LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX100720\
Data File : VX018819.D
Acq On : 07 Oct 2020 18:31
Operator : JC/SP
Sample : L4240-10DL 5X
Misc : 25.0mL/MSVOA X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : BG3S8DL

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	2.343	198	206	220	rBV	106385	181376	1.26%	0.509%
2	2.825	276	285	287	rBV2	280368	533798	3.69%	1.498%
3	2.874	287	293	308	rVB	2005382	4159893	28.79%	11.678%
4	3.154	327	339	354	rBV	3270417	7403172	51.23%	20.782%
5	3.501	385	396	426	rBV	6454724	14450249	100.00%	40.565%
6	4.117	483	497	511	rBV2	189550	587777	4.07%	1.650%
7	4.282	511	524	531	rVV2	171214	517201	3.58%	1.452%
8	4.373	531	539	550	rVB	334139	933266	6.46%	2.620%
9	4.544	555	567	580	rBV2	78907	283231	1.96%	0.795%
10	5.135	652	664	688	rVB	80605	268129	1.86%	0.753%
11	6.044	800	813	829	rBV2	182973	532180	3.68%	1.494%
12	6.830	933	942	951	rBV	141442	338188	2.34%	0.949%
13	7.367	1021	1030	1038	rBV	119554	254319	1.76%	0.714%
14	8.696	1243	1248	1255	rVB	275629	444922	3.08%	1.249%
15	9.427	1362	1368	1377	rBV	439266	603427	4.18%	1.694%
16	10.122	1472	1482	1488	rBV2	991751	1746356	12.09%	4.902%
17	11.232	1657	1664	1675	rVB	134571	176678	1.22%	0.496%
18	12.006	1786	1791	1795	rBV	188244	238308	1.65%	0.669%
19	12.079	1795	1803	1809	rVB2	420142	869748	6.02%	2.442%
20	12.360	1844	1849	1860	rVB	389099	524272	3.63%	1.472%
21	13.628	2051	2057	2063	rBV	453433	576097	3.99%	1.617%

Sum of corrected areas: 35622587

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX100720\
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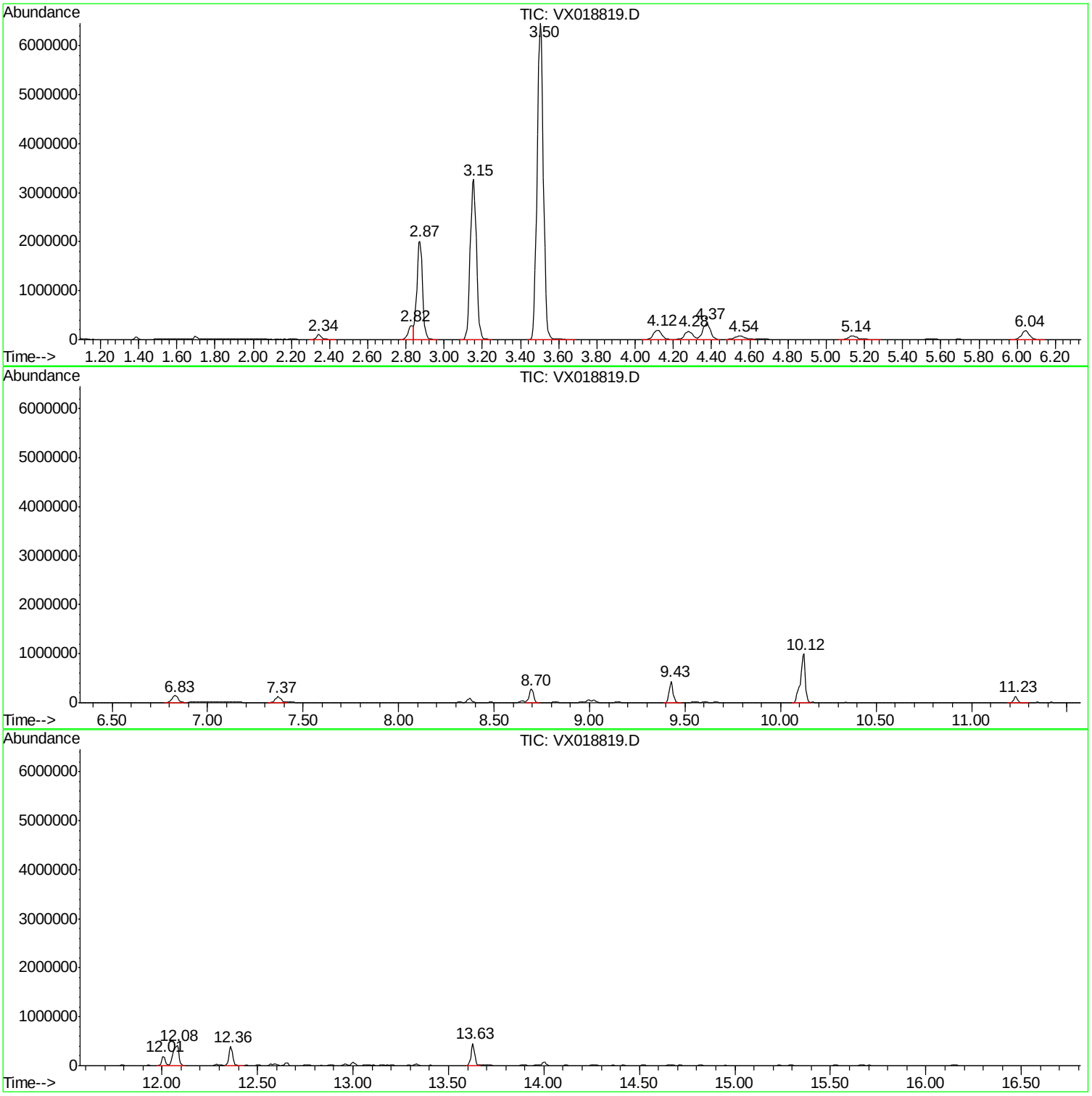
Misc : 25.0mL/MSVOA X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BG3S8DL

