LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV080818\
Data File : VV006934.D
Acq On : 08 Aug 2018 15:24
Operator : SY/MD
Sample : J4357-19
Misc : 25 mL/MSVOA V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : ESWT7

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_V\METHOD\SOMVTR080718WMA.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	64	rBV	7693717	9004754	100.00%	32.494%
2	1.119	65	71	92	rVB	6487355	6126957	68.04%	22.109%
3	1.228	98	105	117	rVB	1729500	1445144	16.05%	5.215%
4	1.318	125	133	143	rBV2	1204408	1183939	13.15%	4.272%
5	1.585	211	216	223	rVB	96982	97174	1.08%	0.351%
6	1.649	229	236	246	rVB	287562	350168	3.89%	1.264%
7	2.131	378	386	399	rVB	196576	289080	3.21%	1.043%
8	2.604	526	533	545	rVB	79049	133265	1.48%	0.481%
9	2.794	583	592	604	rVB	118181	198168	2.20%	0.715%
10	3.803	888	906	927	rBV2	50497	132249	1.47%	0.477%
11	3.967	938	957	1010	rBV2	1026347	2586153	28.72%	9.332%
12	4.408	1076	1094	1116	rBV	131059	312897	3.47%	1.129%
13	4.726	1174	1193	1210	rBV2	80744	199647	2.22%	0.720%
14	5.099	1291	1309	1337	rBV2	319129	761418	8.46%	2.748%
15	5.671	1472	1487	1505	rBV	248815	490615	5.45%	1.770%
16	5.964	1564	1578	1598	rBV	169185	321889	3.57%	1.162%
17	6.125	1614	1628	1639	rBV2	181739	373726	4.15%	1.349%
18	7.035	1900	1911	1924	rBV2	79965	143636	1.60%	0.518%
19	7.366	2000	2014	2032	rBV	300613	521089	5.79%	1.880%
20	8.022	2201	2218	2237	rBV	404832	680042	7.55%	2.454%
21	8.150	2245	2258	2292	rBV2	291429	686734	7.63%	2.478%
22	8.903	2479	2492	2512	rBV	347459	578658	6.43%	2.088%
23	10.266	2905	2916	2940	rVB	128245	204518	2.27%	0.738%
24	11.301	3226	3238	3267	rBV	273174	470942	5.23%	1.699%
25	11.678	3343	3355	3380	rVB	248106	419380	4.66%	1.513%

