LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU021419\
Data File : VU029477.D
Acq On : 14 Feb 2019 23:53
Operator : JC/SP
Sample : K1438-16
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : ESXD8

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\SOMUTR021219WMA.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	1.183	21	29	50	rBV	8521366	7725315	100.00%	37.326%
2	1.302	55	66	88	rBV	1444204	1722698	22.30%	8.323%
3	1.399	89	96	107	rBV	2840283	2885725	37.35%	13.943%
4	1.679	177	183	192	rBV	68777	83431	1.08%	0.403%
5	1.756	199	207	230	rVB	417031	568745	7.36%	2.748%
6	1.945	257	266	281	rVB	296358	402813	5.21%	1.946%
7	2.273	358	368	382	rBV	152519	244436	3.16%	1.181%
8	2.444	413	421	439	rVB	60593	109350	1.42%	0.528%
9	2.788	519	528	546	rVB	110086	209257	2.71%	1.011%
10	2.981	578	588	608	rVB3	71425	153415	1.99%	0.741%
11	4.084	913	931	952	rBV2	74644	198590	2.57%	0.960%
12	4.222	952	974	1010	rBV2	627505	1701462	22.02%	8.221%
13	4.646	1090	1106	1126	rBV	94518	222717	2.88%	1.076%
14	4.987	1193	1212	1230	rBV	96346	234861	3.04%	1.135%
15	5.334	1301	1320	1348	rVB2	186247	526446	6.81%	2.544%
16	5.884	1477	1491	1515	rBV	209155	408514	5.29%	1.974%
17	6.328	1616	1629	1642	rBV	120260	242929	3.14%	1.174%
18	6.408	1642	1654	1668	rVB	71512	154531	2.00%	0.747%
19	7.225	1897	1908	1933	rBV	63922	121629	1.57%	0.588%
20	7.563	1991	2013	2032	rBV	262202	468154	6.06%	2.262%
21	8.312	2234	2246	2288	rBV	365427	655154	8.48%	3.165%
22	9.087	2475	2487	2509	rBV	301007	502440	6.50%	2.428%
23	10.431	2893	2905	2918	rBV	110045	178646	2.31%	0.863%
24	11.482	3218	3232	3256	rBV	311290	517049	6.69%	2.498%
25	11.858	3337	3349	3372	rBV	275433	458720	5.94%	2.216%

Sum of corrected areas: 20697027

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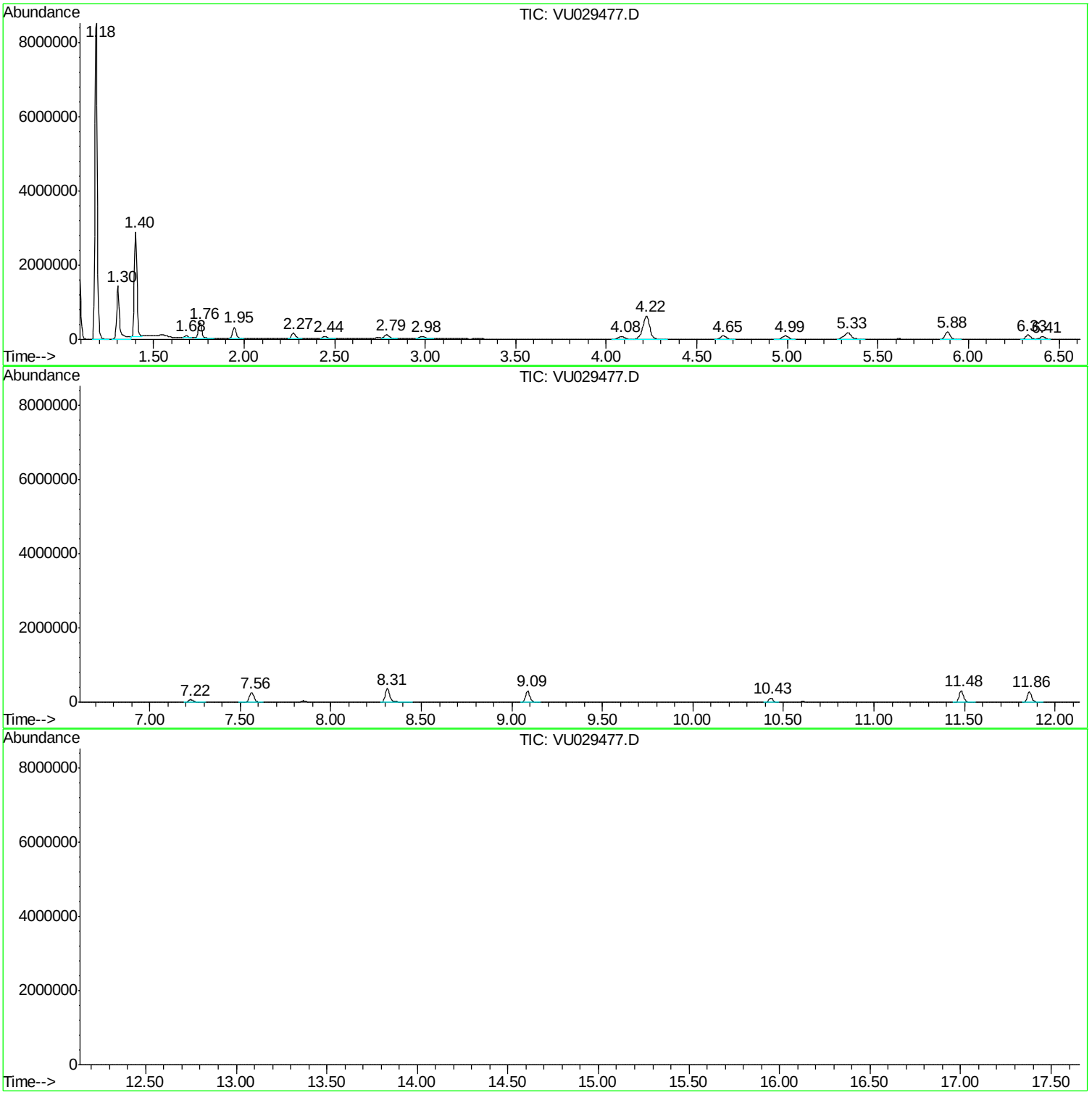
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ESXD8

