LSC Area Percent Report

Data Path : W:\HPCHEM1\MSVOA V\DATA\VV050318\
Data File : VV005764.D
Acq On : 03 May 2018 15:53
Operator : SY/MD
Sample : J2658-15
Misc : 25.0 mL/MSVOA V/WATER
ALS Vial : 1 Sample Multiplier: 1

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 : W:\HPCHEM1\MSVOA_V\METHOD\SOMVTR043018WMA.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	1.032	27	44	66	rBV	5192107	5923086	100.00%	42.161%
2	1.122	66	72	88	rVB	293209	344955	5.82%	2.455%
3	1.231	100	106	112	rVB	76833	71650	1.21%	0.510%
4	1.318	124	133	141	rBV2	269417	399876	6.75%	2.846%
5	1.585	208	216	228	rVB	105981	133659	2.26%	0.951%
6	1.652	229	237	245	rVB	79588	97346	1.64%	0.693%
7	1.829	285	292	311	rVB4	56888	106587	1.80%	0.759%
8	2.135	377	387	397	rBV	228972	328103	5.54%	2.335%
9	3.964	940	956	972	rBV2	99405	293198	4.95%	2.087%
10	4.411	1072	1095	1122	rBV2	143474	356289	6.02%	2.536%
11	5.102	1293	1310	1338	rBV3	332960	823143	13.90%	5.859%
12	5.672	1471	1487	1504	rBV	249018	496881	8.39%	3.537%
13	6.128	1612	1629	1658	rBV	181138	414093	6.99%	2.948%
14	7.038	1895	1912	1934	rBV	90898	170298	2.88%	1.212%
15	7.366	2001	2014	2027	rBV	346661	622907	10.52%	4.434%
16	7.437	2029	2036	2047	rVB2	51252	88404	1.49%	0.629%
17	7.672	2099	2109	2124	rBV2	54878	99011	1.67%	0.705%
18	8.144	2241	2256	2291	rBV	399611	856605	14.46%	6.097%
19	8.903	2480	2492	2525	rBV	366564	650197	10.98%	4.628%
20	9.064	2531	2542	2557	rBV	55016	91252	1.54%	0.650%
21	10.269	2903	2917	2933	rBV	140983	226975	3.83%	1.616%
22	11.205	3197	3208	3226	rBV2	38946	68840	1.16%	0.490%
23	11.302	3226	3238	3259	rVV	347721	587553	9.92%	4.182%
24	11.681	3344	3356	3381	rVB	362049	597721	10.09%	4.255%
25	12.401	3568	3580	3594	rBV	126468	200207	3.38%	1.425%