Sum of corrected areas: 27712242

LSC Report - Integrated Chromatogram

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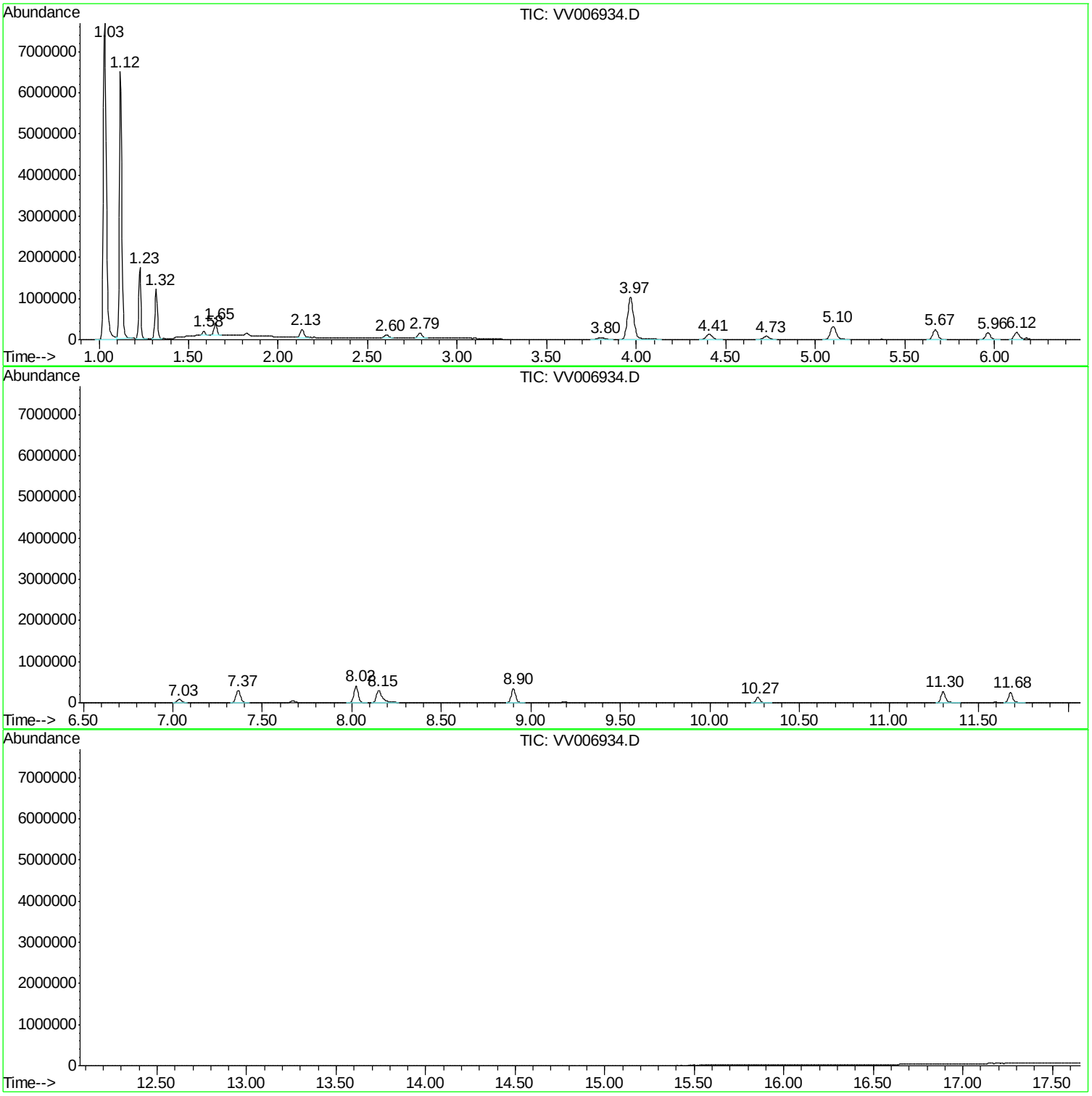
Data File : VV006934.D
Acq On : 08 Aug 2018 15:24
Operator : SY/MD
Sample : J4357-19
Misc : 25 mL/MSVOA_V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : ESWT7

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR080718WMA.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 : VV006934.D
Acq On : 08 Aug 2018 15:24
Operator : SY/MD
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Misc : 25 mL/MSVOA_V/WATER
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Instrument : MSVOA_V
ClientSampleId : ESWT7

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR080718WMA.M
Quant Title : TRACE VOA SOM01.0

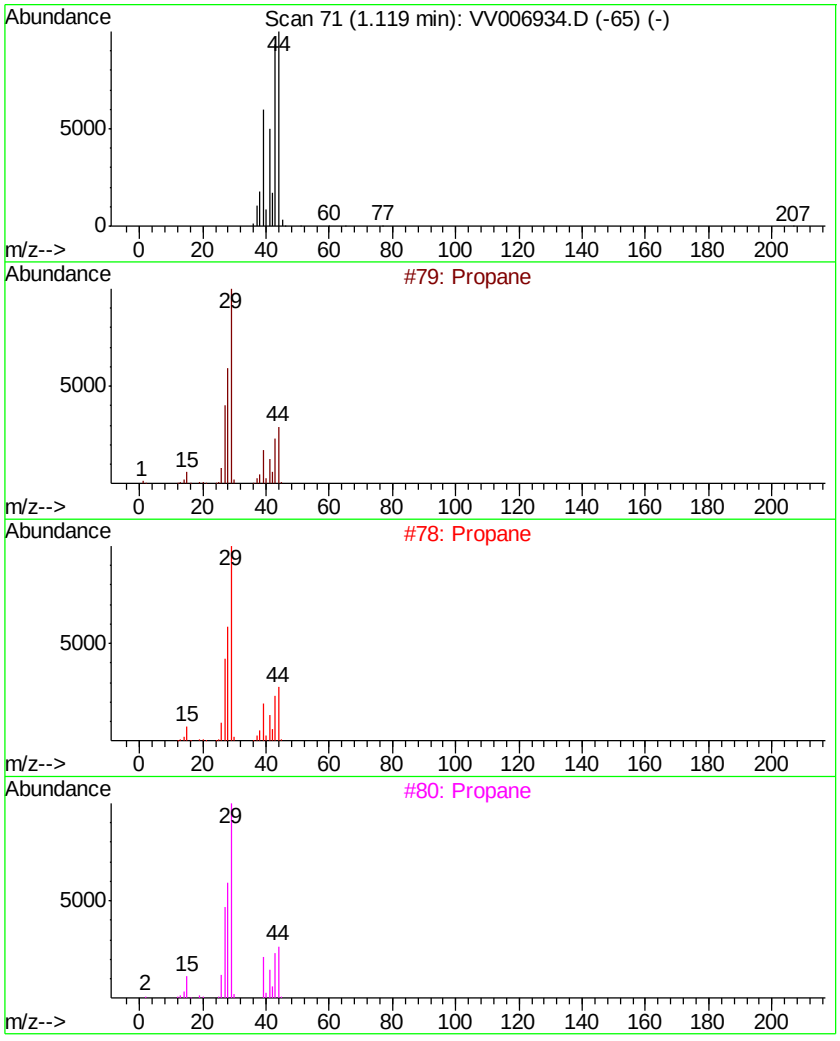
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

