LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV122319\
Data File : VV014169.D
Acq On : 23 Dec 2019 19:55
Operator : SY/MD
Sample : K6404-05
Misc : 25.0mL/MSVOA V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : BFDZ4

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\SOMVTR122319WMA.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	25	rVB	1229987	1129572	77.99%	7.081%
2	1.190	25	31	37	rVV	138820	131361	9.07%	0.823%
3	1.229	37	43	49	rVB	143273	129110	8.91%	0.809%
4	1.315	61	70	79	rBV2	547579	774127	53.45%	4.853%
5	1.370	83	87	91	rVV	26166	25824	1.78%	0.162%
6	1.393	91	94	99	rVV	19011	18525	1.28%	0.116%
7	1.434	99	107	120	rVB5	80689	113163	7.81%	0.709%
8	1.582	145	153	163	rVB	200661	237332	16.39%	1.488%
9	1.650	167	174	185	rVB	73820	92178	6.36%	0.578%
10	1.785	208	216	222	rBV	80479	99415	6.86%	0.623%
11	1.827	222	229	236	rBV3	51146	71748	4.95%	0.450%
12	1.920	252	258	267	rVB3	18177	28607	1.98%	0.179%
13	2.003	276	284	293	rBV2	26604	36285	2.51%	0.227%
14	2.129	314	323	334	rBV	357820	511206	35.30%	3.205%
15	2.184	336	340	352	rVB	24879	35086	2.42%	0.220%
16	2.319	371	382	401	rVB	316740	467302	32.26%	2.929%
17	2.473	416	430	437	rBV	11817	27680	1.91%	0.174%
18	2.560	451	457	466	rVB4	12584	19730	1.36%	0.124%
19	2.798	522	531	542	rVB3	30137	58397	4.03%	0.366%
20	2.933	564	573	579	rBV6	9896	18353	1.27%	0.115%
21	2.987	580	590	603	rVB5	19411	42313	2.92%	0.265%
22	3.077	609	618	629	rVB5	15117	29626	2.05%	0.186%
23	3.923	868	881	912	rBV	174144	461908	31.89%	2.896%
24	4.396	1012	1028	1047	rBV	244616	596272	41.17%	3.738%
25	5.093	1226	1245	1278	rBV3	563237	1448325	100.00%	9.079%
26	5.659	1409	1421	1440	rBV2	423588	856065	59.11%	5.367%
27	6.113	1546	1562	1576	rBV	318725	654049	45.16%	4.100%
28	7.026	1832	1846	1867	rBV	144988	279291	19.28%	1.751%
29	7.357	1936	1949	1963	rBV	636238	1118260	77.21%	7.010%
30	7.431	1963	1972	1985	rVB	82729	143867	9.93%	0.902%
31	7.662	2033	2044	2063	rBV	89325	167428	11.56%	1.050%
32	8.132	2176	2190	2219	rBV	534500	1215594	83.93%	7.620%
33	8.286	2229	2238	2248	rVB4	23756	41208	2.85%	0.258%
34	8.891	2414	2426	2450	rBV	619262	1037254	71.62%	6.502%

LSC Area Percent Report

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Acq On : 23 Dec 2019 19:55
Operator : SY/MD
Sample : K6404-05
Misc : 25.0mL/MSVOA V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : BFDZ4

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\SOMVTR122319WMA.M
Title : TRACE VOA SOM01.0

35	9.055	2467	2477	2486	rBV2	18028	29718	2.05%	0.186%
36	9.177	2495	2515	2528	rBV	63348	119760	8.27%	0.751%
37	9.585	2633	2642	2656	rVB	36007	61658	4.26%	0.387%
38	9.855	2715	2726	2738	rBV	18288	33999	2.35%	0.213%
39	10.257	2834	2851	2865	rVB	218458	364884	25.19%	2.287%
40	10.489	2913	2923	2941	rBV4	15588	34848	2.41%	0.218%
41	10.582	2943	2952	2955	rBV5	10631	14685	1.01%	0.092%
42	10.778	3002	3013	3024	rBV	13413	27694	1.91%	0.174%
43	10.955	3055	3068	3078	rBV2	36668	63569	4.39%	0.399%
44	11.196	3133	3143	3152	rBV3	35597	61931	4.28%	0.388%
45	11.289	3161	3172	3192	rBV2	645542	1153756	79.66%	7.233%
46	11.379	3192	3200	3209	rVB	16141	29275	2.02%	0.184%
47	11.572	3250	3260	3269	rBV	11552	23024	1.59%	0.144%
48	11.665	3278	3289	3311	rBV2	635134	1168814	80.70%	7.327%
49	12.389	3504	3514	3527	rBV2	98745	148211	10.23%	0.929%
50	13.305	3789	3799	3812	rBV2	24925	44170	3.05%	0.277%
51	13.546	3862	3874	3885	rBV	275992	438165	30.25%	2.747%
52	14.681	4217	4227	4238	rBV	8502	17250	1.19%	0.108%