Sum of corrected areas: 14048836

LSC Report - Integrated Chromatogram

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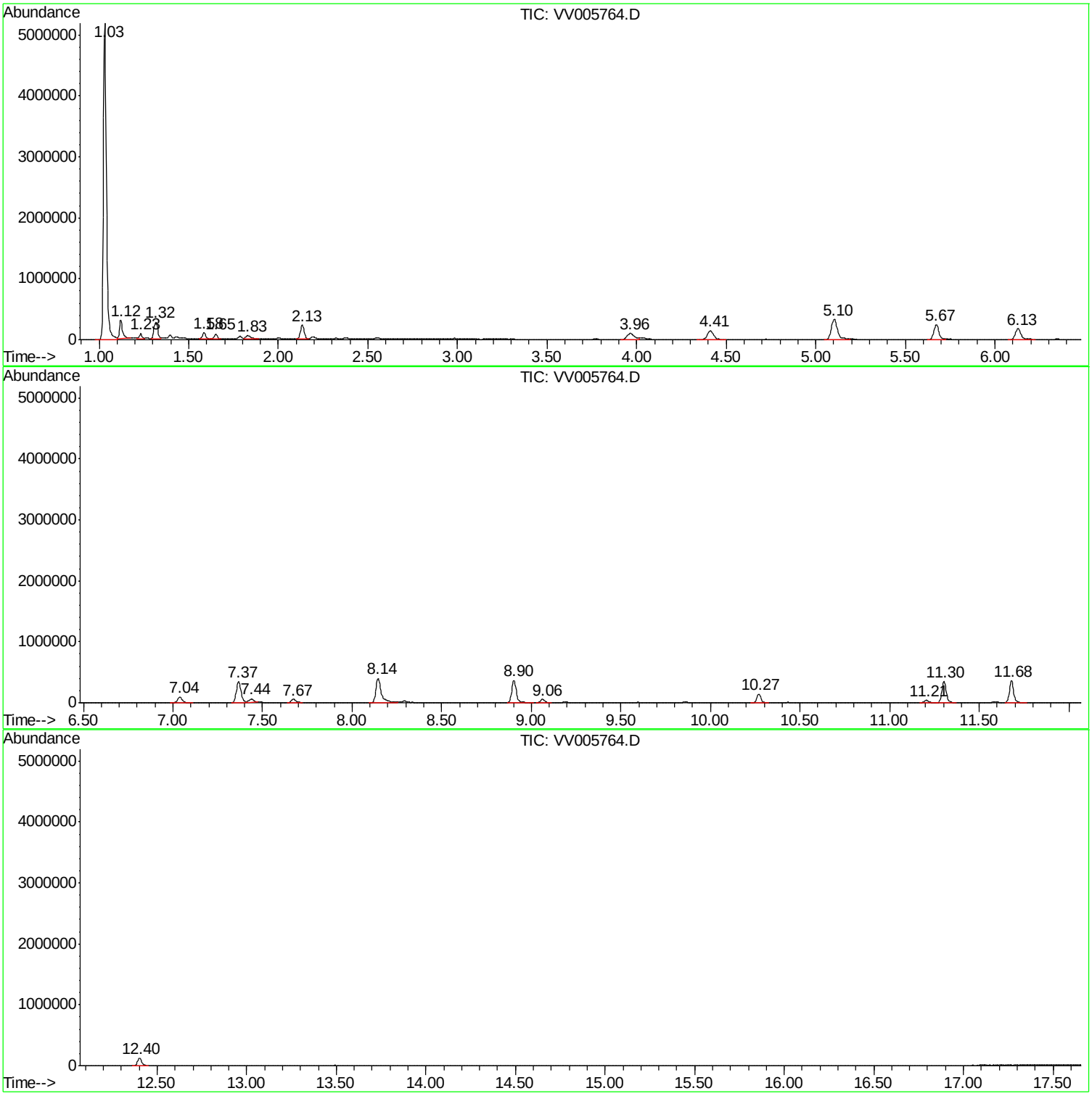
ALS Vial : 1 Sample Multiplier: 1

Quant Method : W:\HPCHEM1\MSVOA_V\METHOD\SOMVTR043018WMA.M
Quant Title : TRACE VOA SOM01.0

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



Library Search Compound Report

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Data File : VV005764.D
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Operator : SY/MD
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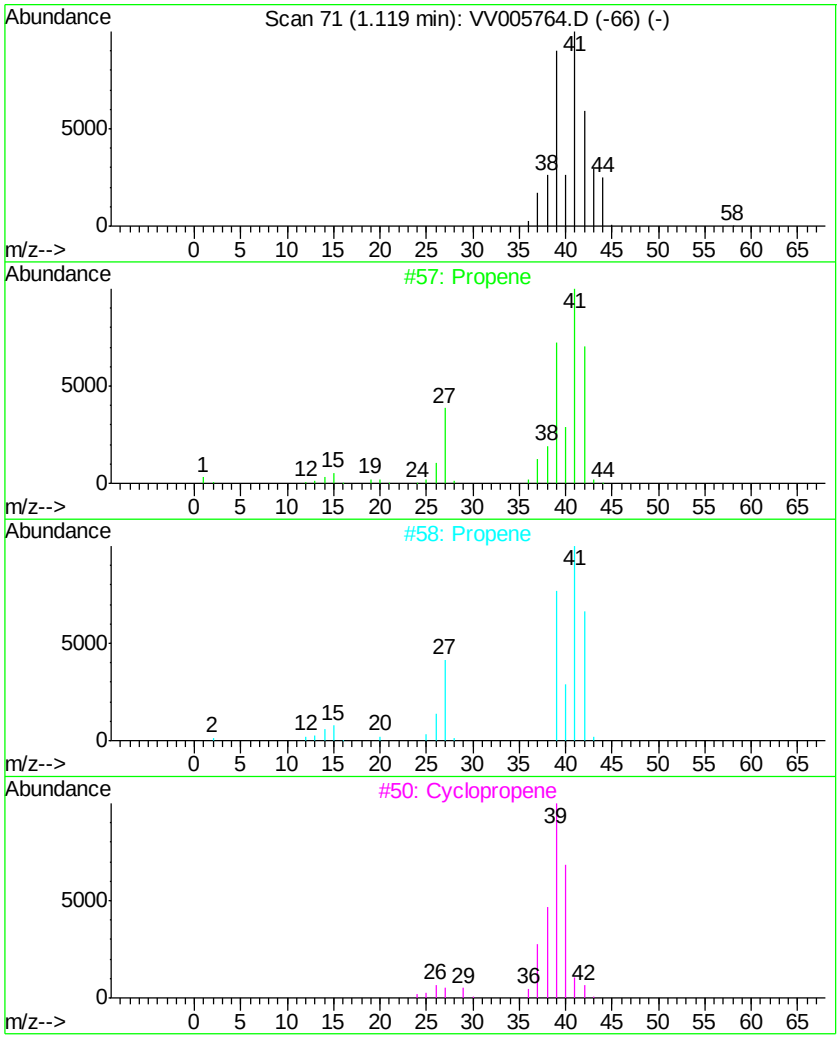
Quant Method : W:\HPCHEM1\MSVOA_V\METHOD\SOMVTR043018WMA.M
Quant Title : TRACE VOA SOM01.0