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR021219WMA.M
Quant Title : TRACE VOA SOM01.0

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU021419\
Data File : VU029477.D
Acq On : 14 Feb 2019 23:53
Operator : JC/SP
Sample : K1438-16
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : ESXD8

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR021219WMA.M
Quant Title : TRACE VOA SOM01.0

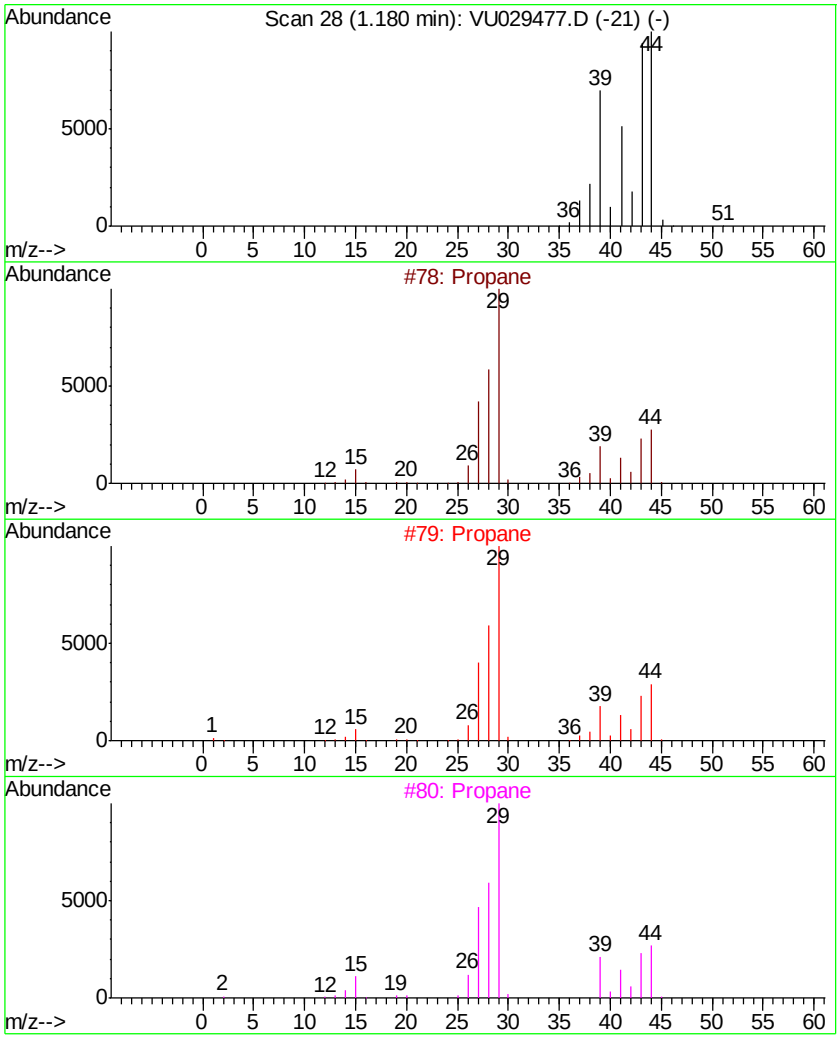
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