Sum of corrected areas: 15951872

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Acq On : 23 Dec 2019 19:55
Operator : SY/MD
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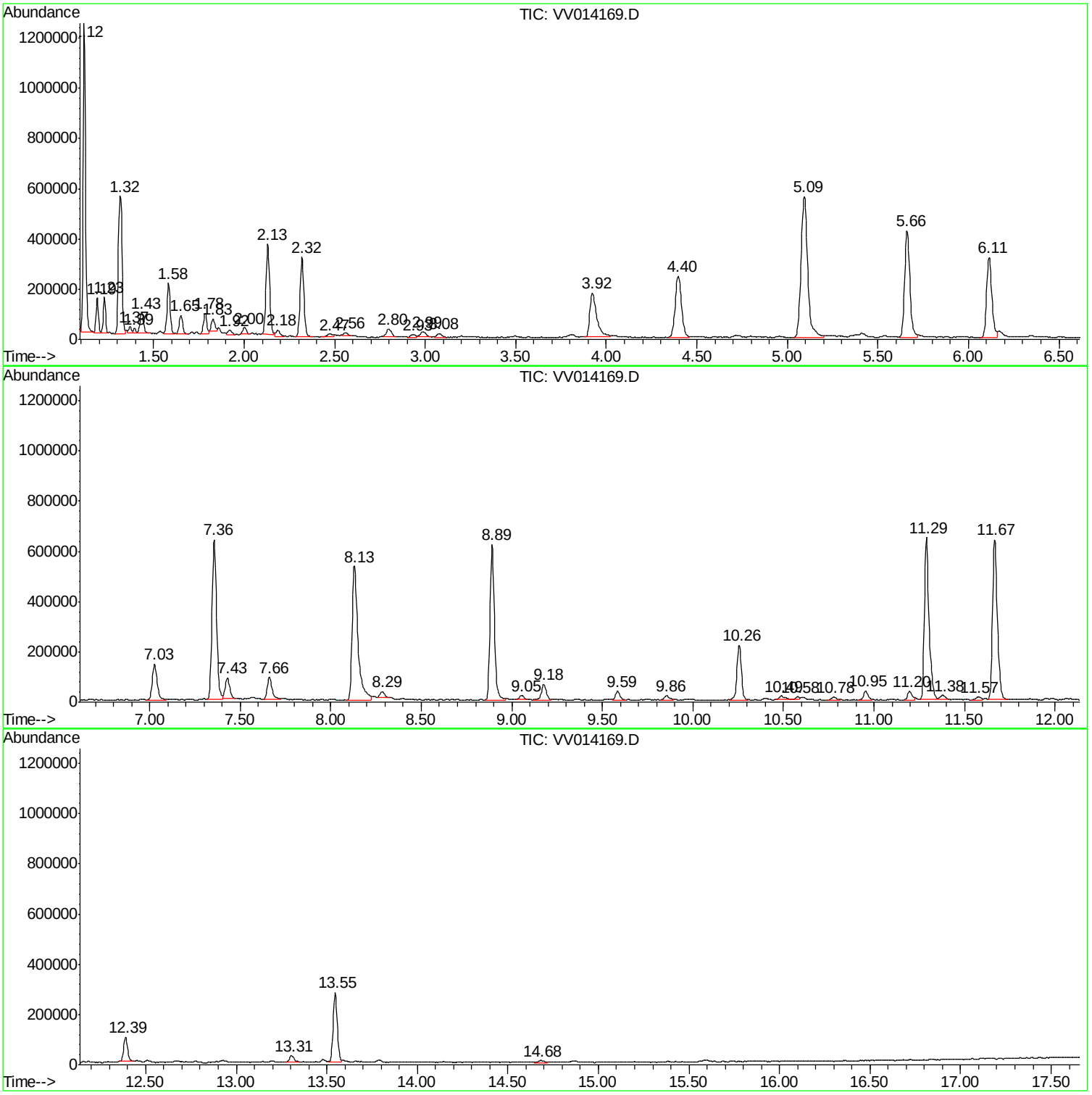
Misc : 25.0mL/MSVOA V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : BFDZ4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR122319WMA.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_V\DATA\VV122319\
Data File : VV014169.D
Acq On : 23 Dec 2019 19:55
Operator : SY/MD
Sample : K6404-05
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : BFDZ4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR122319WMA.M
Quant Title : TRACE VOA SOM01.0