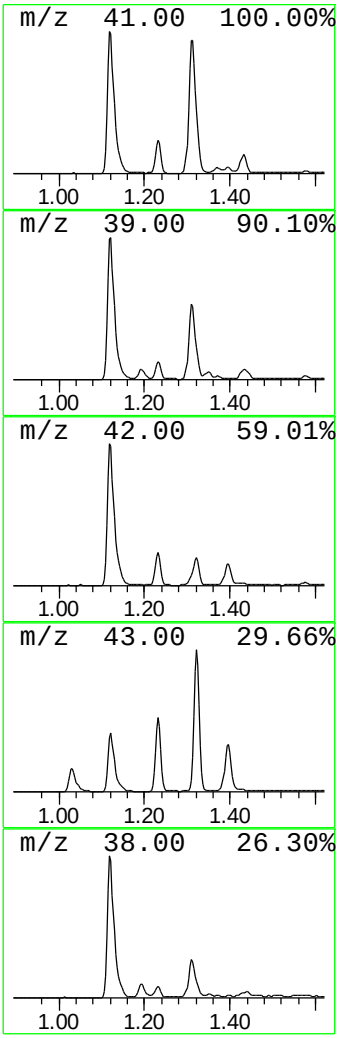
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.12	3.47 ug/L	344955	1,4-Difluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propene	42	C3H6	000115-07-1	83
2	Propene	42	C3H6	000115-07-1	42
3	Cyclopropene	40	C3H4	002781-85-3	5
4	Cyclopropane	42	C3H6	000075-19-4	4
5	Cyclopropane	42	C3H6	000075-19-4	4





Library Search Compound Report

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Data File : VV005764.D
Acq On : 03 May 2018 15:53
Operator : SY/MD
Sample : J2658-15
Misc : 25.0 mL/MSVOA V/WATER
ALS Vial : 1 Sample Multiplier: 1

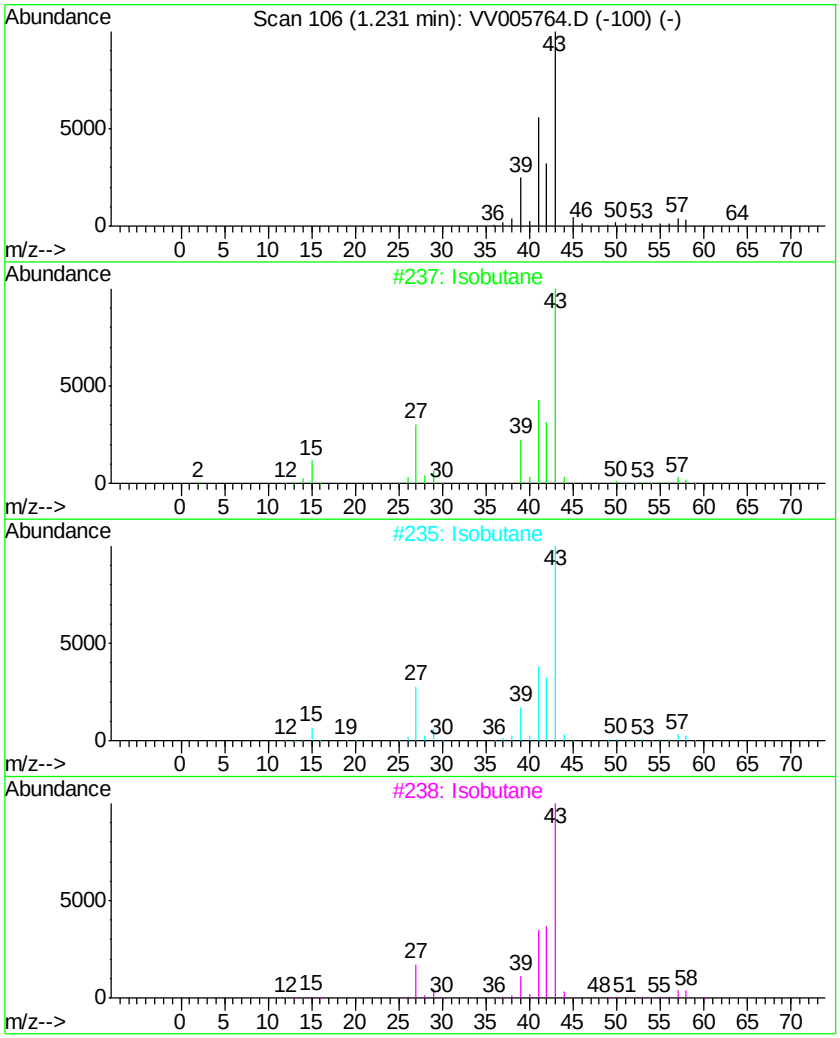
Quant Method : W:\HPCHEM1\MSVOA_V\METHOD\SOMVTR043018WMA.M
Quant Title : TRACE VOA SOM01.0

