LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV112219\
Data File : VV013742.D
Acq On : 22 Nov 2019 18:35
Operator : SY/MD
Sample : K5941-15
Misc : 25.0mL/MSVOA V/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : B0AC9

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\SOMVTR112219WMA.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	1.116	3	8	21	rVB	1195018	1053960	80.15%	7.529%
2	1.225	36	42	47	rBV	115589	95921	7.29%	0.685%
3	1.312	60	69	82	rBV2	591733	886226	67.39%	6.331%
4	1.428	99	105	113	rVB	71405	72274	5.50%	0.516%
5	1.579	143	152	165	rVB2	178575	228027	17.34%	1.629%
6	1.647	166	173	182	rBV	77415	91904	6.99%	0.657%
7	1.782	207	215	222	rBV	141528	174376	13.26%	1.246%
8	1.827	222	229	242	rVB3	107828	186961	14.22%	1.336%
9	1.917	252	257	265	rVB3	14936	15910	1.21%	0.114%
10	2.000	275	283	290	rBV2	43044	59206	4.50%	0.423%
11	2.129	314	323	333	rBV	292649	414350	31.51%	2.960%
12	2.190	334	342	359	rVB	67118	117515	8.94%	0.839%
13	2.315	373	381	394	rBV	28083	46542	3.54%	0.332%
14	2.466	416	428	442	rBV6	25226	67829	5.16%	0.485%
15	2.540	442	451	453	rBV2	12606	17915	1.36%	0.128%
16	2.788	515	528	540	rBV3	18642	41093	3.12%	0.294%
17	2.984	574	589	602	rBV3	46984	103432	7.87%	0.739%
18	3.077	606	618	629	rVB4	20633	40478	3.08%	0.289%
19	3.209	642	659	666	rBV4	9773	31066	2.36%	0.222%
20	3.933	872	884	913	rBV2	167748	474685	36.10%	3.391%
21	4.399	1010	1029	1056	rBV3	267000	847862	64.48%	6.057%
22	4.794	1148	1152	1167	rVB3	7592	15684	1.19%	0.112%
23	5.093	1223	1245	1273	rBV2	491984	1255454	95.47%	8.968%
24	5.421	1338	1347	1353	rBV10	11518	23040	1.75%	0.165%
25	5.659	1408	1421	1442	rBV	390743	797517	60.65%	5.697%
26	5.958	1501	1514	1532	rBB10	24251	64180	4.88%	0.458%
27	6.113	1549	1562	1578	rBV	277548	569056	43.27%	4.065%
28	7.026	1831	1846	1869	rBV	143417	269587	20.50%	1.926%
29	7.357	1935	1949	1966	rBV	589700	1019927	77.56%	7.286%
30	7.662	2034	2044	2067	rVB	87715	158175	12.03%	1.130%
31	8.019	2147	2155	2163	rVB5	10640	18197	1.38%	0.130%
32	8.132	2177	2190	2230	rBV2	584367	1314981	100.00%	9.394%
33	8.479	2289	2298	2309	rVB2	7684	14792	1.12%	0.106%
34	8.891	2412	2426	2446	rBV	606539	1000801	76.11%	7.149%

LSC Area Percent Report

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Misc : 25.0mL/MSVOA V/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : B0AC9

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\SOMVTR112219WMA.M
Title : TRACE VOA SOM01.0

35	9.852	2716	2725	2735	rBV	7816	14564	1.11%	0.104%
36	10.257	2839	2851	2865	rBV	225542	358630	27.27%	2.562%
37	11.093	3100	3111	3125	rBV6	10162	23015	1.75%	0.164%
38	11.289	3161	3172	3191	rBV	595063	939000	71.41%	6.708%
39	11.575	3249	3261	3277	rBV4	47106	97409	7.41%	0.696%
40	11.665	3277	3289	3306	rVB	621773	976963	74.29%	6.979%