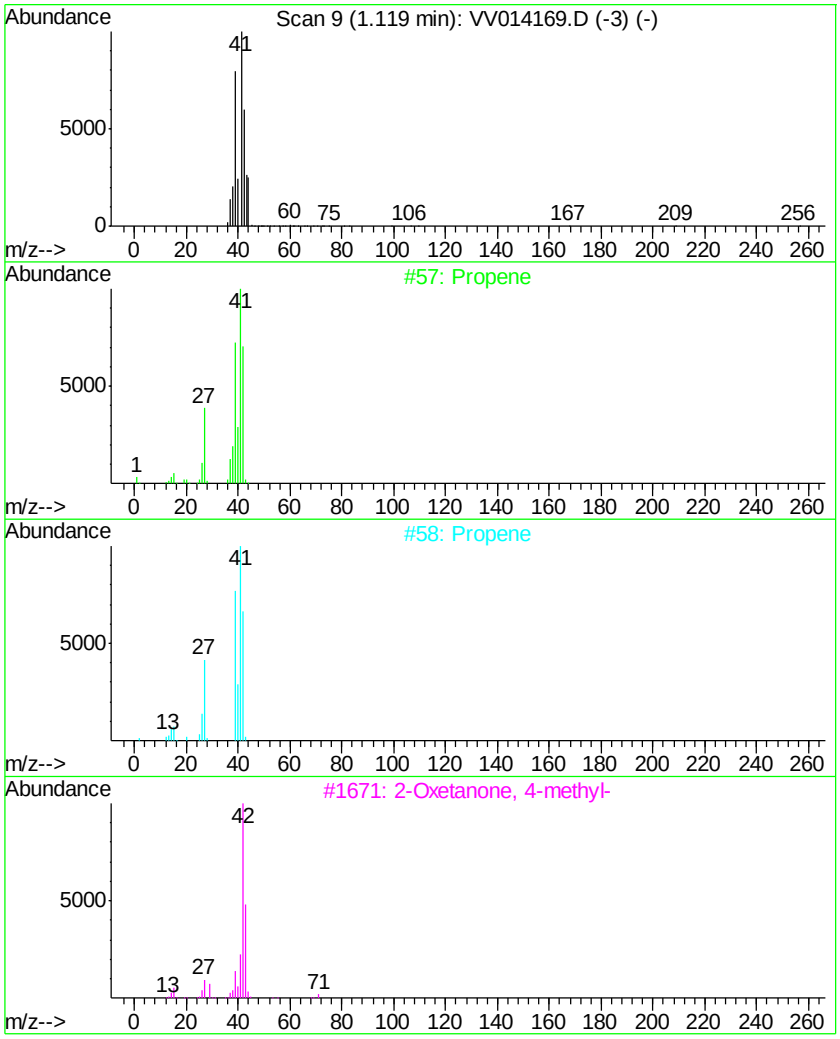
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

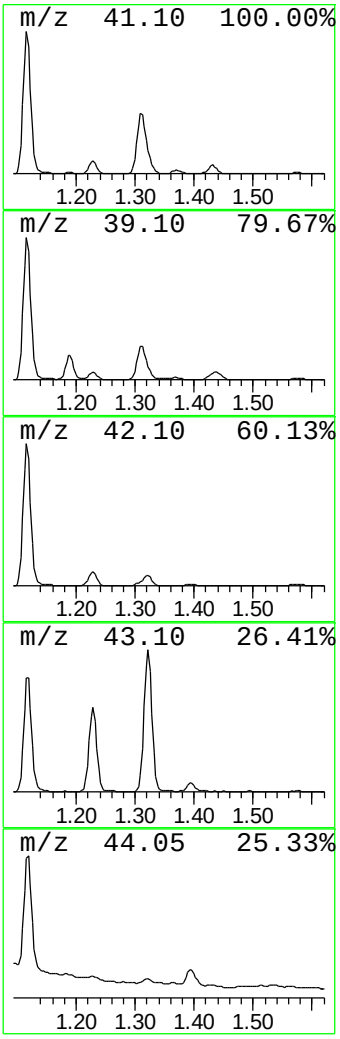
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.12	6.60 ug/L	1129570	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	2-Oxetanone, 4-methyl-	86	C4H6O2	003068-88-0	9
4	Cyclopropane	42	C3H6	000075-19-4	9
5	Cyclopropene	40	C3H4	002781-85-3	9





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV122319\
Data File : VV014169.D
Acq On : 23 Dec 2019 19:55
Operator : SY/MD
Sample : K6404-05
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : BFDZ4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR122319WMA.M
Quant Title : TRACE VOA SOM01.0