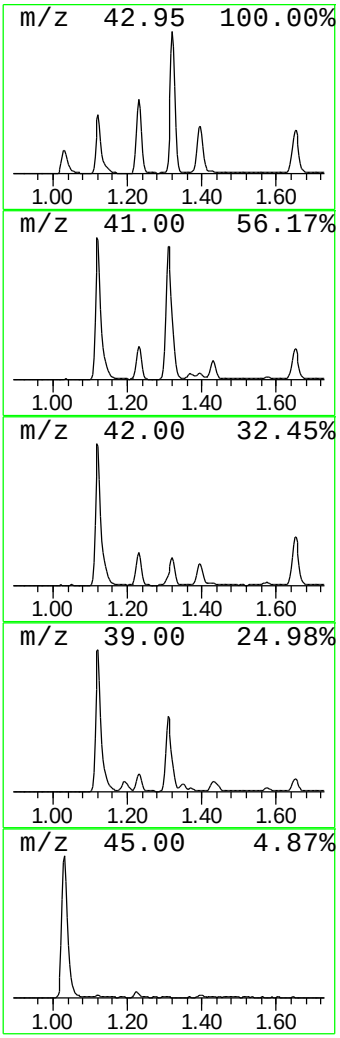
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.23	0.72 ug/L	71650	1,4-Difluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutane	58	C4H10	000075-28-5	42
2	Isobutane	58	C4H10	000075-28-5	9
3	Isobutane	58	C4H10	000075-28-5	9
4	Isobutane	58	C4H10	000075-28-5	9
5	Isobutyl nitrite	103	C4H9NO2	000542-56-3	9





Library Search Compound Report

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Data File : VV005764.D
Acq On : 03 May 2018 15:53
Operator : SY/MD
Sample : J2658-15
Misc : 25.0 mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