Sum of corrected areas: 13998504

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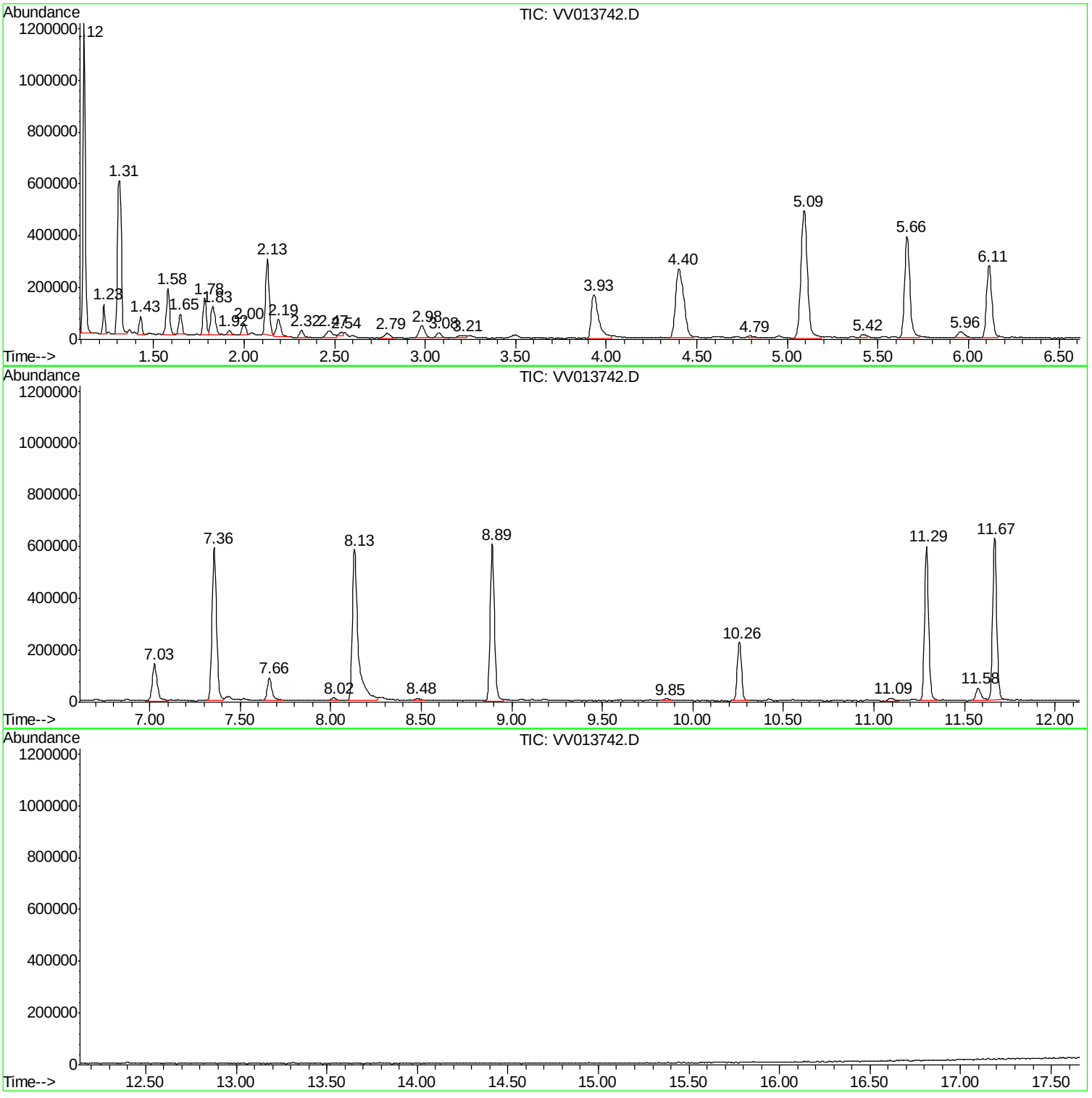
Instrument : MSVOA_V
ClientSampleId : B0AC9

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR112219WMA.M
Quant Title : TRACE VOA SOM01.0

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV112219\
Data File : VV013742.D
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Quant Title : TRACE VOA SOM01.0