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX100720\
Data File : VX018819.D
Acq On : 07 Oct 2020 18:31
Operator : JC/SP
Sample : L4240-10DL 5X
Misc : 25.0mL/MSVOA X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : BG3S8DL

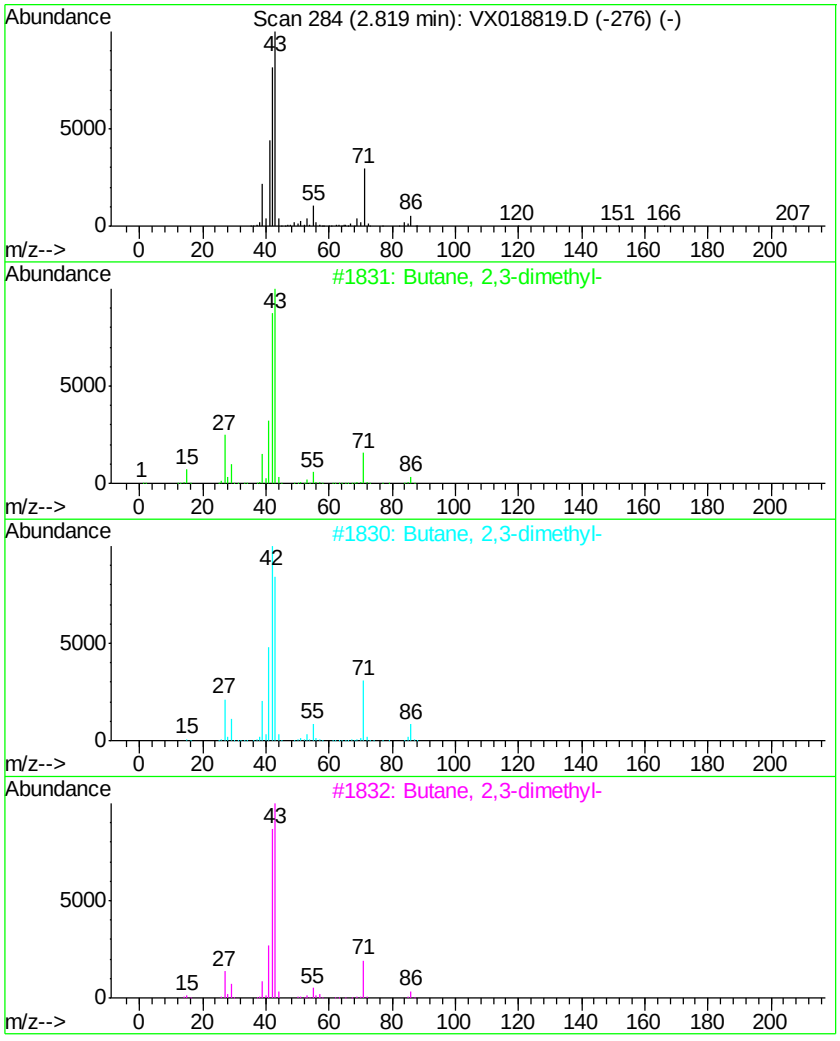
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\SOMXTR100220WMA.M
Quant Title : TRACE VOA SOM01.0