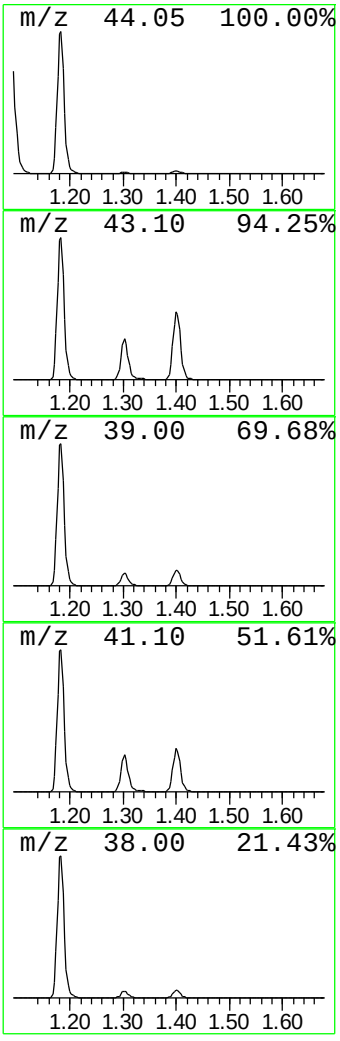
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.18	94.55 ug/L	7725320	1,4-Difluorobenzene	5.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane	44	C3H8	000074-98-6	83
2	Propane	44	C3H8	000074-98-6	45
3	Propane	44	C3H8	000074-98-6	9
4	Propene	42	C3H6	000115-07-1	9
5	Acetaldehyde	44	C2H4O	000075-07-0	5





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU021419\
Data File : VU029477.D
Acq On : 14 Feb 2019 23:53
Operator : JC/SP
Sample : K1438-16
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : ESXD8

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR021219WMA.M
Quant Title : TRACE VOA SOM01.0

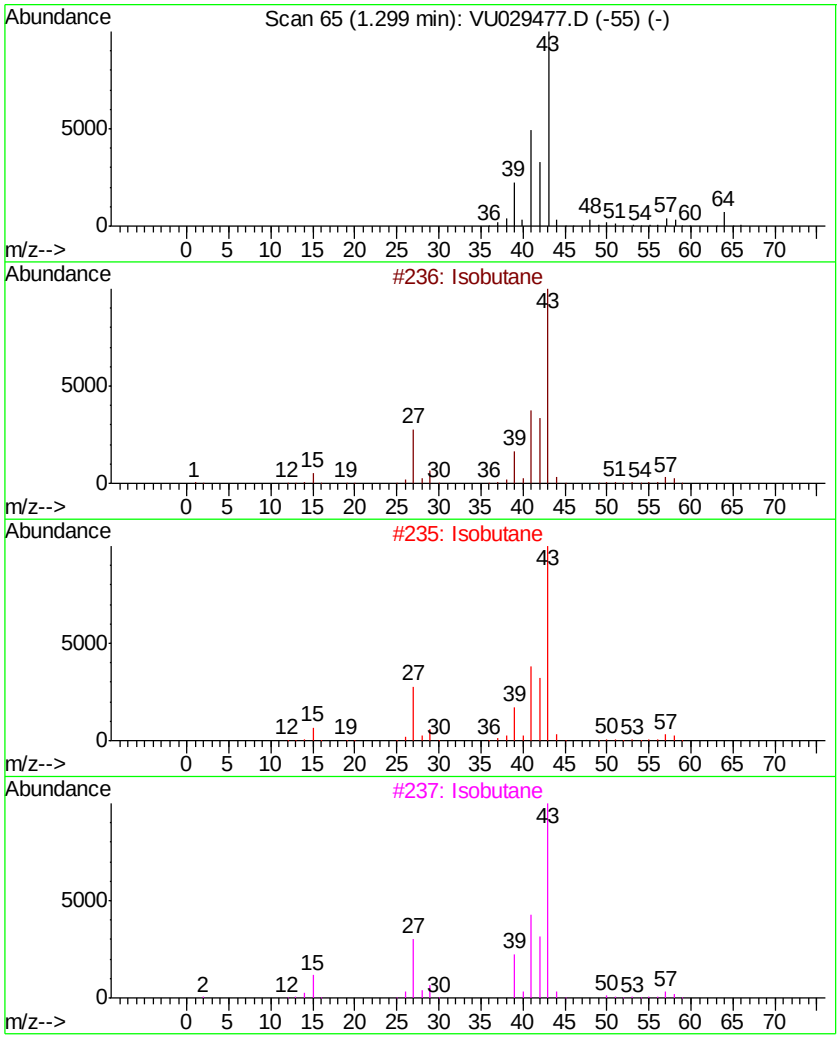
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