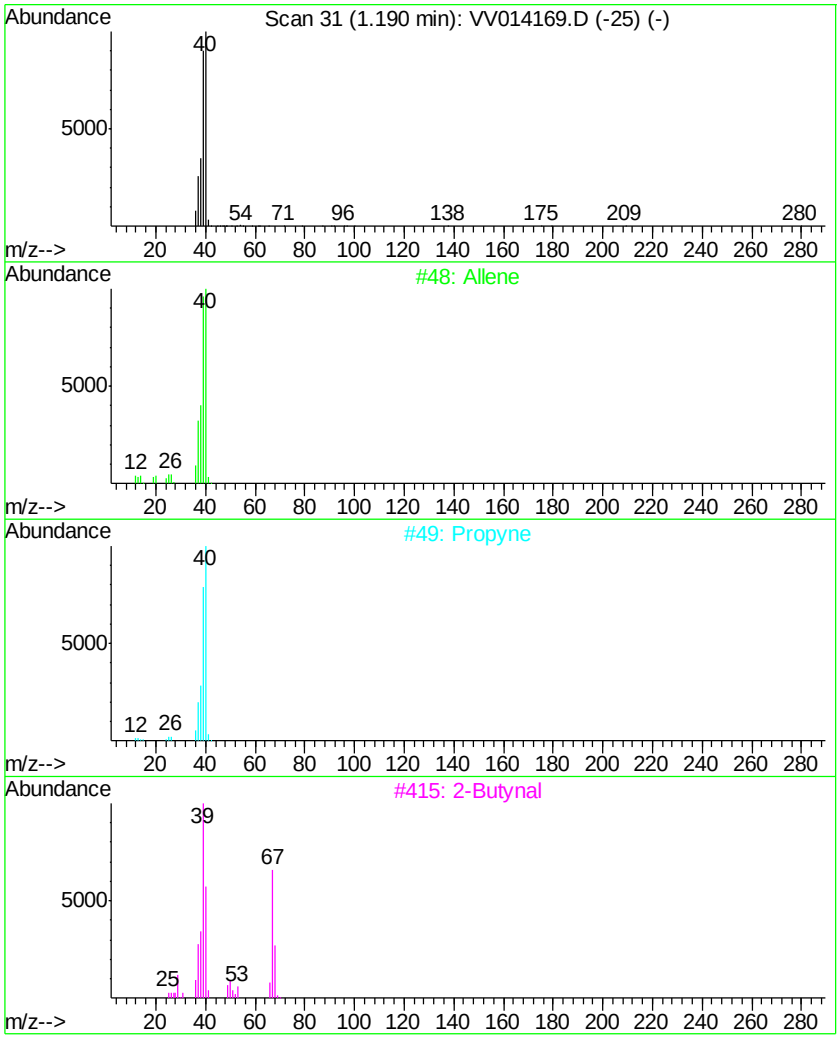
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

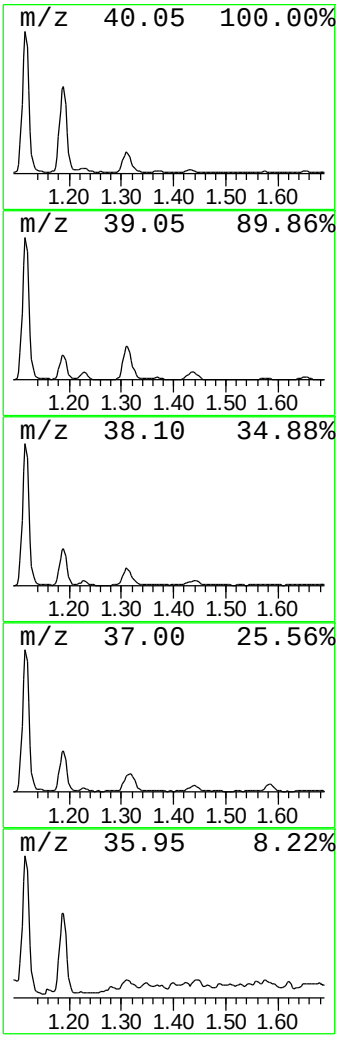
****

Peak Number 2 Allene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.19	0.77 ug/L	131361	1,4-Difluorobenzene	5.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Allene	40	C3H4	000463-49-0	90
2	Propyne	40	C3H4	000074-99-7	90
3	2-Butynal	68	C4H4O	001119-19-3	74
4	1-Propyne, 3-bromo-	118	C3H3Br	000106-96-7	64
5	2H-Pyrano[3,2-b]pyridine	133	C8H7NO	004767-91-3	9





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV122319\
Data File : VV014169.D
Acq On : 23 Dec 2019 19:55
Operator : SY/MD
Sample : K6404-05
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : BFDZ4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR122319WMA.M
Quant Title : TRACE VOA SOM01.0