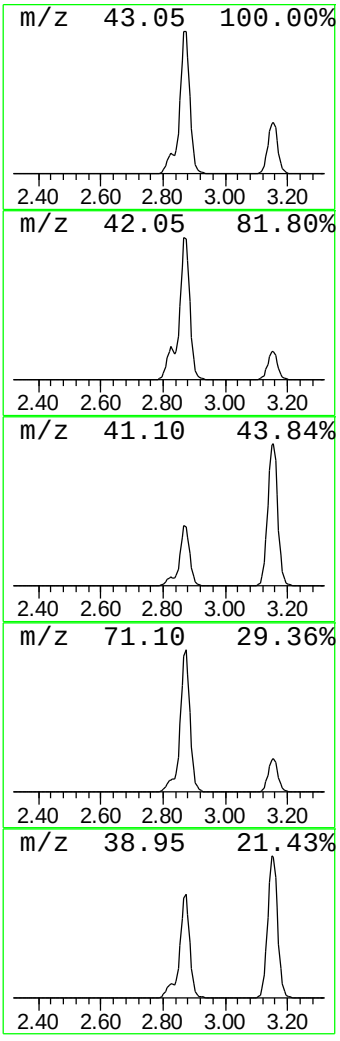
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.82	7.89 ug/L	533798	1,4-Difluorobenzene	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	80
2	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	80
3	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	78
4	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	53
5	Tetrahydrofuran	72	C4H8O	000109-99-9	36





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX100720\
Data File : VX018819.D
Acq On : 07 Oct 2020 18:31
Operator : JC/SP
Sample : L4240-10DL 5X
Misc : 25.0mL/MSVOA X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : BG3S8DL

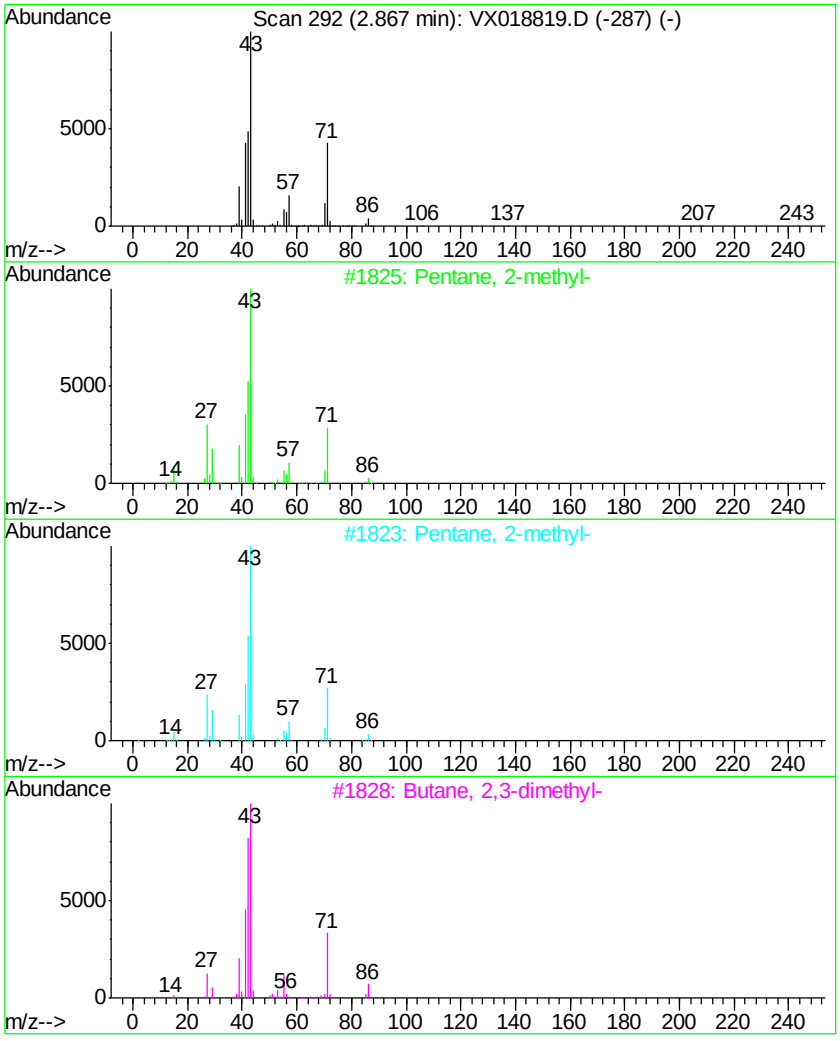
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\SOMXTR100220WMA.M
Quant Title : TRACE VOA SOM01.0

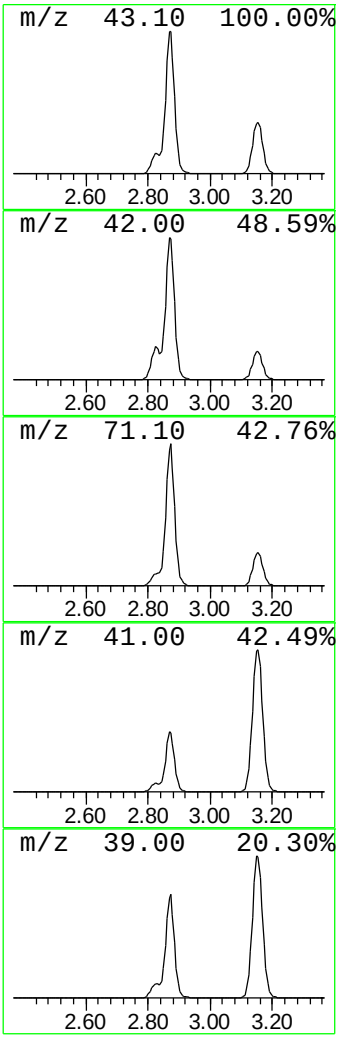
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.87	61.50 ug/L	4159890	1,4-Difluorobenzene	6.83