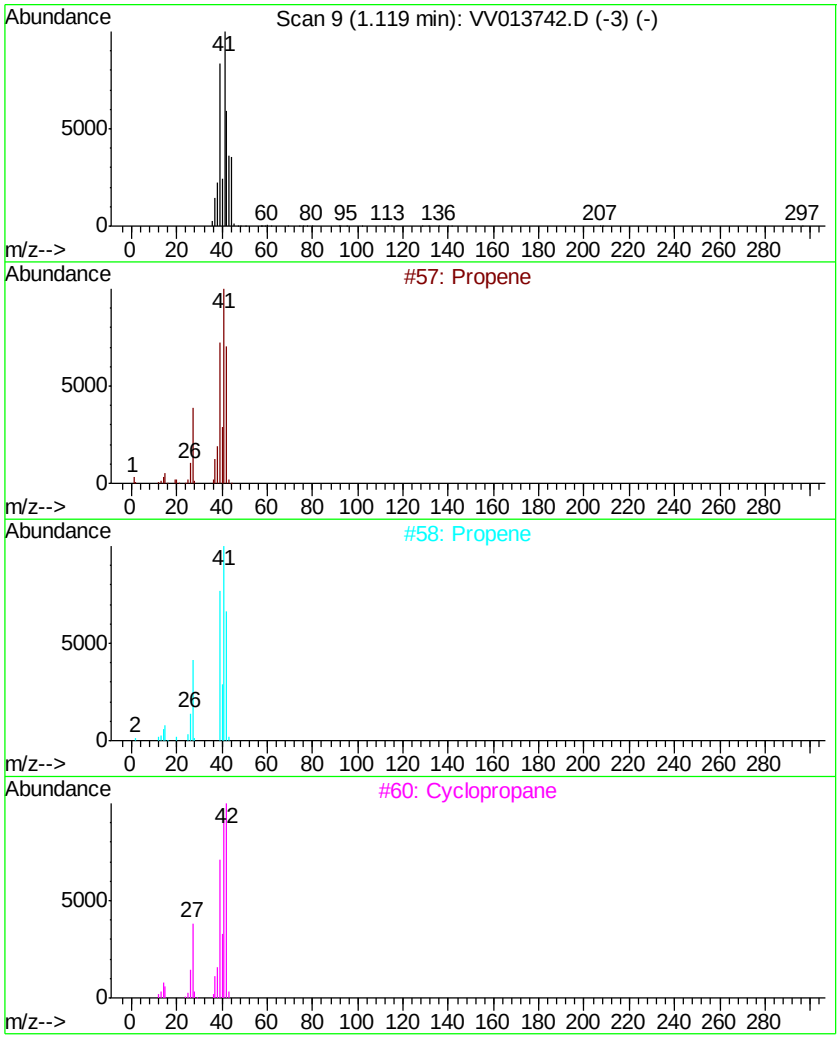
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

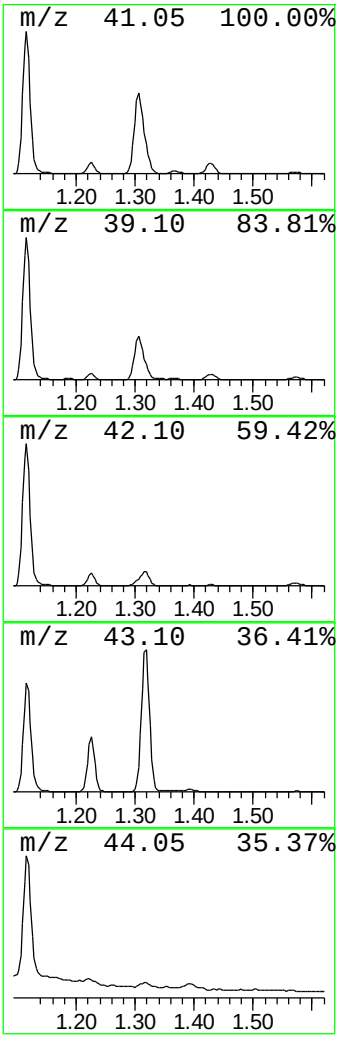
****

Peak Number 1 (DEL) Alkane: Cyclic1.12 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.12	6.61 ug/L	1053960	1,4-Difluorobenzene	5.66

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





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Operator : SY/MD
Sample : K5941-15
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ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : B0AC9

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR112219WMA.M
Quant Title : TRACE VOA SOM01.0

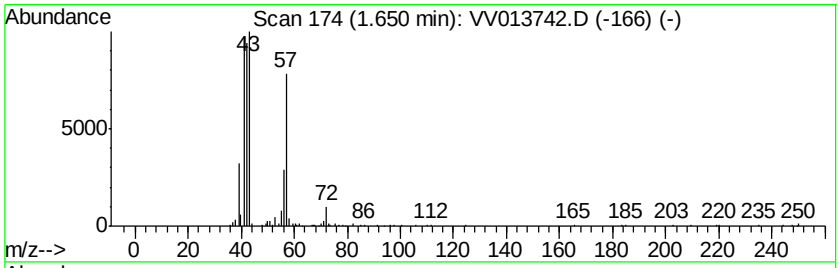
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