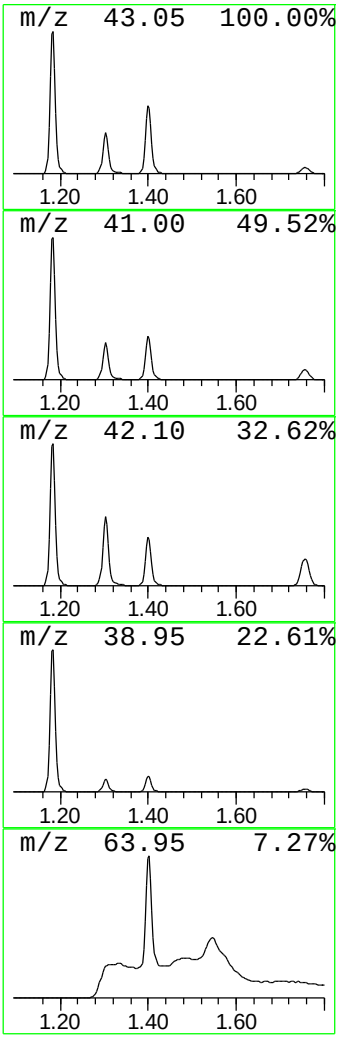
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.30	21.08 ug/L	1722700	1,4-Difluorobenzene	5.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutane	58	C4H10	000075-28-5	72
2	Isobutane	58	C4H10	000075-28-5	64
3	Isobutane	58	C4H10	000075-28-5	59
4	Isobutane	58	C4H10	000075-28-5	53
5	Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU021419\
Data File : VU029477.D
Acq On : 14 Feb 2019 23:53
Operator : JC/SP
Sample : K1438-16
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : ESXD8

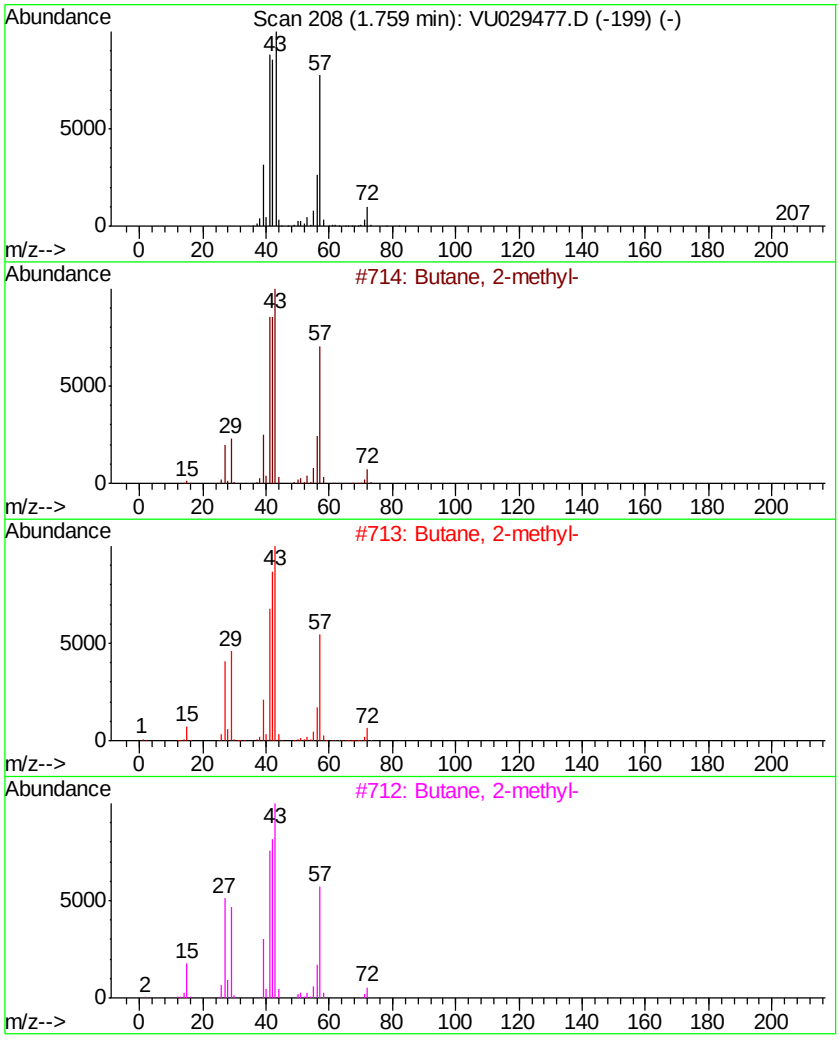
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR021219WMA.M
Quant Title : TRACE VOA SOM01.0

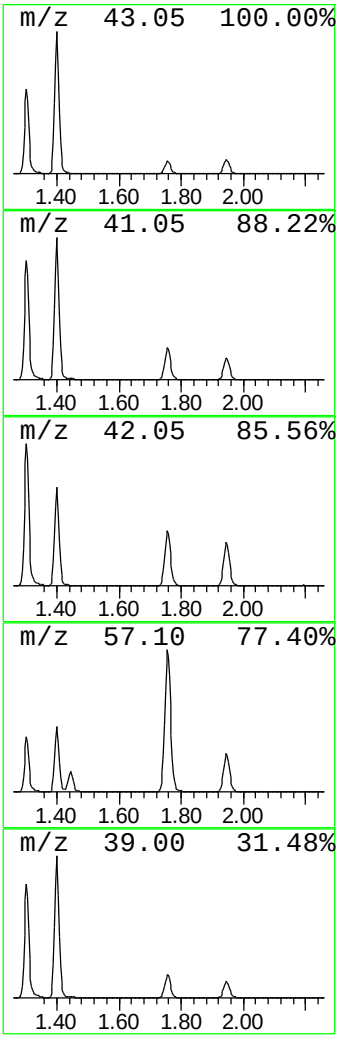
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.76	6.96 ug/L	568745	1,4-Difluorobenzene	5.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	94
2	Butane, 2-methyl-	72	C5H12	000078-78-4	86
3	Butane, 2-methyl-	72	C5H12	000078-78-4	80
4	3-Buten-1-ol	72	C4H8O	000627-27-0	38
5	Pentane	72	C5H12	000109-66-0	33