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	49
4	Pentane	72	C5H12	000109-66-0	46
5	1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	40





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX100720\
Data File : VX018819.D
Acq On : 07 Oct 2020 18:31
Operator : JC/SP
Sample : L4240-10DL 5X
Misc : 25.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : BG3S8DL

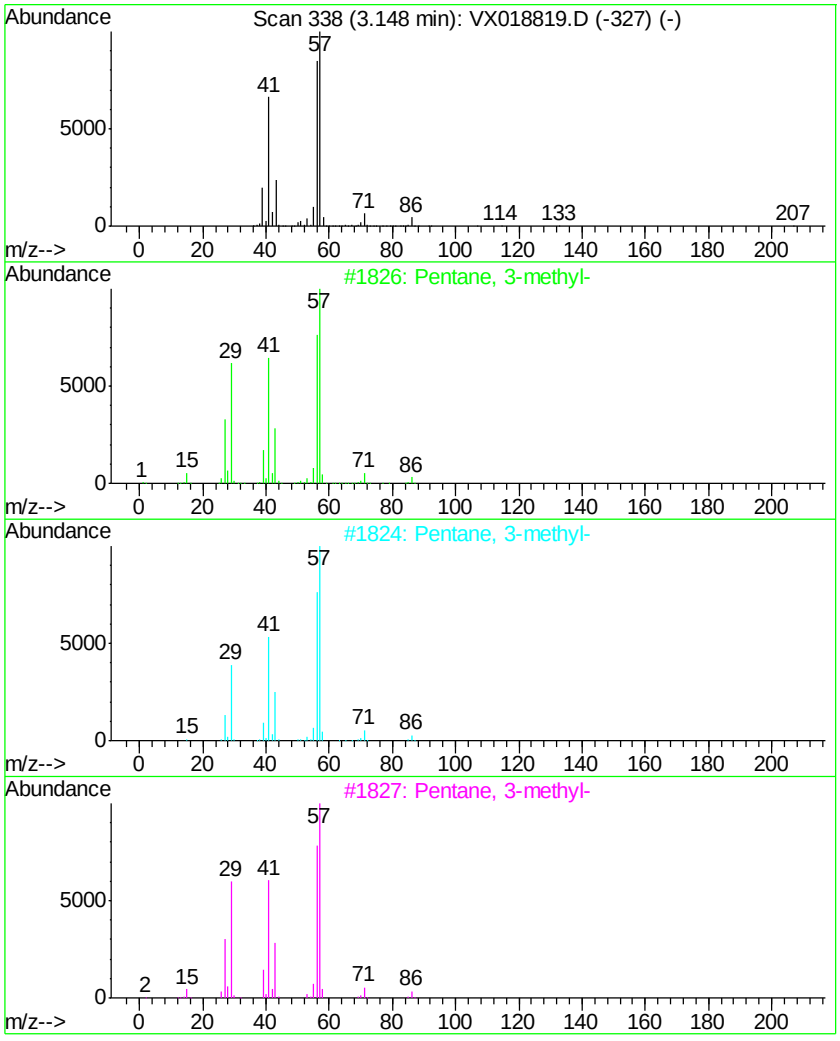
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\SOMXTR100220WMA.M
Quant Title : TRACE VOA SOM01.0

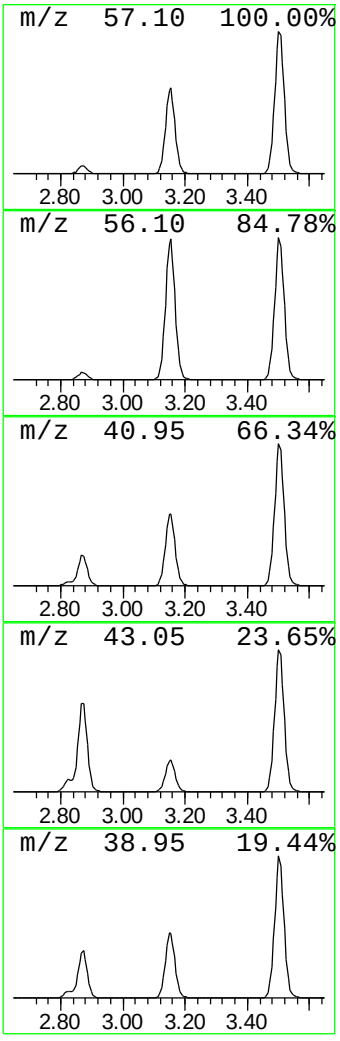
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.15	109.45 ug/L	7403170	1,4-Difluorobenzene	6.83