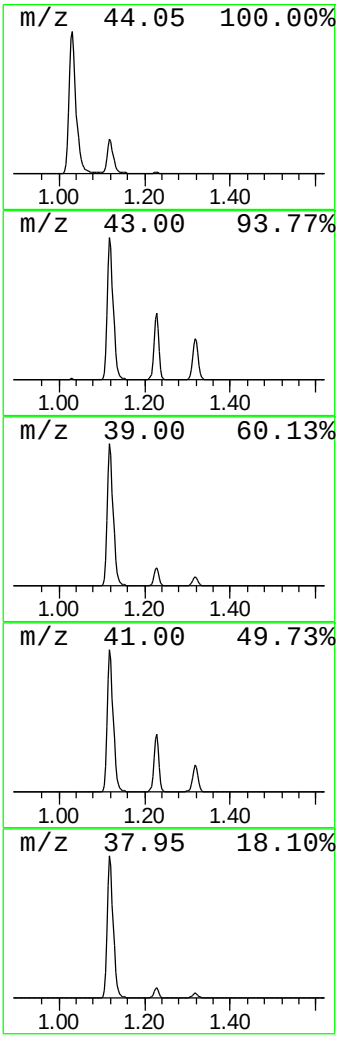
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.12	62.44 ug/L	6126960	1,4-Difluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane	44	C3H8	000074-98-6	83
2	Propane	44	C3H8	000074-98-6	78
3	Propane	44	C3H8	000074-98-6	9
4	Acetaldehyde	44	C2H4O	000075-07-0	5
5	Ethylene oxide	44	C2H4O	000075-21-8	5





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV080818\
Data File : VV006934.D
Acq On : 08 Aug 2018 15:24
Operator : SY/MD
Sample : J4357-19
Misc : 25 mL/MSVOA_V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : ESWT7

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR080718WMA.M
Quant Title : TRACE VOA SOM01.0