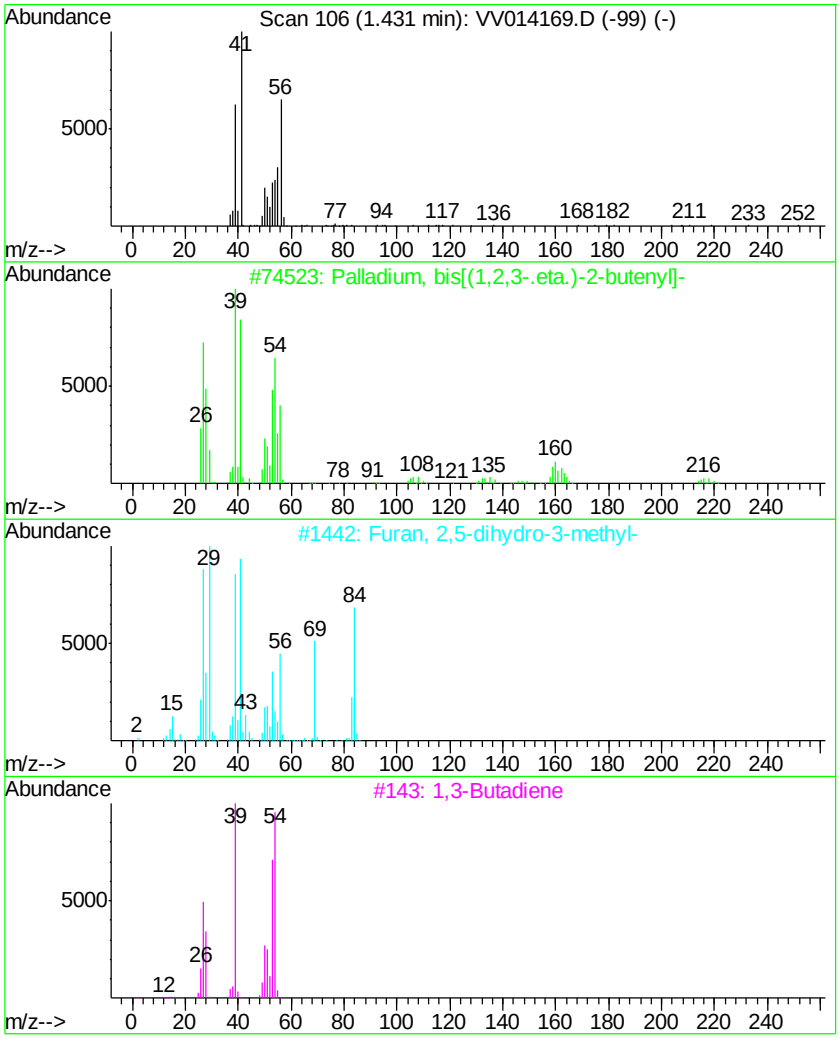
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

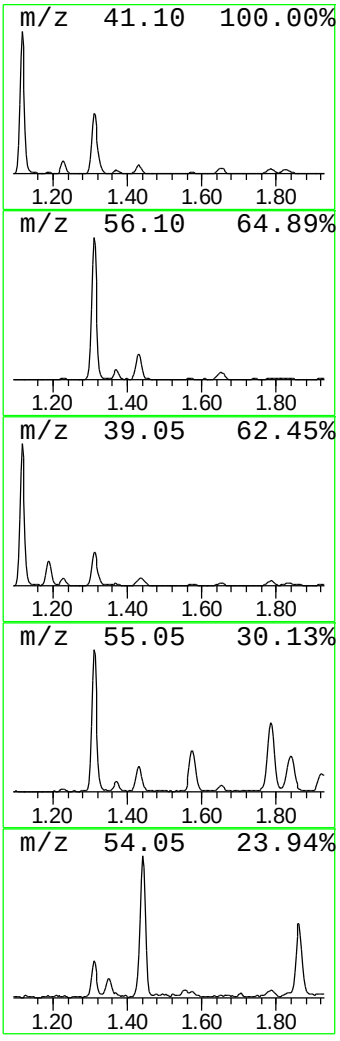
****

Peak Number 3 Palladium, bis[(1,2,3-.eta.... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.43	0.66 ug/L	113163	1,4-Difluorobenzene	5.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Palladium, bis[(1,2,3-.eta.)-2-b...	216	C8H14Pd	063817-37-8	78
2	Furan, 2,5-dihydro-3-methyl-	84	C5H8O	001708-31-2	78
3	1,3-Butadiene	54	C4H6	000106-99-0	72
4	1-Methylcyclopropene	54	C4H6	003100-04-7	72
5	1,3-Butadiene	54	C4H6	000106-99-0	64





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV122319\
Data File : VV014169.D
Acq On : 23 Dec 2019 19:55
Operator : SY/MD
Sample : K6404-05
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : BFDZ4