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	90
4	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	43
5	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	43





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX100720\
Data File : VX018819.D
Acq On : 07 Oct 2020 18:31
Operator : JC/SP
Sample : L4240-10DL 5X
Misc : 25.0mL/MSVOA X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : BG3S8DL

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

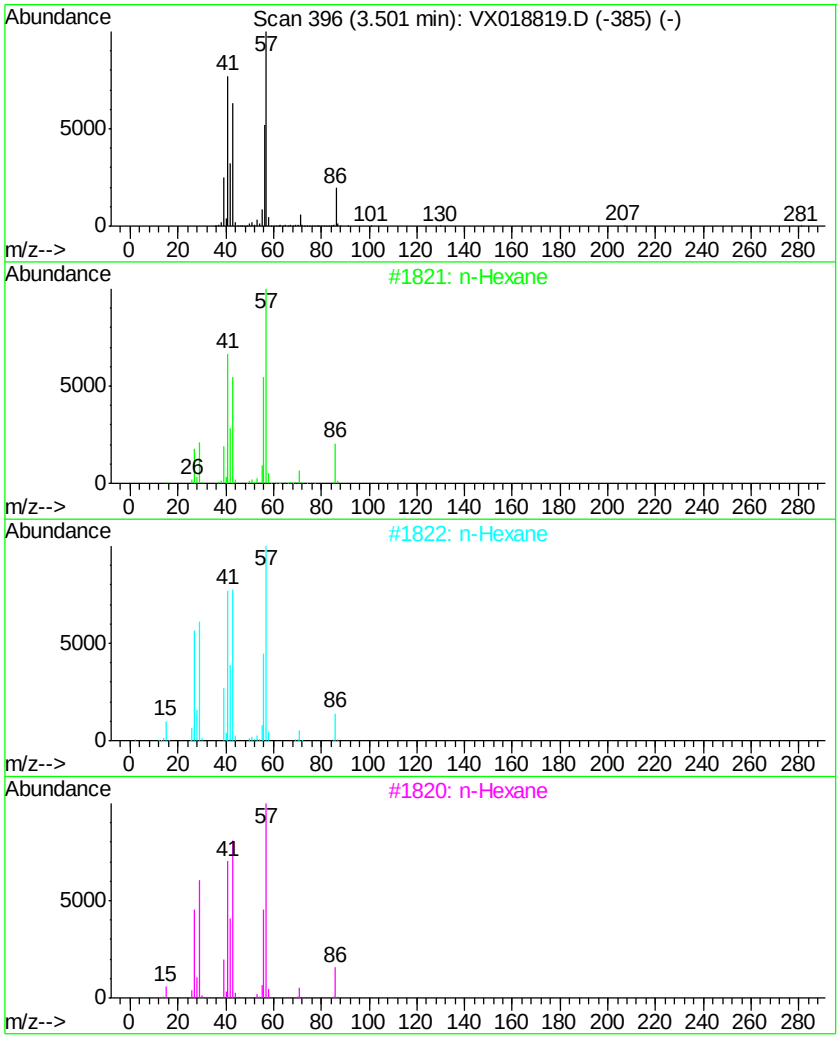
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

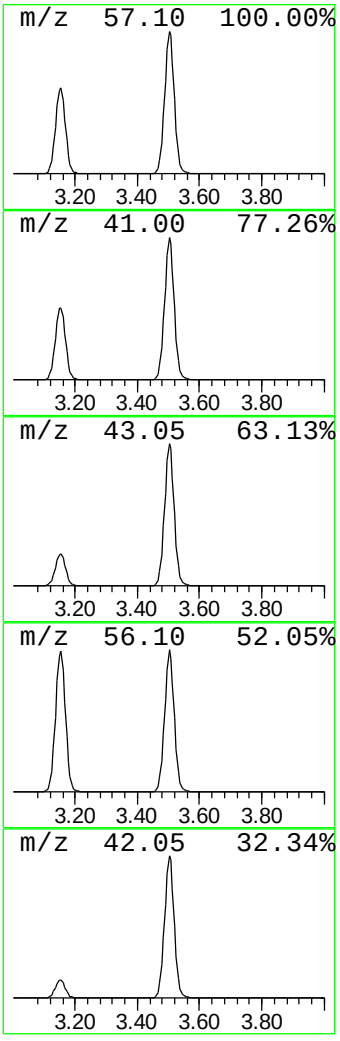
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.50	213.64 ug/L	14450200	1,4-Difluorobenzene	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexane	86	C6H14	000110-54-3	94
2	n-Hexane	86	C6H14	000110-54-3	64
3	n-Hexane	86	C6H14	000110-54-3	59
4	Butanal, 2-methyl-	86	C5H10O	000096-17-3	43
5	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	43