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

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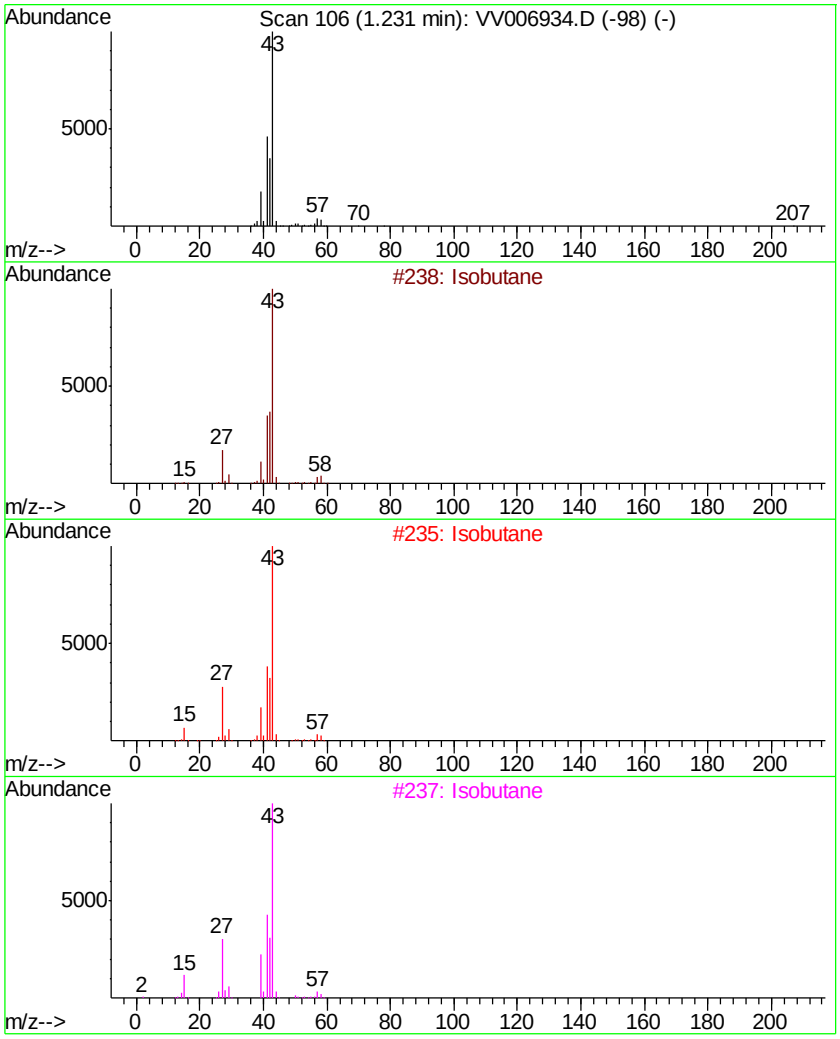
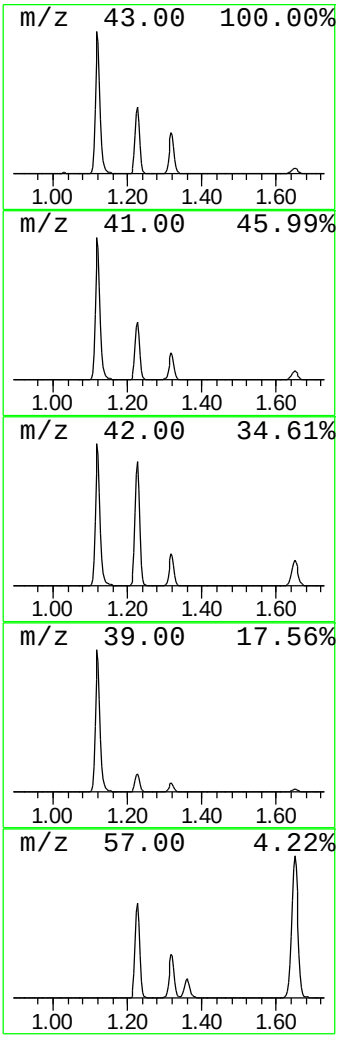
Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.23	14.73 ug/L	1445140	1,4-Difluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutane	58	C4H10	000075-28-5	80
2	Isobutane	58	C4H10	000075-28-5	72
3	Isobutane	58	C4H10	000075-28-5	64
4	Isobutane	58	C4H10	000075-28-5	64
5	Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9





Library Search Compound Report

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Data File : VV006934.D
Acq On : 08 Aug 2018 15:24
Operator : SY/MD
Sample : J4357-19
Misc : 25 mL/MSVOA_V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : ESWT7

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR080718WMA.M
Quant Title : TRACE VOA SOM01.0