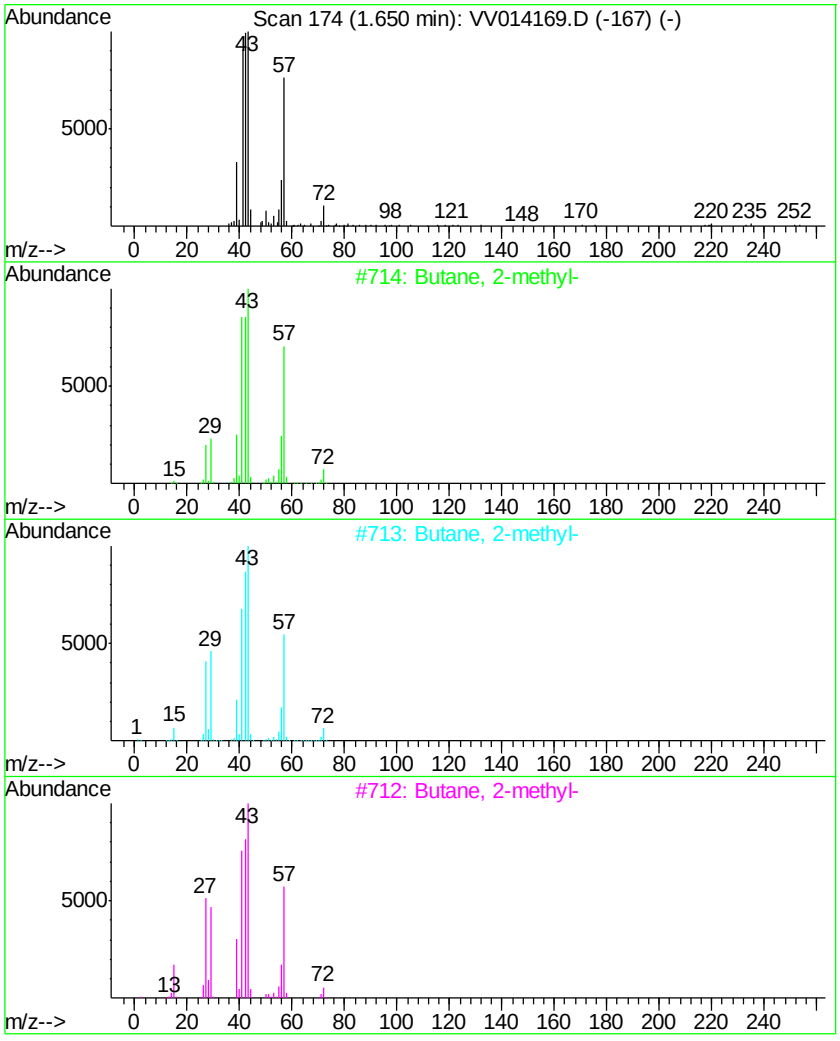
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR122319WMA.M
Quant Title : TRACE VOA SOM01.0

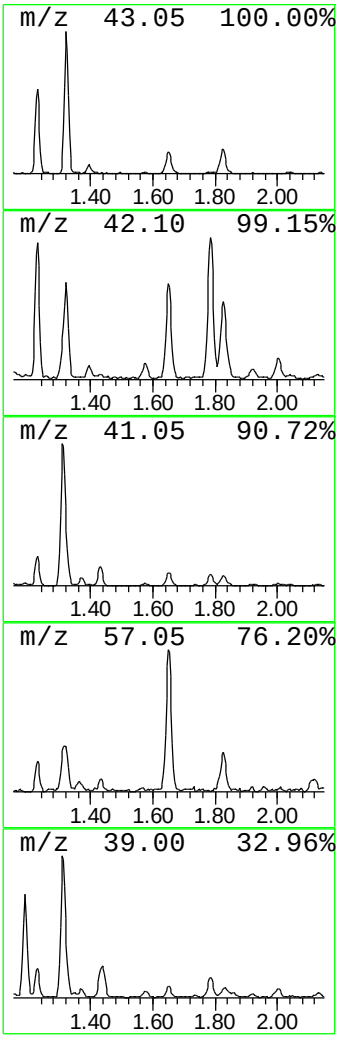
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.65	0.54 ug/L	92178	1,4-Difluorobenzene	5.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	90
2	Butane, 2-methyl-	72	C5H12	000078-78-4	87
3	Butane, 2-methyl-	72	C5H12	000078-78-4	87
4	3-Buten-1-ol	72	C4H8O	000627-27-0	43
5	Taurultam	136	C3H8N2O2S	038668-01-8	36





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV122319\
Data File : VV014169.D
Acq On : 23 Dec 2019 19:55
Operator : SY/MD
Sample : K6404-05
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : BFDZ4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR122319WMA.M
Quant Title : TRACE VOA SOM01.0