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU021419\
Data File : VU029477.D
Acq On : 14 Feb 2019 23:53
Operator : JC/SP
Sample : K1438-16
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : ESXD8

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR021219WMA.M
Quant Title : TRACE VOA SOM01.0

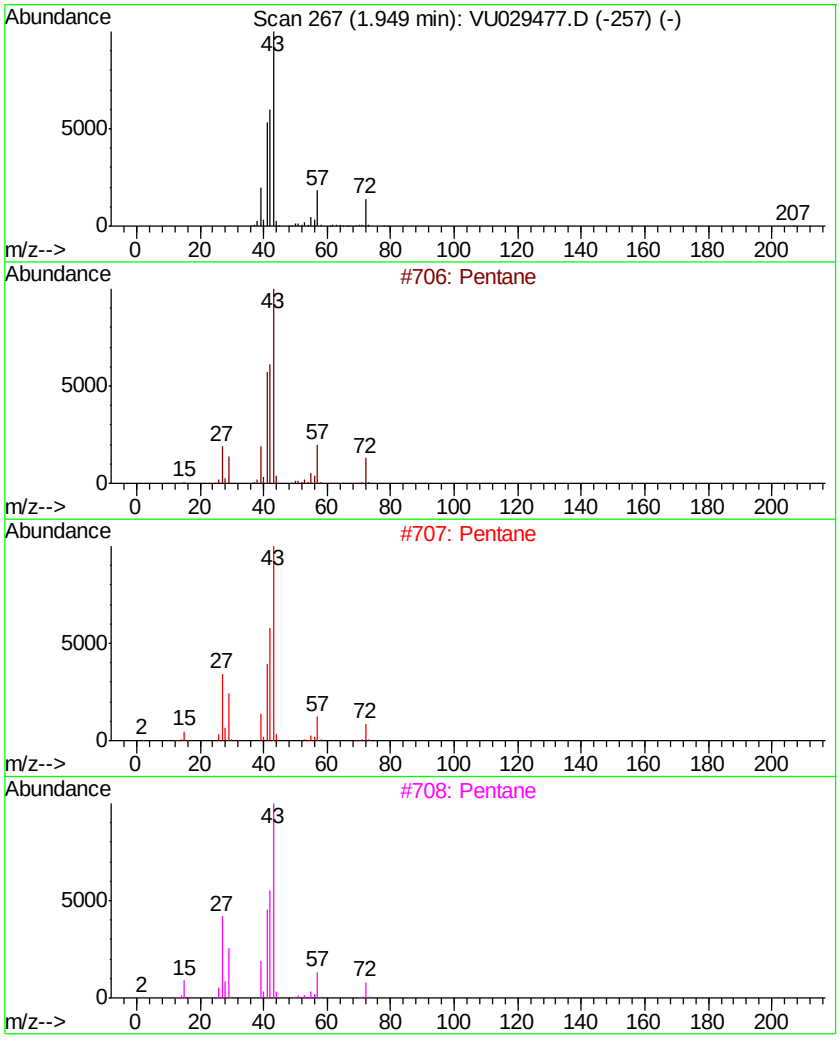
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

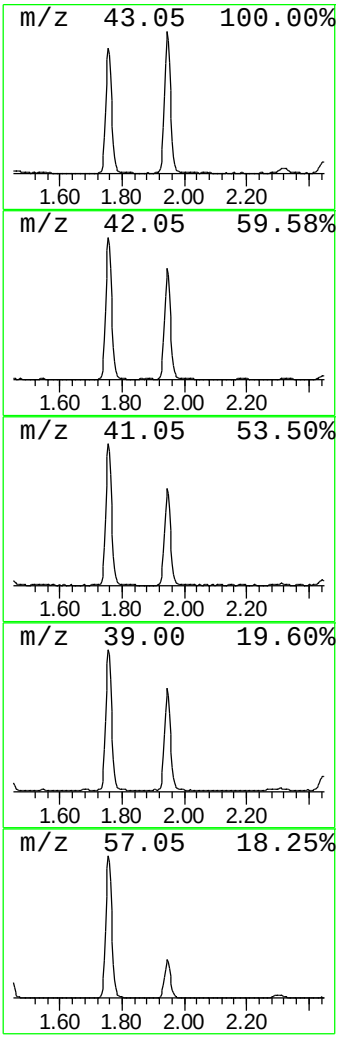
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.95	4.93 ug/L	402813	1,4-Difluorobenzene	5.88