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX100720\
Data File : VX018819.D
Acq On : 07 Oct 2020 18:31
Operator : JC/SP
Sample : L4240-10DL 5X
Misc : 25.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : BG3S8DL

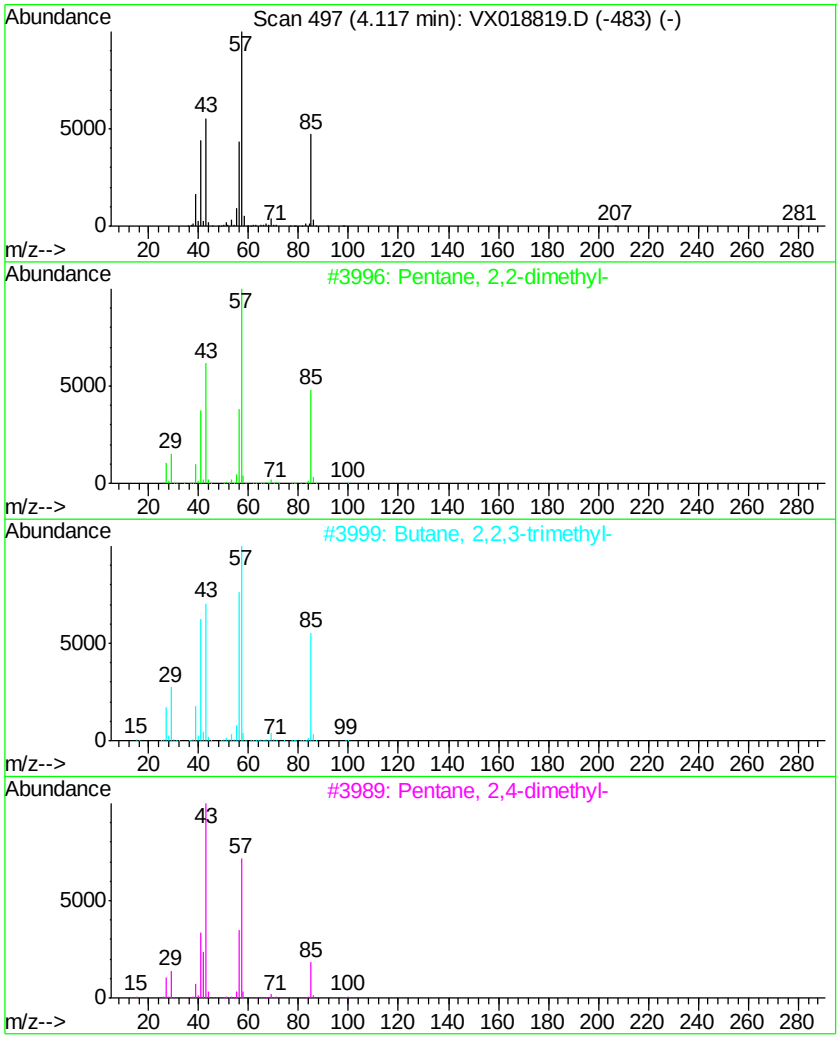
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\SOMXTR100220WMA.M
Quant Title : TRACE VOA SOM01.0

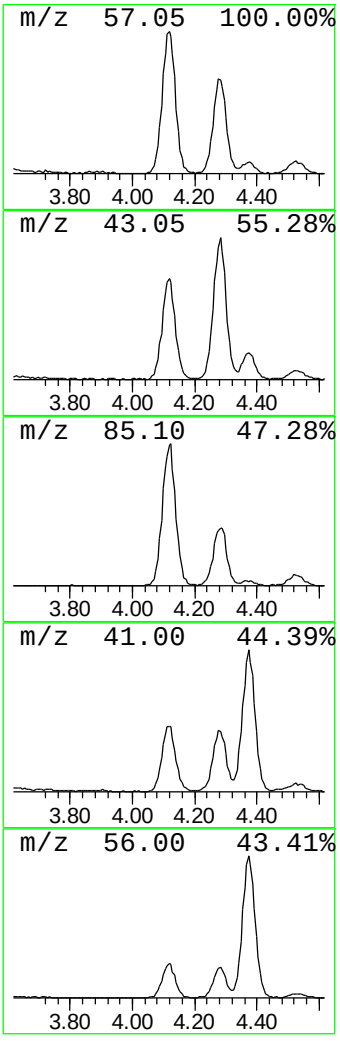
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.12	8.69 ug/L	587777	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	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	78
3	Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	78
4	Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	74
5	Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	74





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX100720\
Data File : VX018819.D
Acq On : 07 Oct 2020 18:31
Operator : JC/SP
Sample : L4240-10DL 5X
Misc : 25.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : BG3S8DL