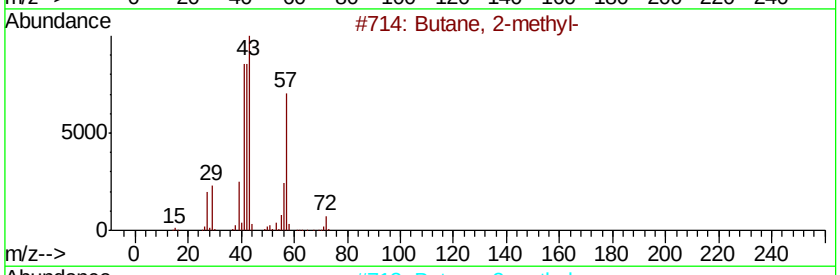
****

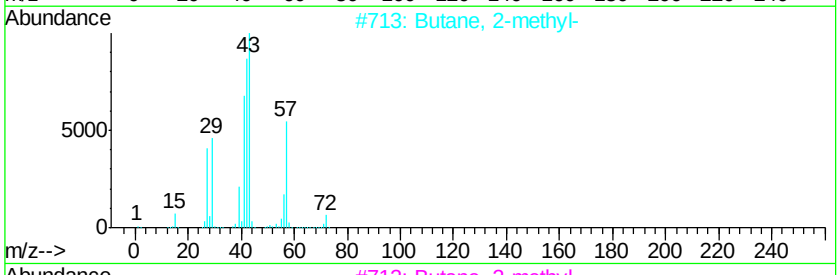
Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 6

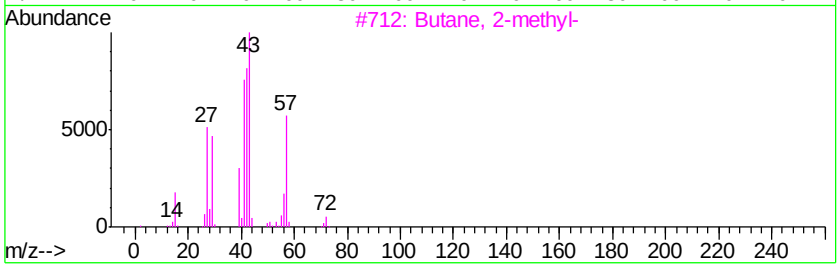
R.T.	EstConc	Area	Relative to ISTD	R.T.
1.65	0.58 ug/L	91904	1,4-Difluorobenzene	5.66

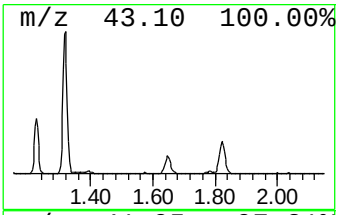
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	91
2	Butane, 2-methyl-	72	C5H12	000078-78-4	80
3	Butane, 2-methyl-	72	C5H12	000078-78-4	80
4	3-Buten-1-ol	72	C4H8O	000627-27-0	43
5	Pentane	72	C5H12	000109-66-0	28

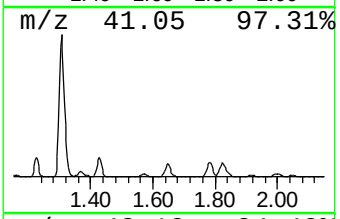


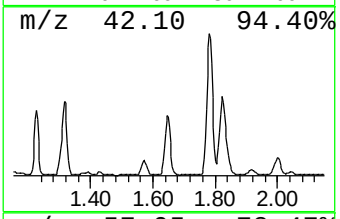


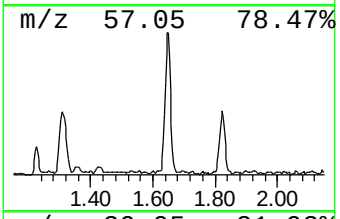


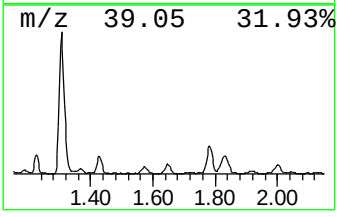












Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV112219\
Data File : VV013742.D
Acq On : 22 Nov 2019 18:35
Operator : SY/MD
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Instrument : MSVOA_V
ClientSampleId : B0AC9

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR112219WMA.M
Quant Title : TRACE VOA SOM01.0