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	64
5	Oxirane, ethyl-	72	C4H8O	000106-88-7	53





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU021419\
Data File : VU029477.D
Acq On : 14 Feb 2019 23:53
Operator : JC/SP
Sample : K1438-16
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : ESXD8

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR021219WMA.M
Quant Title : TRACE VOA SOM01.0

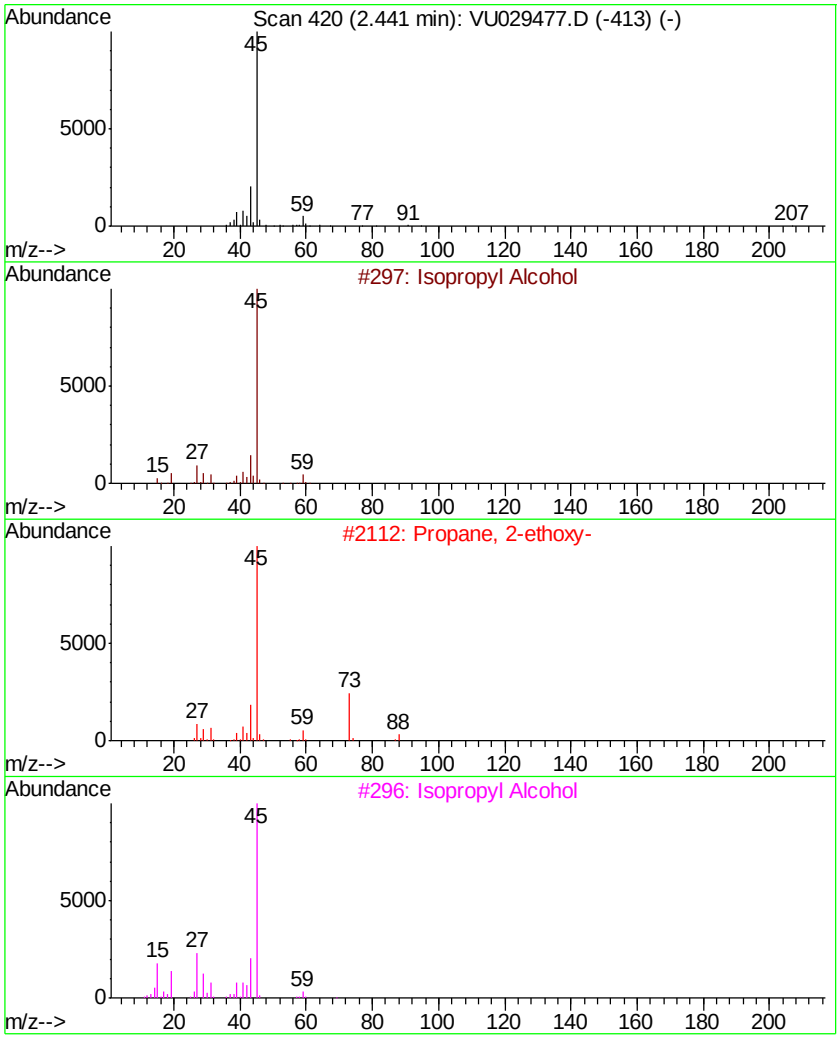
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

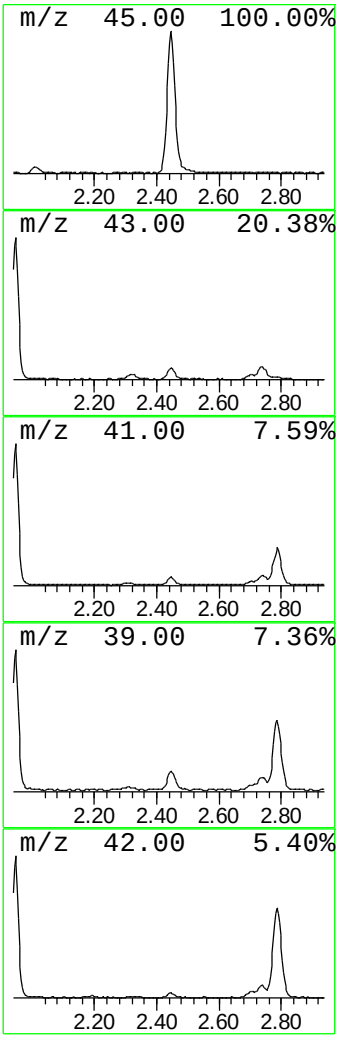
****

Peak Number 5 Isopropyl Alcohol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.44	1.34 ug/L	109350	1,4-Difluorobenzene	5.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	80
2	Propane, 2-ethoxy-	88	C5H12O	000625-54-7	64
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	56
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	50
5	2-Pentanol	88	C5H12O	006032-29-7	9





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Operator : JC/SP
Sample : K1438-16
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : ESXD8

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR021219WMA.M
Quant Title : TRACE VOA SOM01.0

