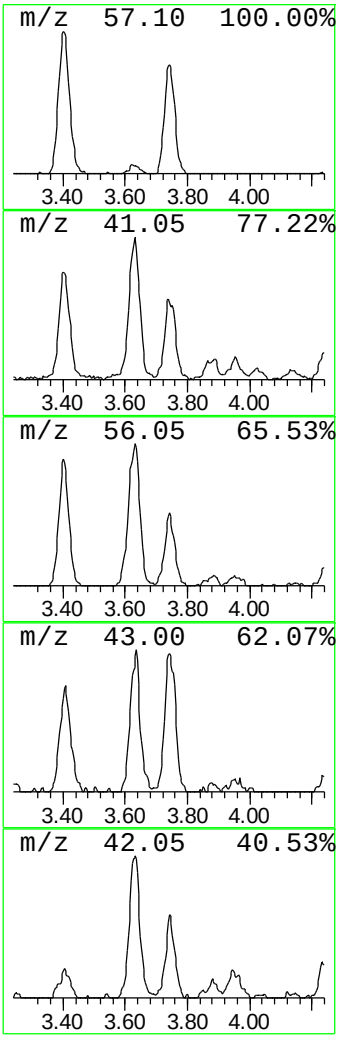
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 (DEL) Alkane: Straight-Chai... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.74	0.68 ug/L	85370	1,4-Difluorobenzene	6.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexane	86	C6H14	000110-54-3	72
2	n-Hexane	86	C6H14	000110-54-3	64
3	1-Hexene	84	C6H12	000592-41-6	37
4	1-Hexene	84	C6H12	000592-41-6	28
5	Cyanic acid, propyl ester	85	C4H7NO	001768-36-1	28





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU121919\
Data File : VU036289.D
Acq On : 19 Dec 2019 17:46
Operator : JC/MD
Sample : K6282-08
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDW4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR121319WMA.M
Quant Title : TRACE VOA SOM01.0

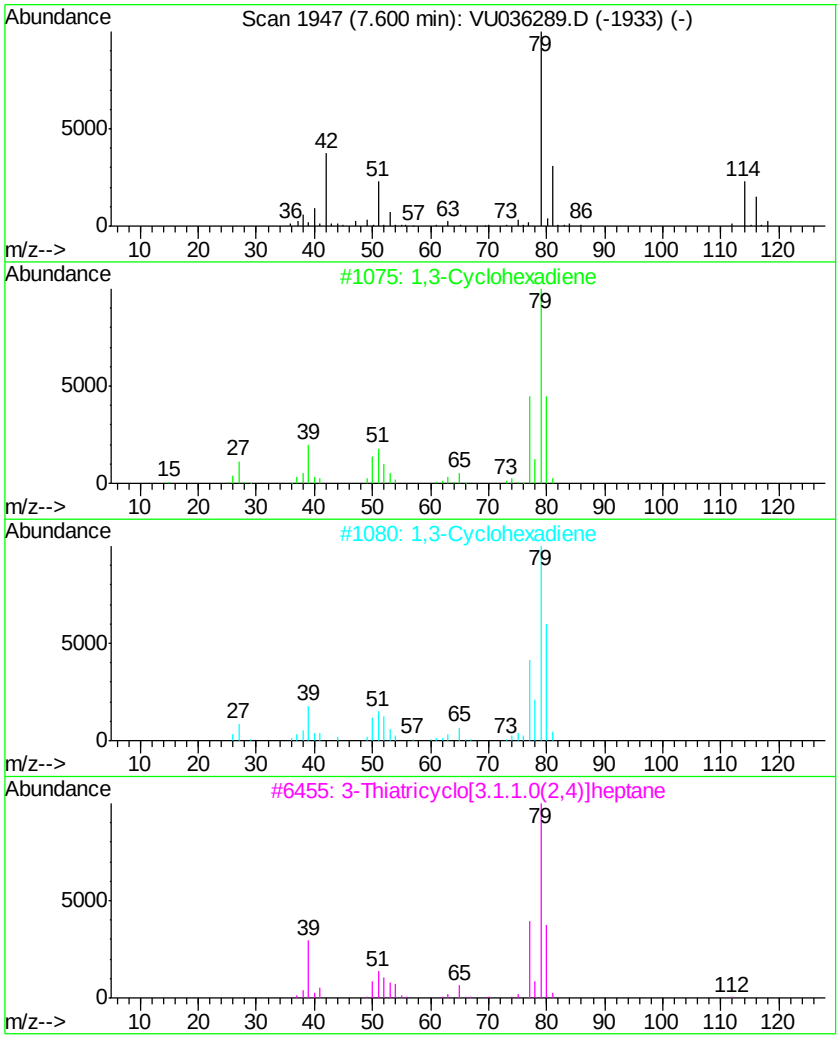
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