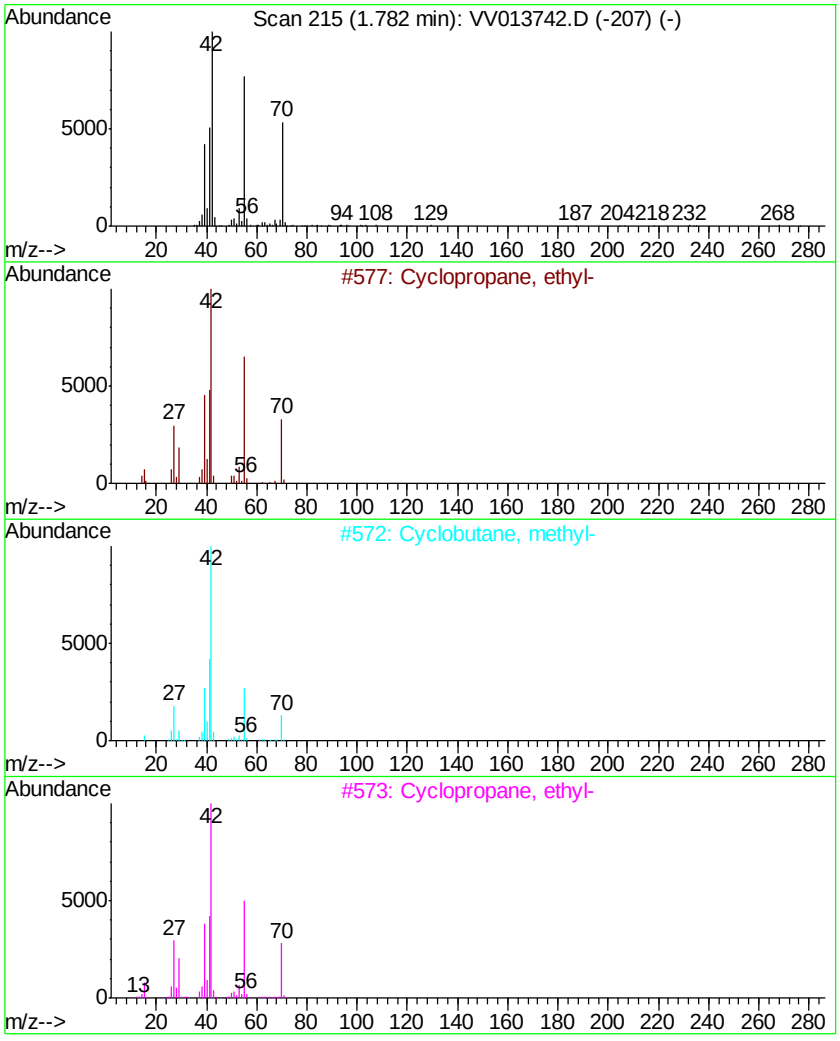
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

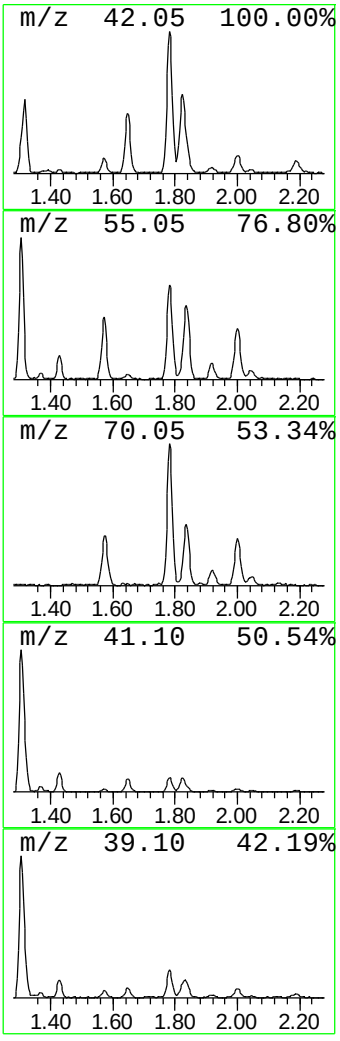
****

Peak Number 3 (DEL) Alkane: Cyclic1.70 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.78	1.09 ug/L	174376	1,4-Difluorobenzene	5.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, ethyl-	70	C5H10	001191-96-4	86
2	Cyclobutane, methyl-	70	C5H10	000598-61-8	68
3	Cyclopropane, ethyl-	70	C5H10	001191-96-4	64
4	1-Pentene	70	C5H10	000109-67-1	64
5	1-Pentene	70	C5H10	000109-67-1	64