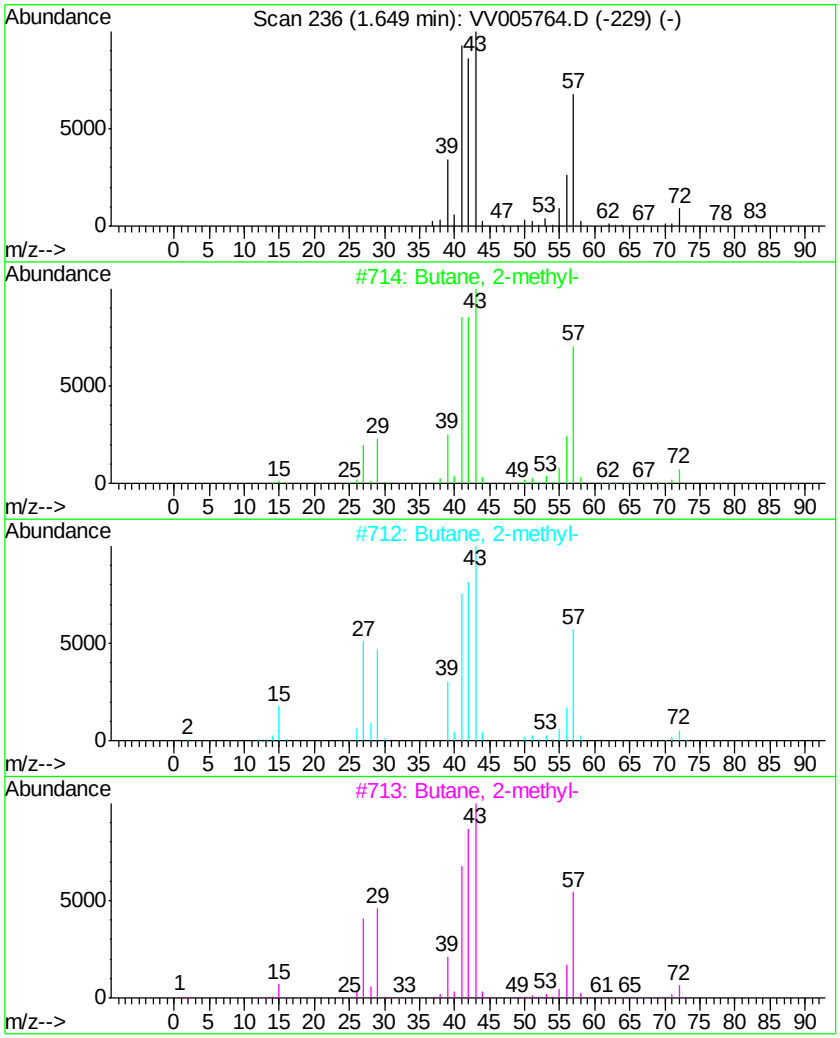
Quant Method : W:\HPCHEM1\MSVOA_V\METHOD\SOMVTR043018WMA.M
Quant Title : TRACE VOA SOM01.0

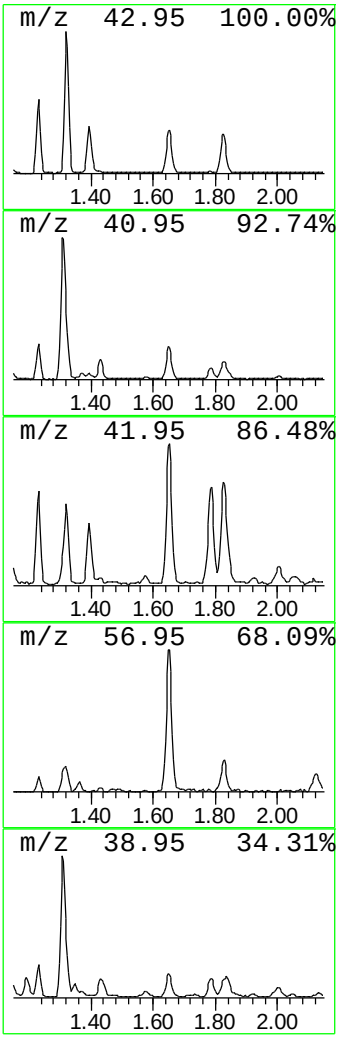
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.65	0.98 ug/L	97346	1,4-Difluorobenzene	5.67

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	80
3	Butane, 2-methyl-	72	C5H12	000078-78-4	80
4	2-Butene-1,4-diol	88	C4H8O2	000110-64-5	47
5	3-Buten-1-ol	72	C4H8O	000627-27-0	47





Library Search Compound Report

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Data File : VV005764.D
Acq On : 03 May 2018 15:53
Operator : SY/MD
Sample : J2658-15
Misc : 25.0 mL/MSVOA V/WATER
ALS Vial : 1 Sample Multiplier: 1