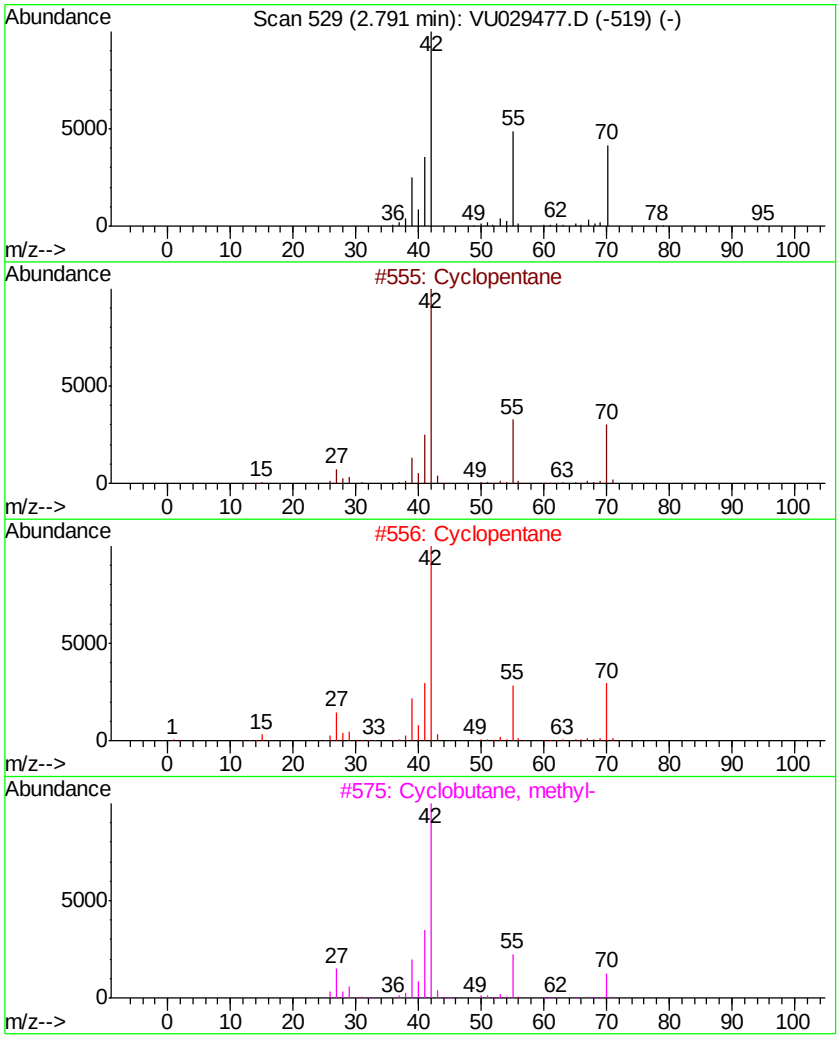
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

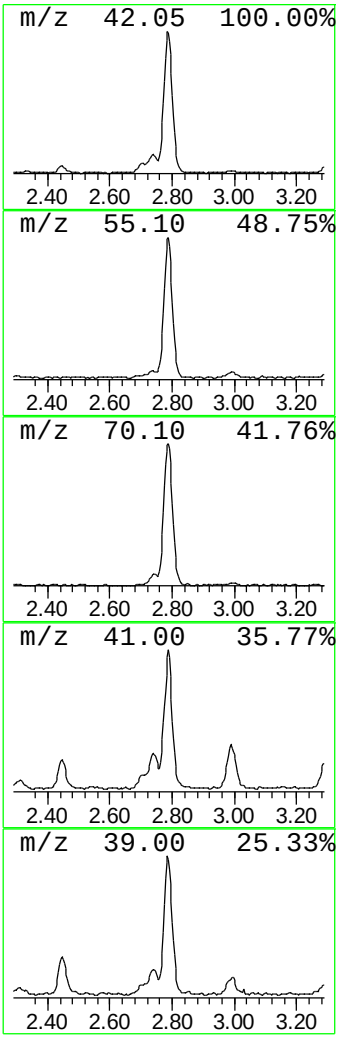
****

Peak Number 6 (DEL) Alkane: Cyclic2.79 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.79	2.56 ug/L	209257	1,4-Difluorobenzene	5.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane	70	C5H10	000287-92-3	86
2	Cyclopentane	70	C5H10	000287-92-3	78
3	Cyclobutane, methyl-	70	C5H10	000598-61-8	72
4	1-Pentene	70	C5H10	000109-67-1	64
5	Cyclobutane, methyl-	70	C5H10	000598-61-8	56





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ALS Vial : 34 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : ESXD8

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR021219WMA.M
Quant Title : TRACE VOA SOM01.0