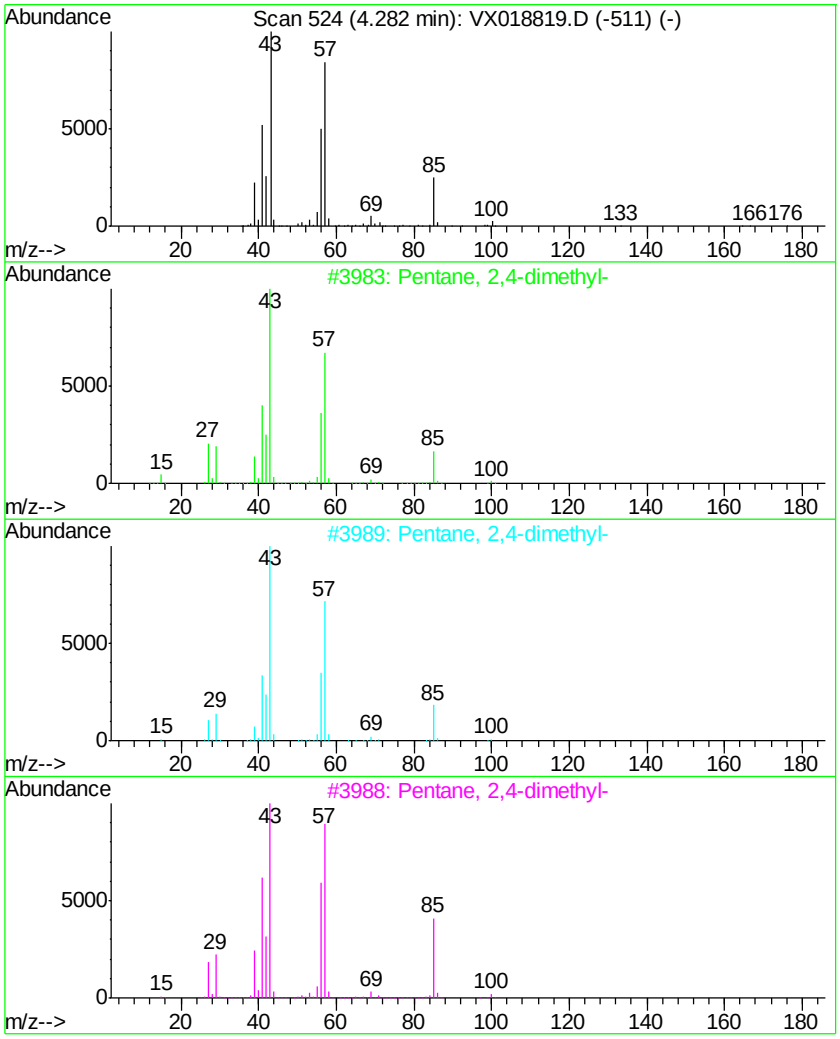
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\SOMXTR100220WMA.M
Quant Title : TRACE VOA SOM01.0

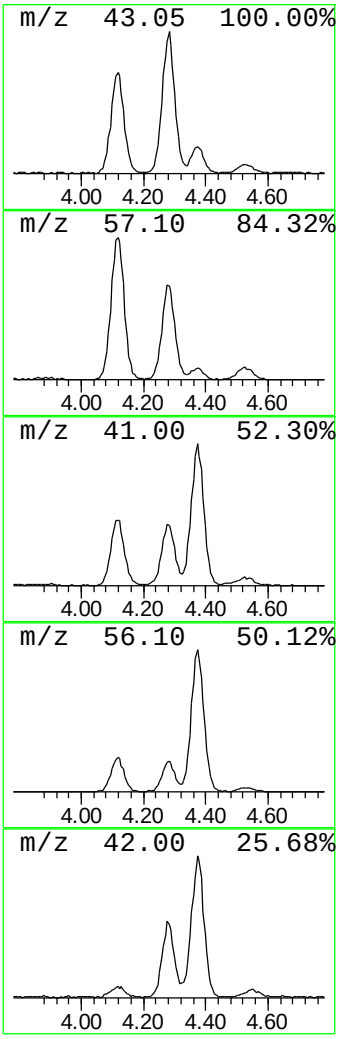
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.28	7.65 ug/L	517201	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	90
3	Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	74
4	Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	59
5	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	59





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX100720\
Data File : VX018819.D
Acq On : 07 Oct 2020 18:31
Operator : JC/SP
Sample : L4240-10DL 5X
Misc : 25.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : BG3S8DL