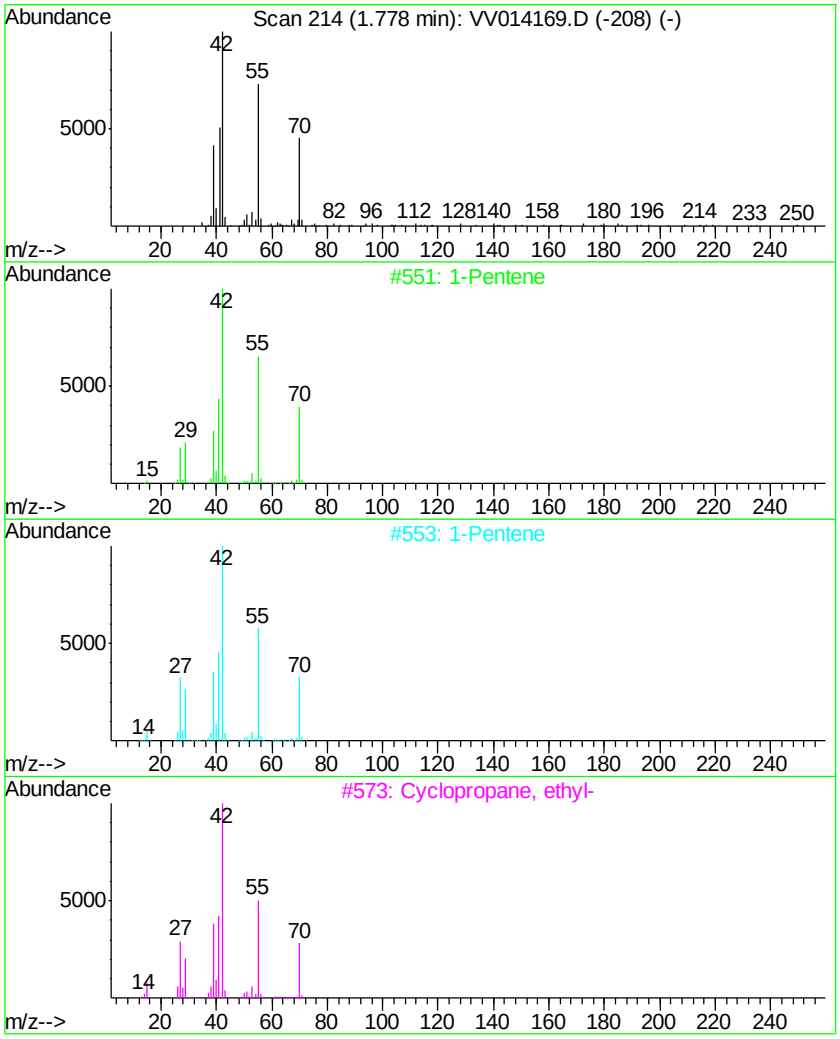
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

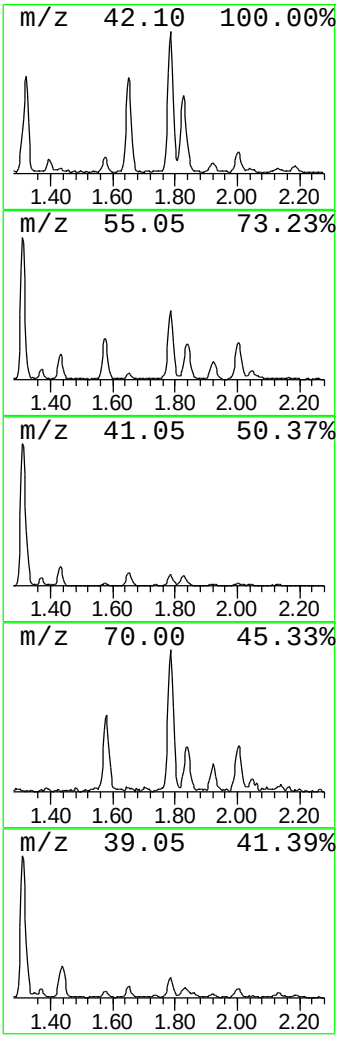
****

Peak Number 5 (DEL) Alkane: Cyclic1.78 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.78	0.58 ug/L	99415	1,4-Difluorobenzene	5.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene	70	C5H10	000109-67-1	76
2	1-Pentene	70	C5H10	000109-67-1	70
3	Cyclopropane, ethyl-	70	C5H10	001191-96-4	62
4	Cyclopropane, ethyl-	70	C5H10	001191-96-4	59
5	Cyclopentane	70	C5H10	000287-92-3	53





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ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : BFDZ4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR122319WMA.M
Quant Title : TRACE VOA SOM01.0