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ClientSampleId : B0AC9

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR112219WMA.M
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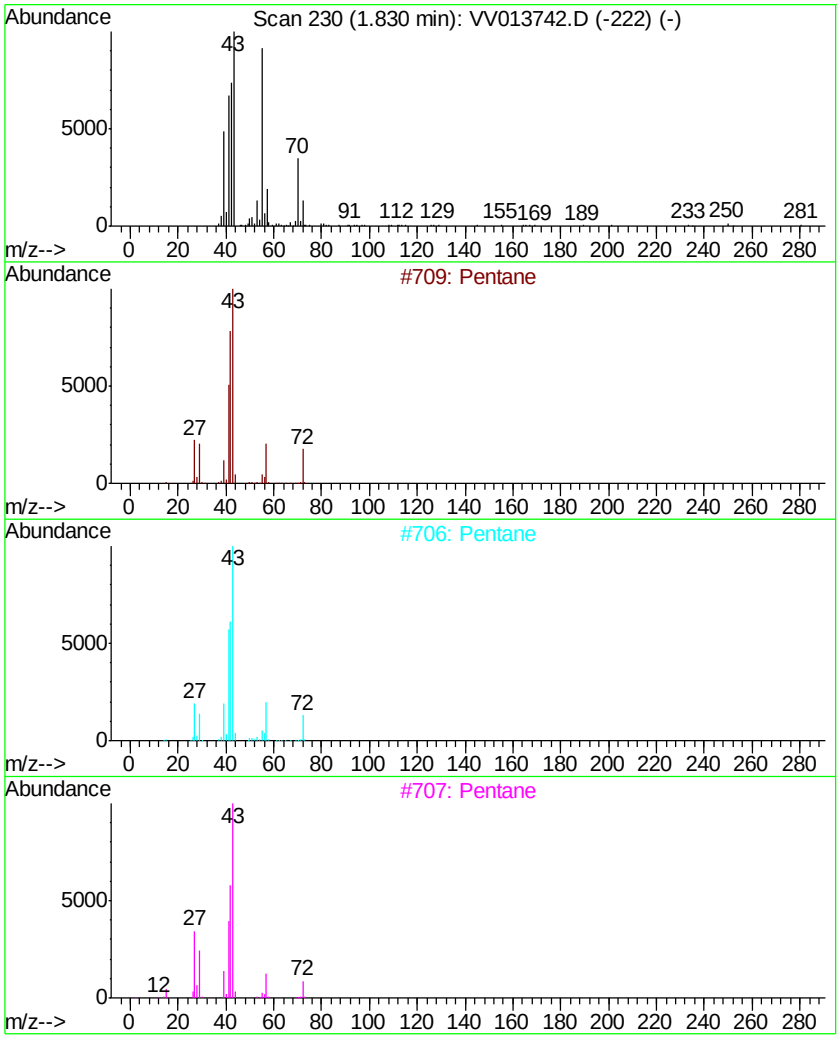
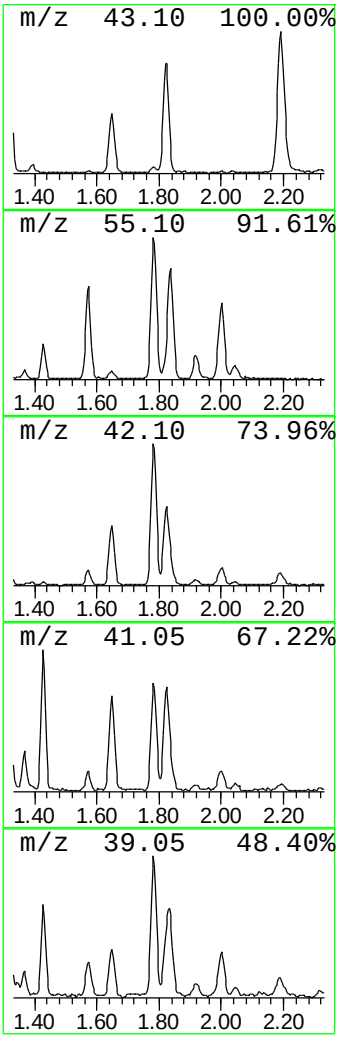
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.83	1.17 ug/L	186961	1,4-Difluorobenzene	5.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	53
2	Pentane	72	C5H12	000109-66-0	53
3	Pentane	72	C5H12	000109-66-0	53
4	Pentane	72	C5H12	000109-66-0	53
5	1-Pentene	70	C5H10	000109-67-1	46





Library Search Compound Report

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ClientSampleId : B0AC9

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR112219WMA.M
Quant Title : TRACE VOA SOM01.0