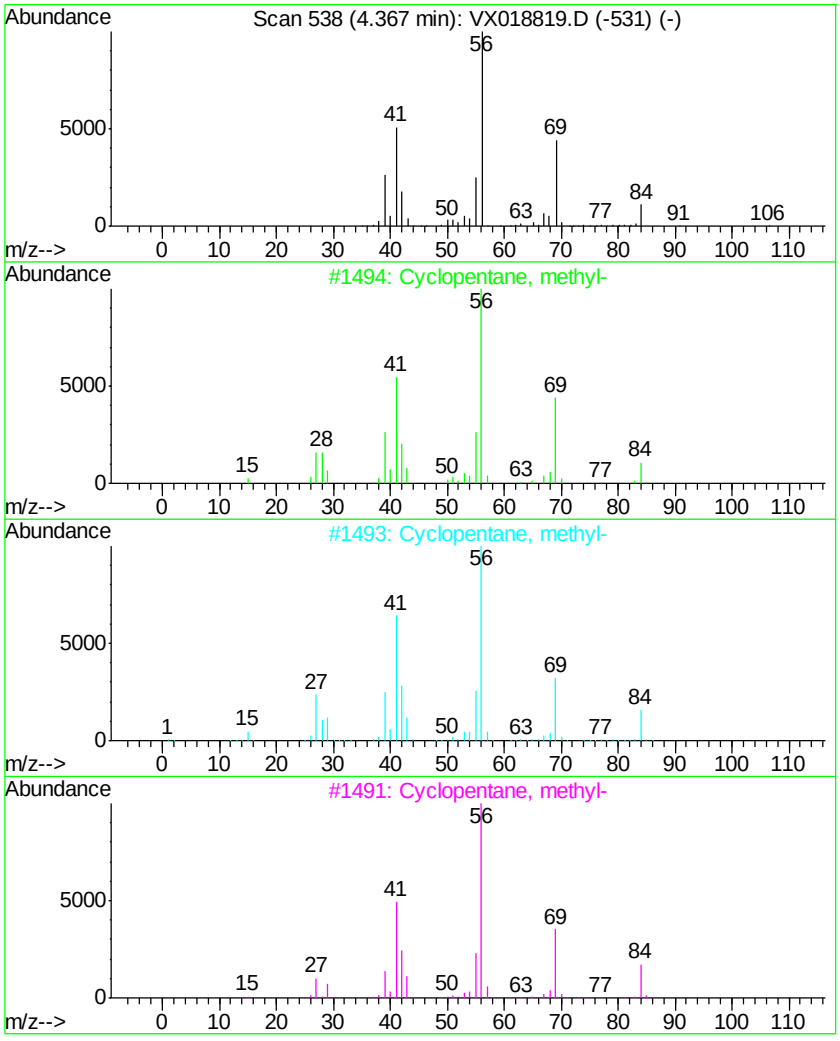
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\SOMXTR100220WMA.M
Quant Title : TRACE VOA SOM01.0

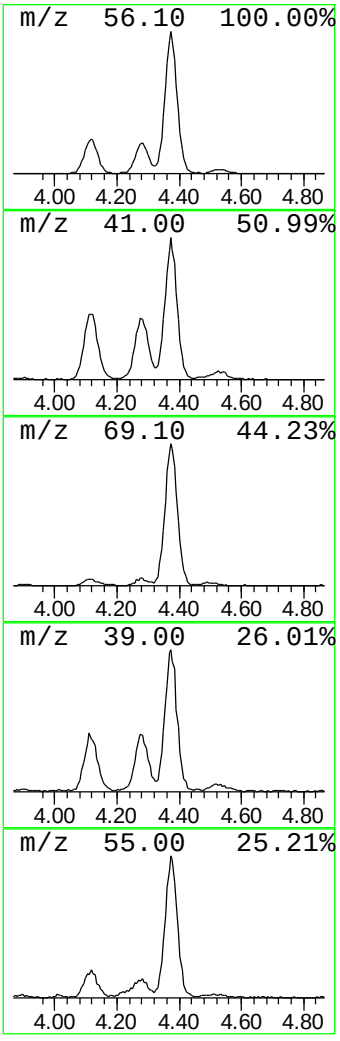
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 (DEL) Alkane: Cyclic4.37 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.37	13.80 ug/L	933266	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	86
3	Cyclopentane, methyl-	84	C6H12	000096-37-7	78
4	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	64
5	Cyclobutane, ethyl-	84	C6H12	004806-61-5	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX100720\
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ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : BG3S8DL

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
(DEL) Alkane: Str...	2.82	7.9	ug/L	533798	1	6.83	338188	5.0
(DEL) Alkane: Str...	2.87	61.5	ug/L	4159890	1	6.83	338188	5.0
(DEL) Alkane: Str...	3.15	109.5	ug/L	7403170	1	6.83	338188	5.0
(DEL) Alkane: Str...	3.50	213.6	ug/L	14450200	1	6.83	338188	5.0
(DEL) Alkane: Str...	4.12	8.7	ug/L	587777	1	6.83	338188	5.0
(DEL) Alkane: Str...	4.28	7.7	ug/L	517201	1	6.83	338188	5.0
(DEL) Alkane: Cyc...	4.37	13.8	ug/L	933266	1	6.83	338188	5.0