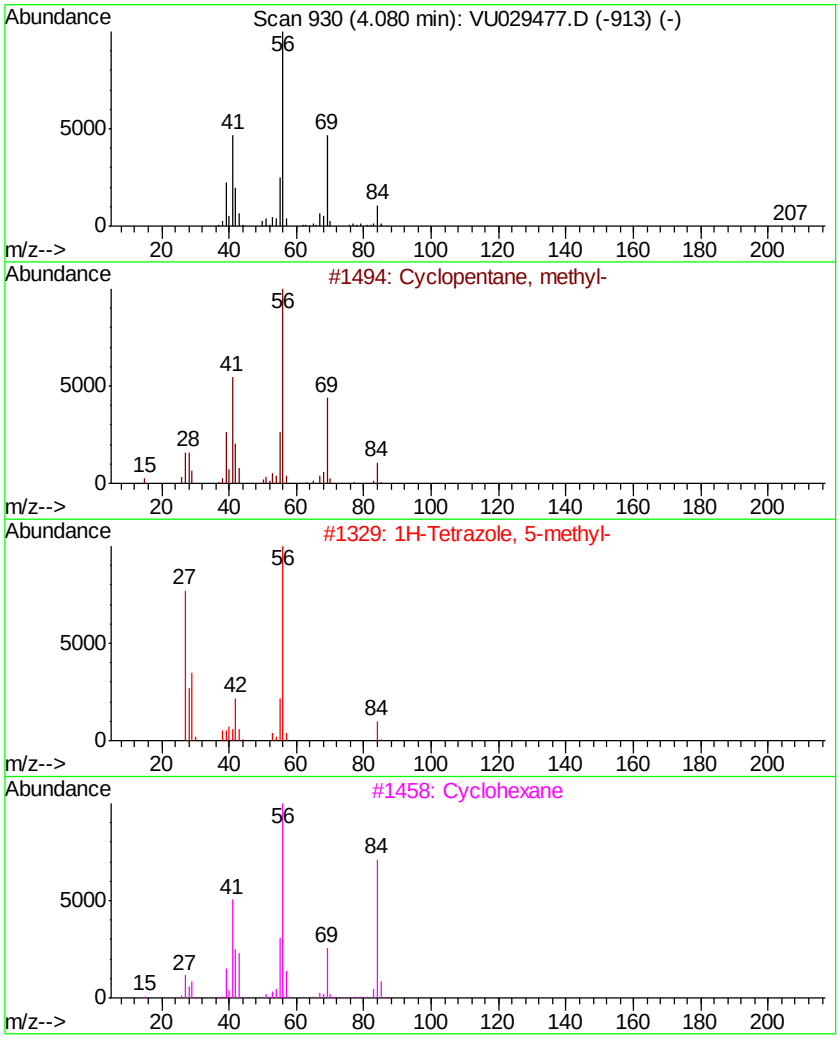
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

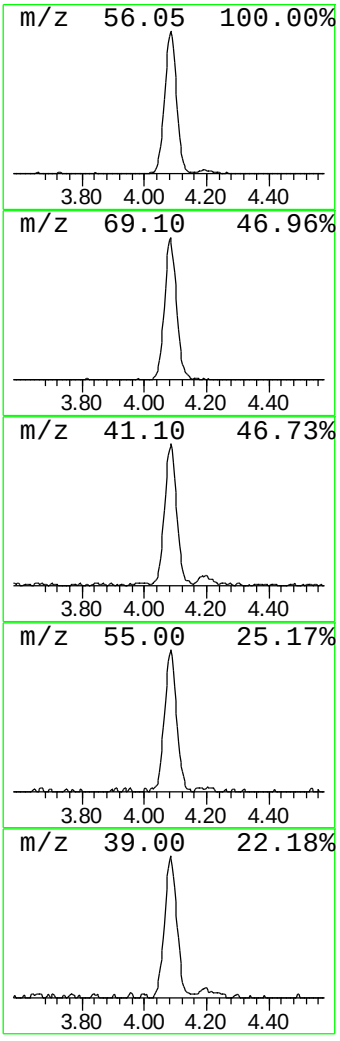
****

Peak Number 7 (DEL) Alkane: Cyclic4.08 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.08	2.43 ug/L	198590	1,4-Difluorobenzene	5.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	80
3	Cyclohexane	84	C6H12	000110-82-7	78
4	Cyclobutane, ethyl-	84	C6H12	004806-61-5	59
5	Cyclobutane, ethyl-	84	C6H12	004806-61-5	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU021419\
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ALS Vial : 34 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : ESXD8

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR021219WMA.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: Str...	1.18	94.5	ug/L	7725320	1	5.88	408514	5.0
(DEL) Alkane: Str...	1.30	21.1	ug/L	1722700	1	5.88	408514	5.0
(DEL) Alkane: Str...	1.76	7.0	ug/L	568745	1	5.88	408514	5.0
(DEL) Alkane: Str...	1.95	4.9	ug/L	402813	1	5.88	408514	5.0
Isopropyl Alcohol	2.44	1.3	ug/L	109350	1	5.88	408514	5.0
(DEL) Alkane: Cyc...	2.79	2.6	ug/L	209257	1	5.88	408514	5.0
(DEL) Alkane: Cyc...	4.08	2.4	ug/L	198590	1	5.88	408514	5.0