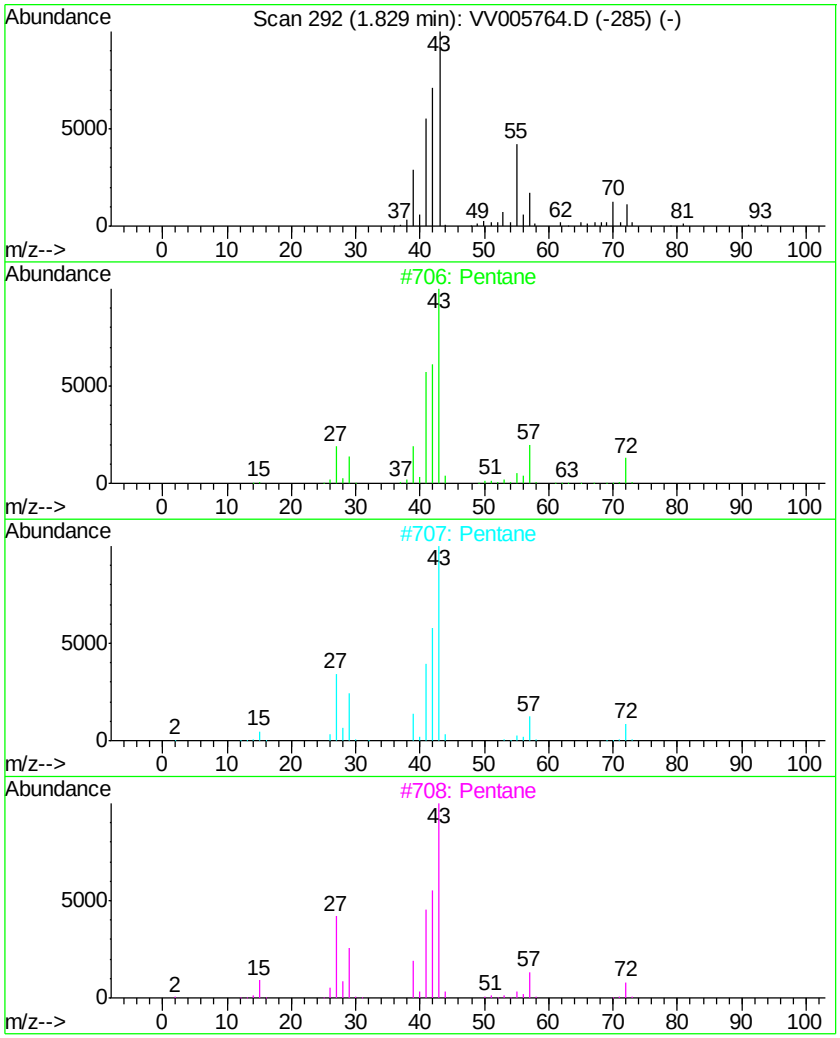
Quant Method : W:\HPCHEM1\MSVOA_V\METHOD\SOMVTR043018WMA.M
Quant Title : TRACE VOA SOM01.0

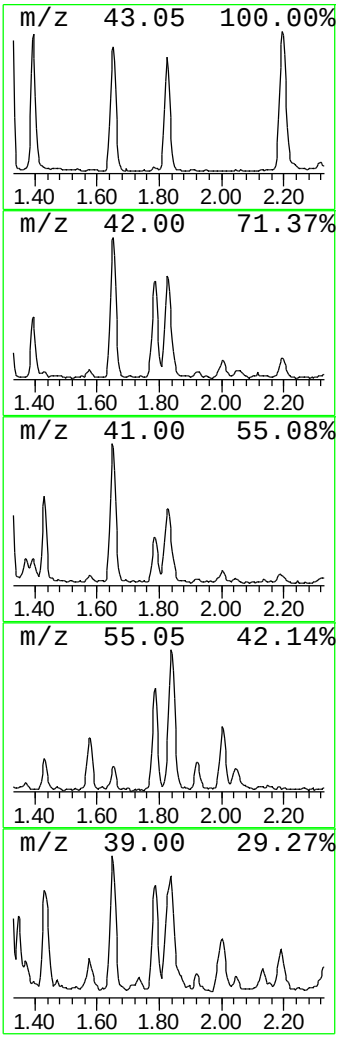
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.83	1.07 ug/L	106587	1,4-Difluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	64
2	Pentane	72	C5H12	000109-66-0	59
3	Pentane	72	C5H12	000109-66-0	59
4	Butane, 2-methyl-	72	C5H12	000078-78-4	50
5	Oxirane, ethyl-	72	C4H8O	000106-88-7	43





Library Search Compound Report

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Operator : SY/MD
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ALS Vial : 1 Sample Multiplier: 1

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Quant Title : TRACE VOA SOM01.0