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

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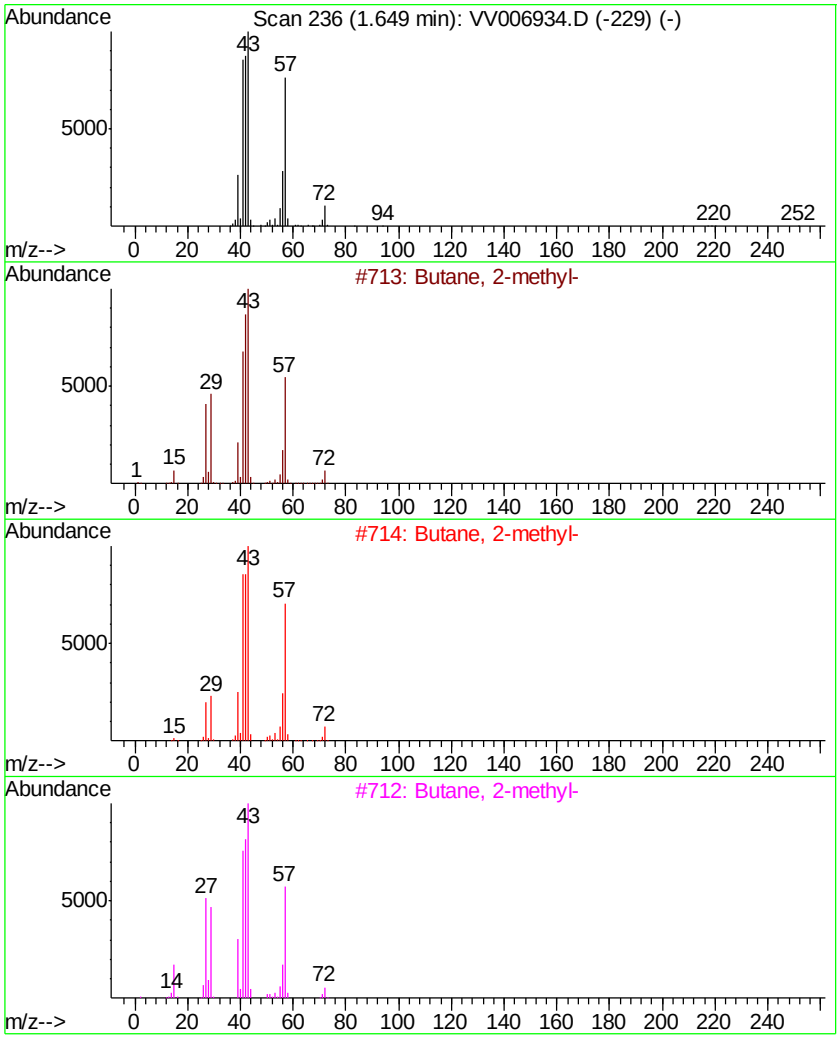
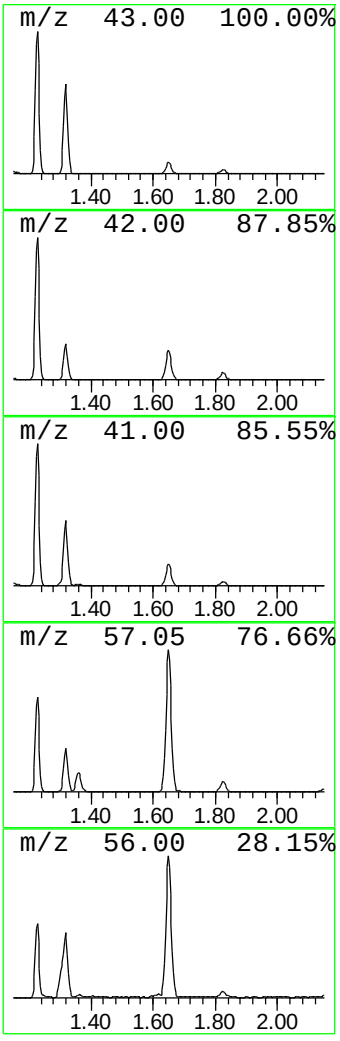
Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.65	3.57 ug/L	350168	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	91
3	Butane, 2-methyl-	72	C5H12	000078-78-4	86
4	Pentane	72	C5H12	000109-66-0	38
5	1,3-Dimethyldiaziridine	72	C3H8N2	026177-36-6	36





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Data File : VV006934.D
Acq On : 08 Aug 2018 15:24
Operator : SY/MD
Sample : J4357-19
Misc : 25 mL/MSVOA_V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : ESWT7

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR080718WMA.M
Quant Title : TRACE VOA SOM01.0