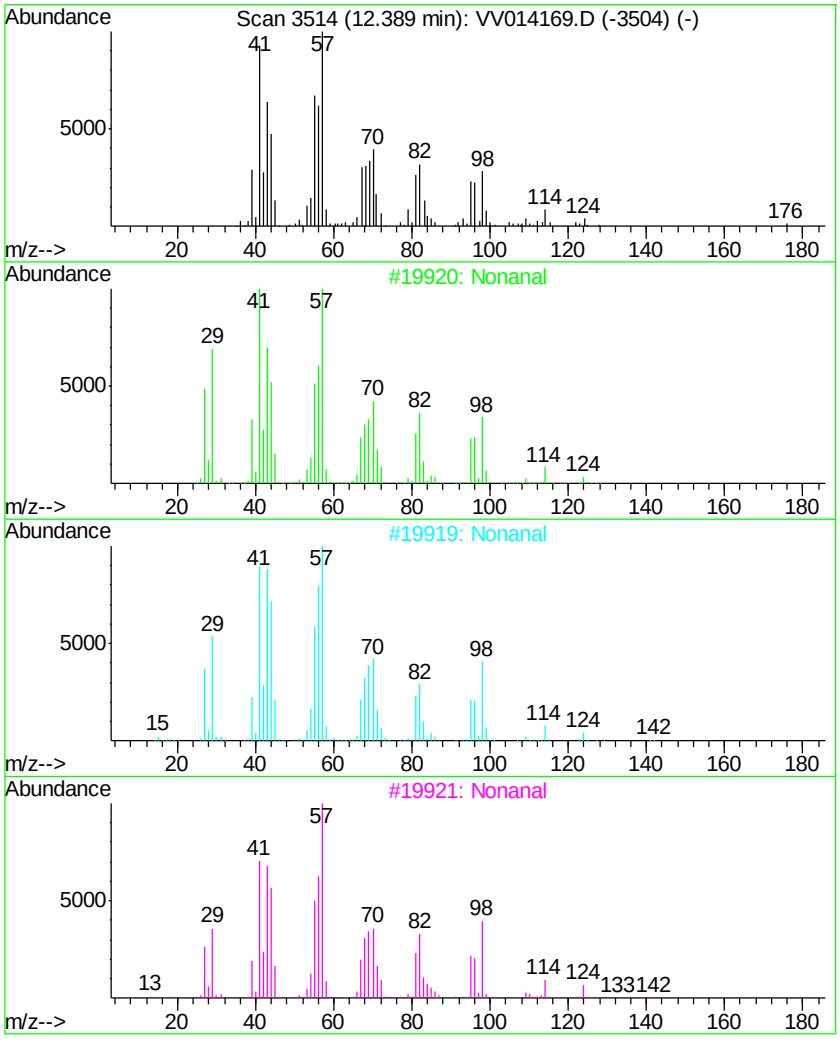
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

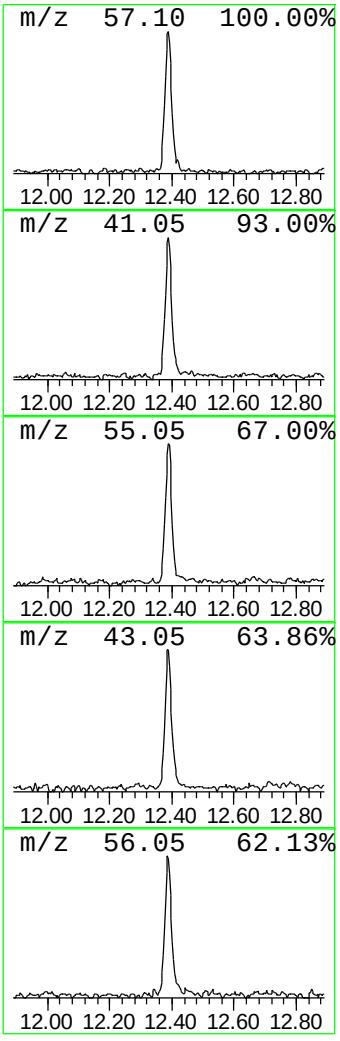
****

Peak Number 7 Nonanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.39	0.64 ug/L	148211	1,4-Dichlorobenzene-d4	11.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanal	142	C9H18O	000124-19-6	91
2	Nonanal	142	C9H18O	000124-19-6	78
3	Nonanal	142	C9H18O	000124-19-6	72
4	2-Heptene	98	C7H14	000592-77-8	35
5	Cyclohexanol, 2-methyl-, trans-	114	C7H14O	007443-52-9	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV122319\
Data File : VV014169.D
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Instrument : MSVOA_V
ClientSampleId : BFDZ4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR122319WMA.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: Cyc...	1.12	6.6	ug/L	1129570	1	5.66	856065	5.0
Allene	1.19	0.8	ug/L	131361	1	5.66	856065	5.0
Palladium, bis[(1...	1.43	0.7	ug/L	113163	1	5.66	856065	5.0
(DEL) Alkane: Str...	1.65	0.5	ug/L	92178	1	5.66	856065	5.0
(DEL) Alkane: Cyc...	1.78	0.6	ug/L	99415	1	5.66	856065	5.0
Nonanal	12.39	0.6	ug/L	148211	3	11.29	1153760	5.0