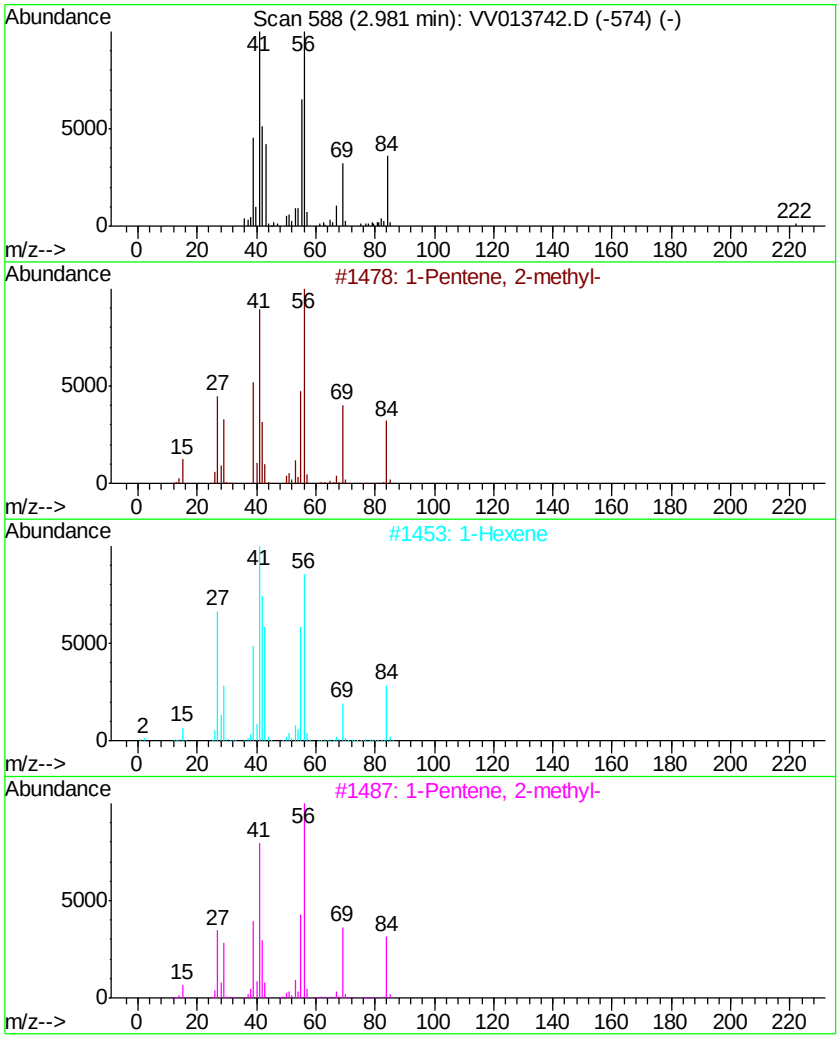
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

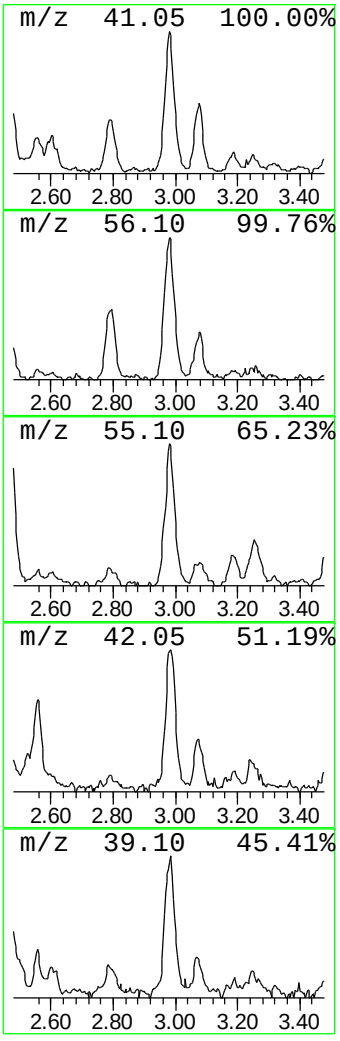
****

Peak Number 5 (DEL) Alkane: Cyclic2.98 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.98	0.65 ug/L	103432	1,4-Difluorobenzene	5.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	72
2	1-Hexene	84	C6H12	000592-41-6	70
3	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	68
4	1-Hexene	84	C6H12	000592-41-6	58
5	1-Heptene	98	C7H14	000592-76-7	50





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ClientSampleId : B0AC9

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Quant Title : TRACE VOA SOM01.0