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

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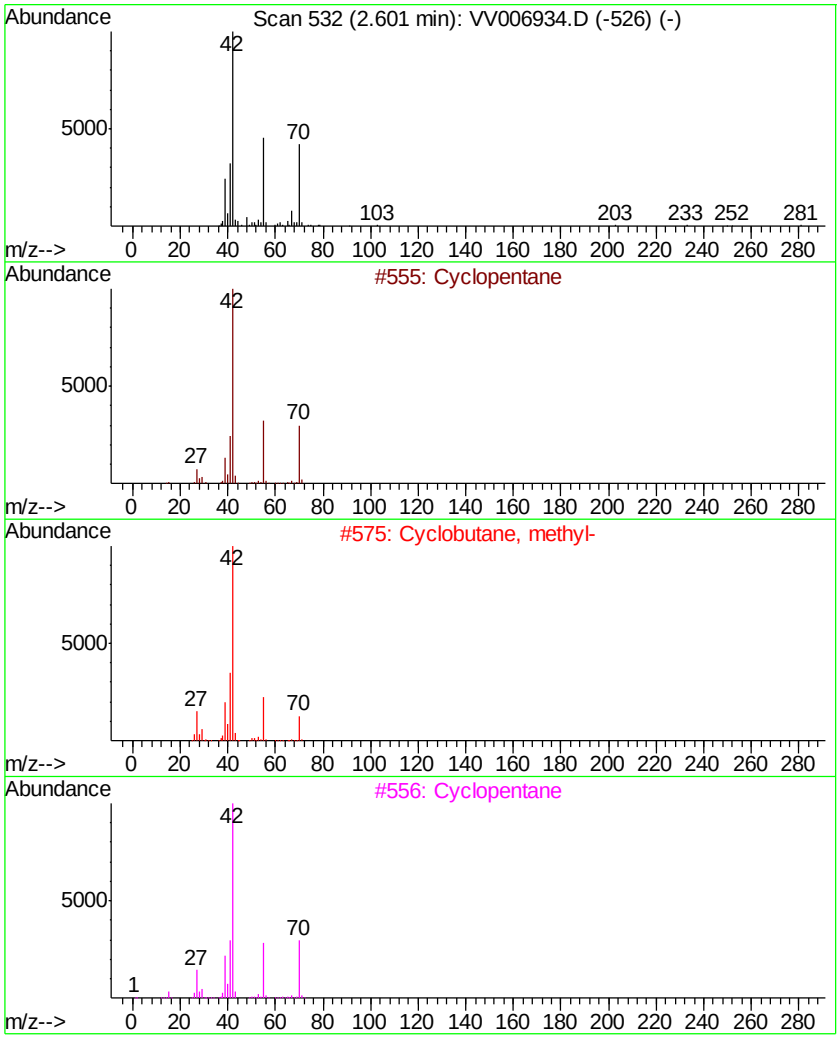
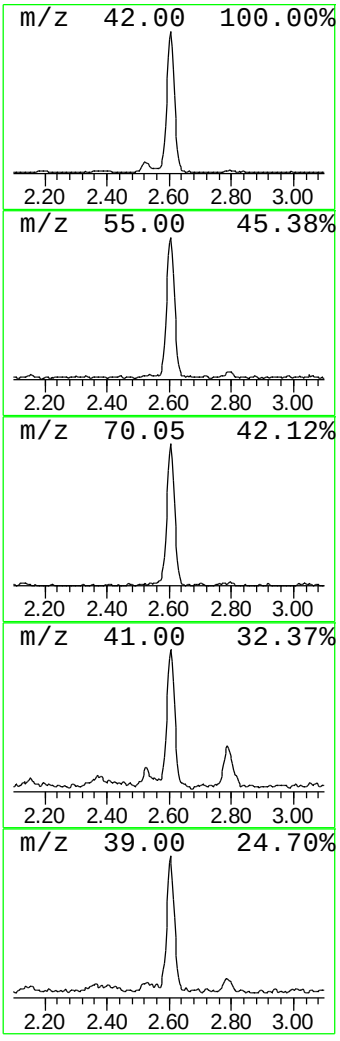
Peak Number 5 (DEL) Alkane: Cyclic2.60 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.60	1.36 ug/L	133265	1,4-Difluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane	70	C5H10	000287-92-3	80
2	Cyclobutane, methyl-	70	C5H10	000598-61-8	80
3	Cyclopentane	70	C5H10	000287-92-3	80
4	Cyclobutane, methyl-	70	C5H10	000598-61-8	72
5	1-Pentene	70	C5H10	000109-67-1	47





Library Search Compound Report

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Data File : VV006934.D
Acq On : 08 Aug 2018 15:24
Operator : SY/MD
Sample : J4357-19
Misc : 25 mL/MSVOA_V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : ESWT7

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR080718WMA.M
Quant Title : TRACE VOA SOM01.0