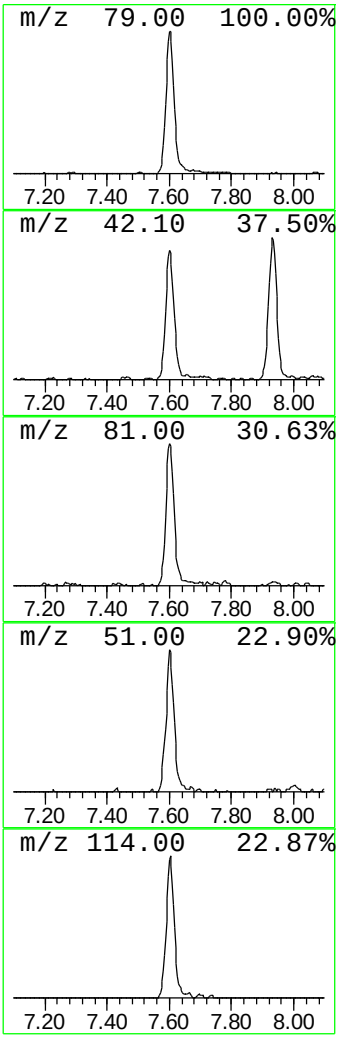
****

Peak Number 10 unknown-01 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.60	1.46 ug/L	183271	1,4-Difluorobenzene	6.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclohexadiene	80	C6H8	000592-57-4	28
2	1,3-Cyclohexadiene	80	C6H8	000592-57-4	25
3	3-Thiatricyclo[3.1.1.0(2,4)]heptane	112	C6H8S	1000221-37-0	25
4	1,4-Cyclohexadiene	80	C6H8	000628-41-1	9
5	2-Propanol, 1,3-dichloro-	128	C3H6Cl2O	000096-23-1	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU121919\
Data File : VU036289.D
Acq On : 19 Dec 2019 17:46
Operator : JC/MD
Sample : K6282-08
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDW4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR121319WMA.M
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: Cyc...	1.37	30.4	ug/L	3802430	1	6.29	625987	5.0
(DEL) Alkane: Str...	1.51	2.1	ug/L	262571	1	6.29	625987	5.0
(DEL) Alkane: Cyc...	1.75	2.1	ug/L	265178	1	6.29	625987	5.0
(DEL) Alkane: Str...	2.02	2.8	ug/L	352605	1	6.29	625987	5.0
(DEL) Alkane: Str...	2.23	4.9	ug/L	611514	1	6.29	625987	5.0
(DEL) Alkane: Cyc...	2.44	1.5	ug/L	187312	1	6.29	625987	5.0
(DEL) Alkane: Cyc...	3.01	0.8	ug/L	103871	1	6.29	625987	5.0
(DEL) Alkane: Cyc...	3.63	1.2	ug/L	153694	1	6.29	625987	5.0
(DEL) Alkane: Str...	3.74	0.7	ug/L	85370	1	6.29	625987	5.0
unknown-01	7.60	1.5	ug/L	183271	1	6.29	625987	5.0