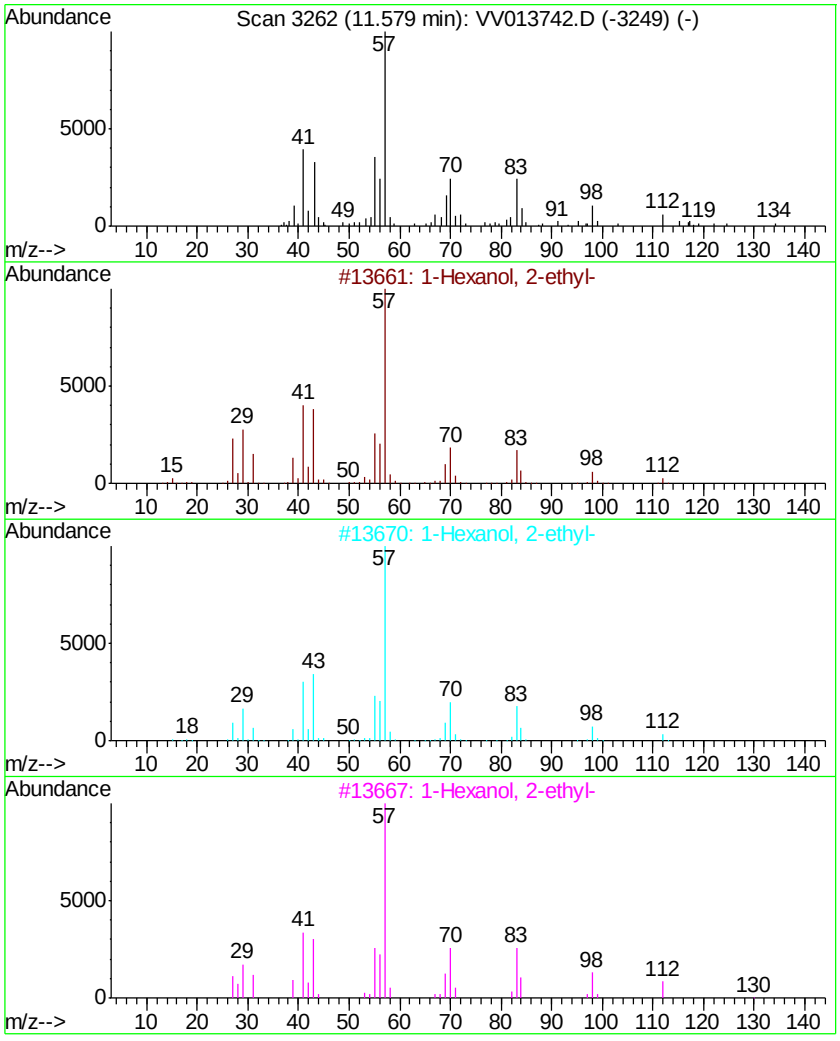
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

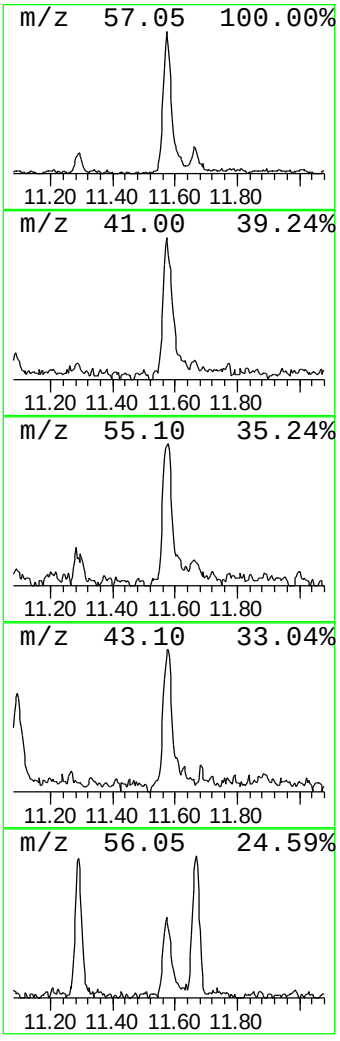
****

Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.58	0.52 ug/L	97409	1,4-Dichlorobenzene-d4	11.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	86
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
3	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
4	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	56
5	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53





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: Cyc...	1.12	6.6	ug/L	1053960	1	5.66	797517	5.0
(DEL) Alkane: Str...	1.65	0.6	ug/L	91904	1	5.66	797517	5.0
(DEL) Alkane: Cyc...	1.78	1.1	ug/L	174376	1	5.66	797517	5.0
(DEL) Alkane: Str...	1.83	1.2	ug/L	186961	1	5.66	797517	5.0
(DEL) Alkane: Cyc...	2.98	0.7	ug/L	103432	1	5.66	797517	5.0
1-Hexanol, 2-ethyl-	11.58	0.5	ug/L	97409	3	11.29	939000	5.0