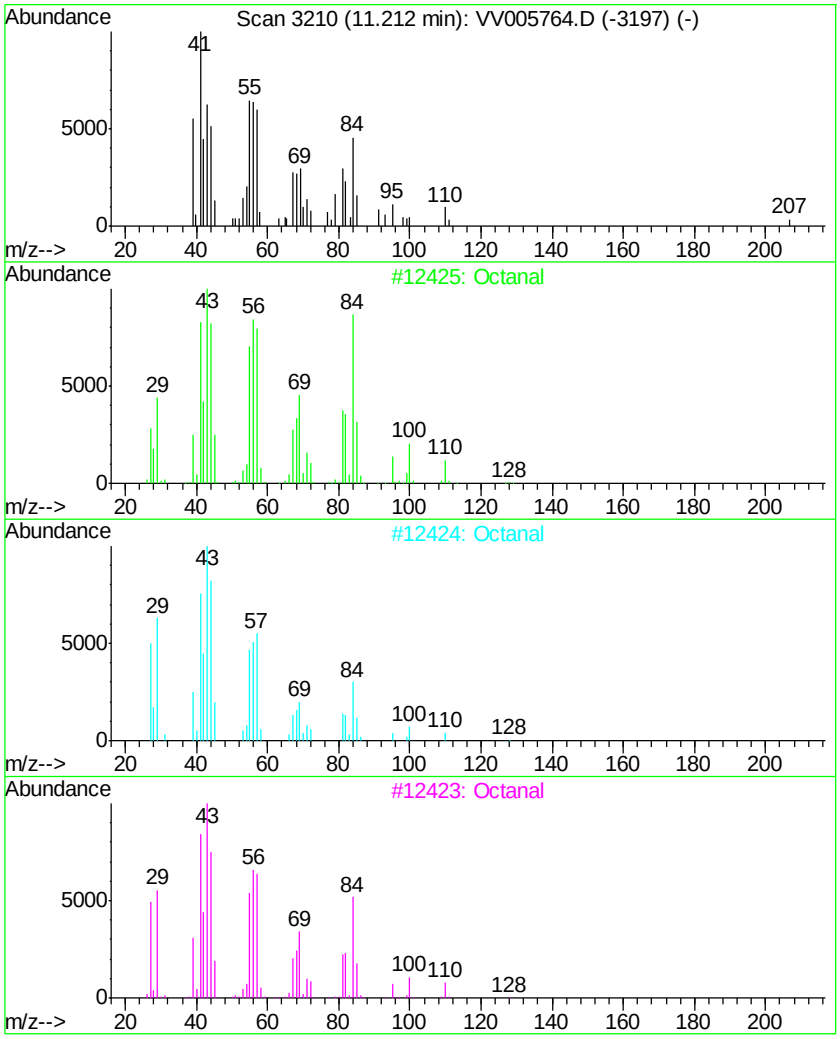
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

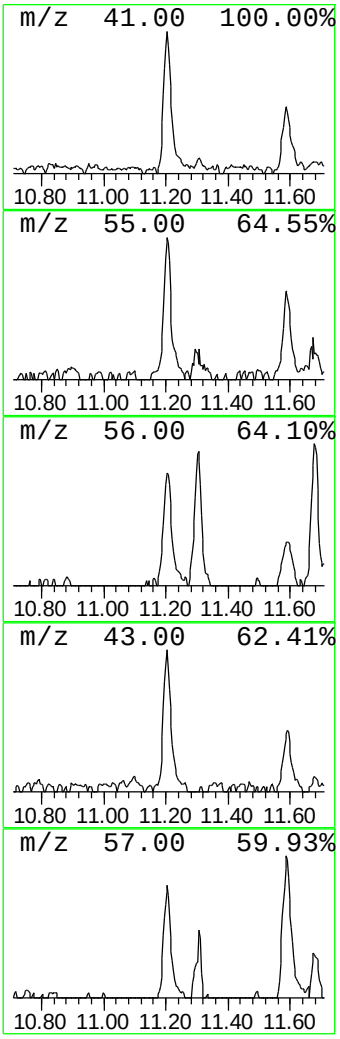
****

Peak Number 7 Octanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.21	0.59 ug/L	68840	1,4-Dichlorobenzene-d4	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanal	128	C8H16O	000124-13-0	64
2	Octanal	128	C8H16O	000124-13-0	59
3	Octanal	128	C8H16O	000124-13-0	59
4	Octanal	128	C8H16O	000124-13-0	53
5	3-Chlorohexane	120	C6H13Cl	002346-81-8	38