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

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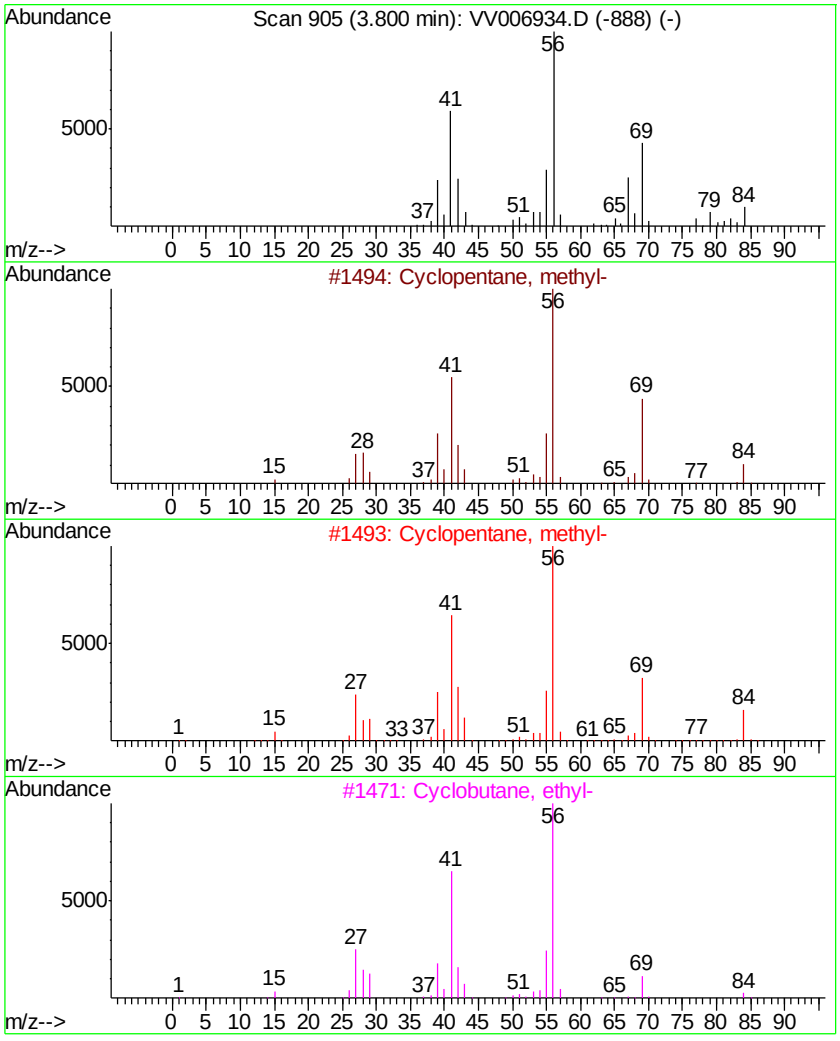
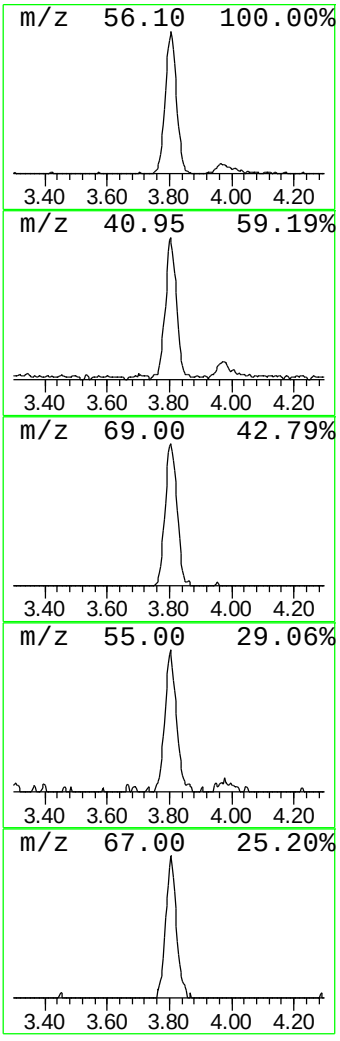
Peak Number 6 (DEL) Alkane: Cyclic3.80 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.80	1.35 ug/L	132249	1,4-Difluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	76
2	Cyclopentane, methyl-	84	C6H12	000096-37-7	59
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	50
4	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	50
5	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	47





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Operator : SY/MD
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Misc : 25 mL/MSVOA_V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : ESWT7

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR080718WMA.M
Quant Title : TRACE VOA SOM01.0