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TIC Library : C:\DATABASE\NIST11.L
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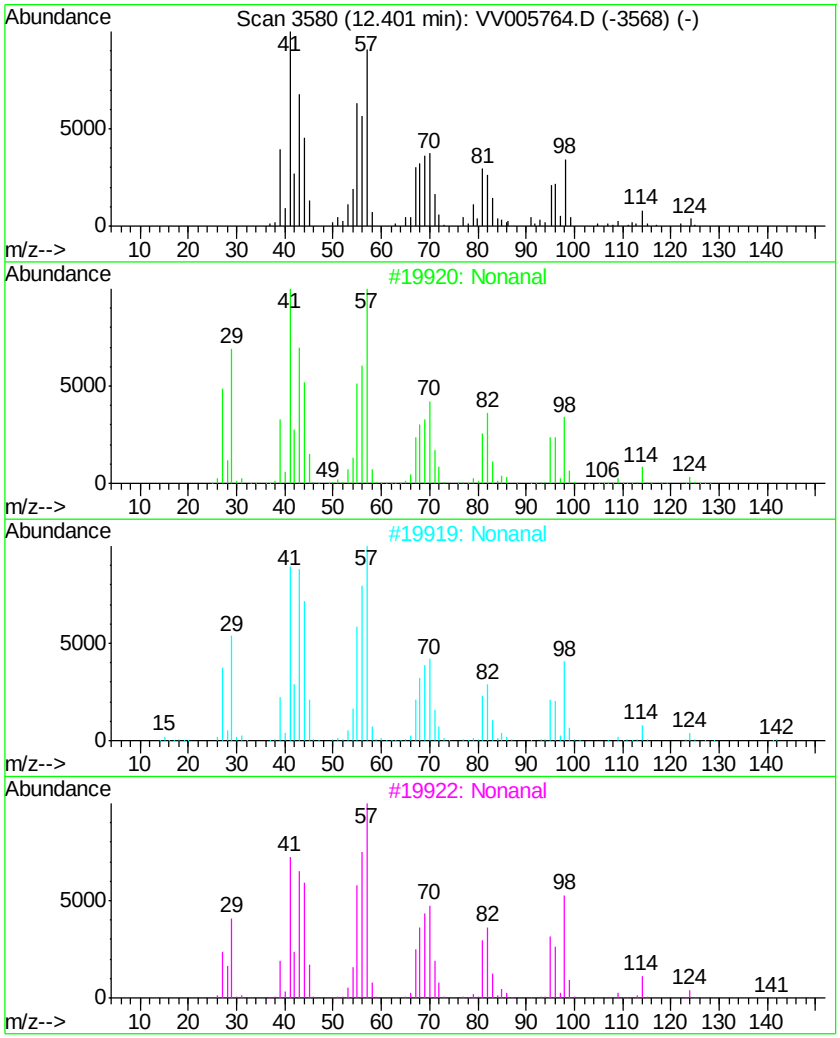
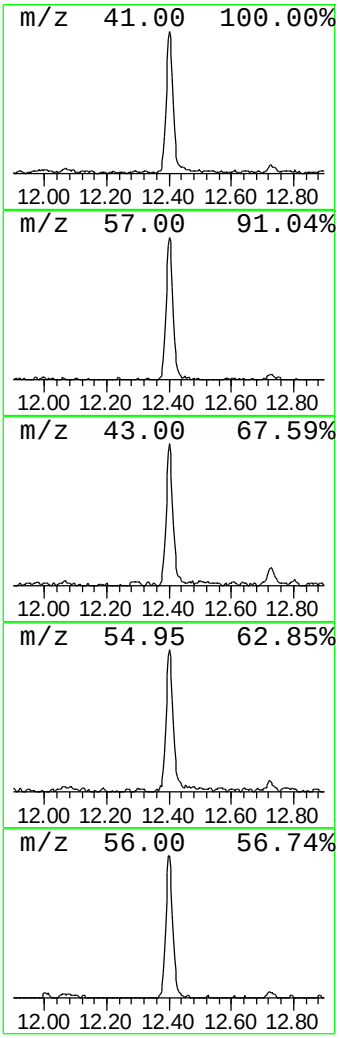
****

Peak Number 8 Nonanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.40	1.70 ug/L	200207	1,4-Dichlorobenzene-d4	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanal	142	C9H18O	000124-19-6	91
2	Nonanal	142	C9H18O	000124-19-6	90
3	Nonanal	142	C9H18O	000124-19-6	86
4	Cyclohexanol, 2-methyl-, cis-	114	C7H14O	007443-70-1	38
5	2-Nonen-1-ol	142	C9H18O	022104-79-6	35





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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
(DEL) Alkane: Str...	1.12	3.5	ug/L	344955	1	5.67	496881	5.0
(DEL) Alkane: Str...	1.23	0.7	ug/L	71650	1	5.67	496881	5.0
(DEL) Alkane: Str...	1.65	1.0	ug/L	97346	1	5.67	496881	5.0
(DEL) Alkane: Str...	1.83	1.1	ug/L	106587	1	5.67	496881	5.0
Octanal	11.21	0.6	ug/L	68840	3	11.30	587553	5.0
Nonanal	12.40	1.7	ug/L	200207	3	11.30	587553	5.0