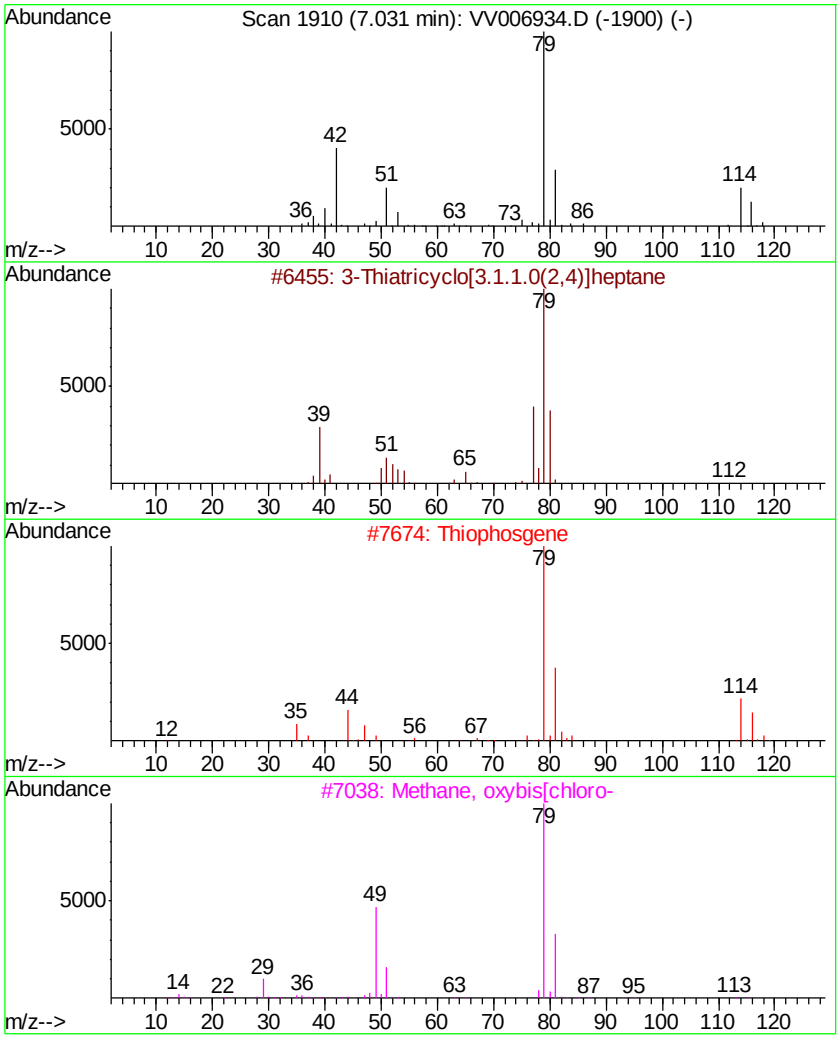
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

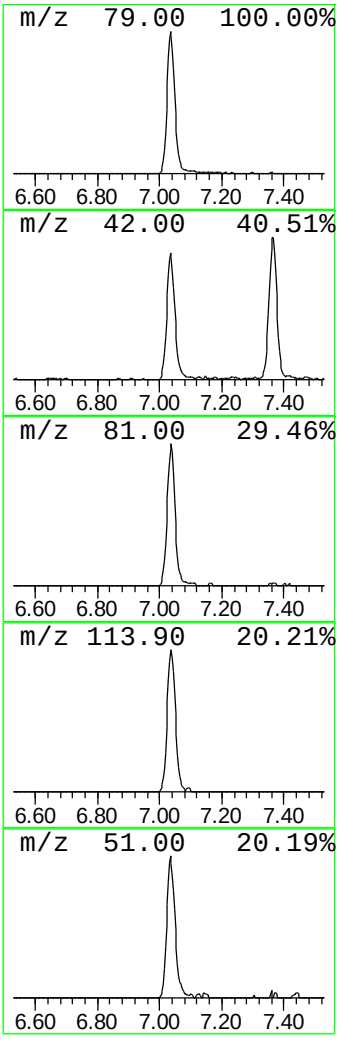
****

Peak Number 7 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.03	1.46 ug/L	143636	1,4-Difluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Thiatricyclo[3.1.1.0(2,4)]heptane	112	C6H8S	1000221-37-0	43
2	Thiophosgene	114	CCl2S	000463-71-8	38
3	Methane, oxybis[chloro-	114	C2H4Cl2O	000542-88-1	37
4	Methane, oxybis[chloro-	114	C2H4Cl2O	000542-88-1	25
5	1,3-Cyclohexadiene	80	C6H8	000592-57-4	25





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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
(DEL) Alkane: Str...	1.12	62.4	ug/L	6126960	1	5.67	490615	5.0
(DEL) Alkane: Str...	1.23	14.7	ug/L	1445140	1	5.67	490615	5.0
(DEL) Alkane: Str...	1.65	3.6	ug/L	350168	1	5.67	490615	5.0
(DEL) Alkane: Cyc...	2.60	1.4	ug/L	133265	1	5.67	490615	5.0
(DEL) Alkane: Cyc...	3.80	1.4	ug/L	132249	1	5.67	490615	5.0
unknown-01	7.03	1.5	ug/L	143636	1	5.67	490615	5.0