LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU072120\
Data File : VU039611.D
Acq On : 21 Jul 2020 20:47
Operator : SY/MD
Sample : L3347-15
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GAY07

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_U\METHOD\SOMUTR072120WMA.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	1.366	3	8	14	rBV	526775	496229	100.00%	8.897%
2	1.398	14	18	28	rVB	112099	117628	23.70%	2.109%
3	1.498	41	49	57	rBV	31122	31399	6.33%	0.563%
4	1.597	71	80	97	rBV3	270504	439347	88.54%	7.878%
5	1.668	97	102	106	rVV2	9549	10681	2.15%	0.192%
6	1.697	106	111	118	rVV2	9315	11981	2.41%	0.215%
7	1.742	118	125	135	rVB	39382	46398	9.35%	0.832%
8	1.922	169	181	196	rVB2	65549	98156	19.78%	1.760%
9	2.006	198	207	217	rVB	37522	51730	10.42%	0.928%
10	2.167	247	257	265	rBV	82092	113968	22.97%	2.043%
11	2.221	265	274	294	rVB4	56724	119726	24.13%	2.147%
12	2.330	301	308	315	rBV	6823	9388	1.89%	0.168%
13	2.427	329	338	348	rBV2	26191	39315	7.92%	0.705%
14	2.478	348	354	367	rVB5	4990	8441	1.70%	0.151%
15	2.581	367	386	398	rBV2	84785	148406	29.91%	2.661%
16	2.649	398	407	427	rVB	7547	17191	3.46%	0.308%
17	2.810	442	457	469	rBV2	7862	17177	3.46%	0.308%
18	2.993	499	514	526	rBV7	8035	21482	4.33%	0.385%
19	3.102	541	548	556	rVB4	4501	7726	1.56%	0.139%
20	3.382	619	635	652	rVB4	17308	39515	7.96%	0.709%
21	3.604	689	704	722	rVB3	24326	58989	11.89%	1.058%
22	3.723	728	741	757	rVB4	8938	19827	4.00%	0.356%
23	3.848	764	780	792	rBV4	3561	7840	1.58%	0.141%
24	3.925	795	804	815	rVB8	2857	6748	1.36%	0.121%
25	4.218	881	895	910	rBV5	6227	14641	2.95%	0.263%
26	4.472	958	974	989	rVB6	3513	8561	1.73%	0.154%
27	4.649	1012	1029	1070	rBV3	86273	245001	49.37%	4.393%
28	5.083	1150	1164	1188	rVB	80870	188729	38.03%	3.384%
29	5.388	1247	1259	1269	rVB6	2805	5297	1.07%	0.095%
30	5.469	1269	1284	1303	rVB5	3511	10740	2.16%	0.193%
31	5.610	1316	1328	1339	rBV7	4105	8018	1.62%	0.144%
32	5.742	1349	1369	1397	rBV3	158487	424750	85.60%	7.616%
33	5.986	1432	1445	1453	rBV6	4205	8723	1.76%	0.156%
34	6.041	1453	1462	1477	rVB7	7323	16761	3.38%	0.301%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU072120\
Data File : VU039611.D
Acq On : 21 Jul 2020 20:47
Operator : SY/MD
Sample : L3347-15
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GAY07

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_U\METHOD\SOMUTR072120WMA.M
Title : TRACE VOA SOM01.0

35	6.153	1487	1497	1505	rBV6	4608	8903	1.79%	0.160%
36	6.266	1515	1532	1554	rBV	149857	290737	58.59%	5.213%
37	6.568	1615	1626	1637	rVB8	3289	7192	1.45%	0.129%
38	6.707	1654	1669	1685	rBV	100259	195126	39.32%	3.499%
39	6.870	1707	1720	1735	rBV4	14462	30341	6.11%	0.544%
40	7.578	1924	1940	1952	rBV2	52149	91891	18.52%	1.648%
41	7.906	2030	2042	2056	rBV	186965	325777	65.65%	5.841%
42	7.977	2056	2064	2076	rVB2	13495	22301	4.49%	0.400%
43	8.189	2118	2130	2143	rBV	32704	56169	11.32%	1.007%
44	8.642	2256	2271	2298	rBV	266713	492656	99.28%	8.833%
45	8.793	2309	2318	2326	rBV5	4358	6699	1.35%	0.120%
46	9.423	2501	2514	2531	rBV	215091	359106	72.37%	6.439%
47	9.697	2588	2599	2609	rBV4	7732	12719	2.56%	0.228%
48	10.102	2715	2725	2738	rBV	17321	27636	5.57%	0.496%
49	10.758	2915	2929	2944	rBV	80447	130863	26.37%	2.346%
50	11.809	3244	3256	3272	rBV	207198	336265	67.76%	6.029%
51	12.189	3361	3374	3389	rBV2	193822	312287	62.93%	5.599%

Sum of corrected areas: 5577177

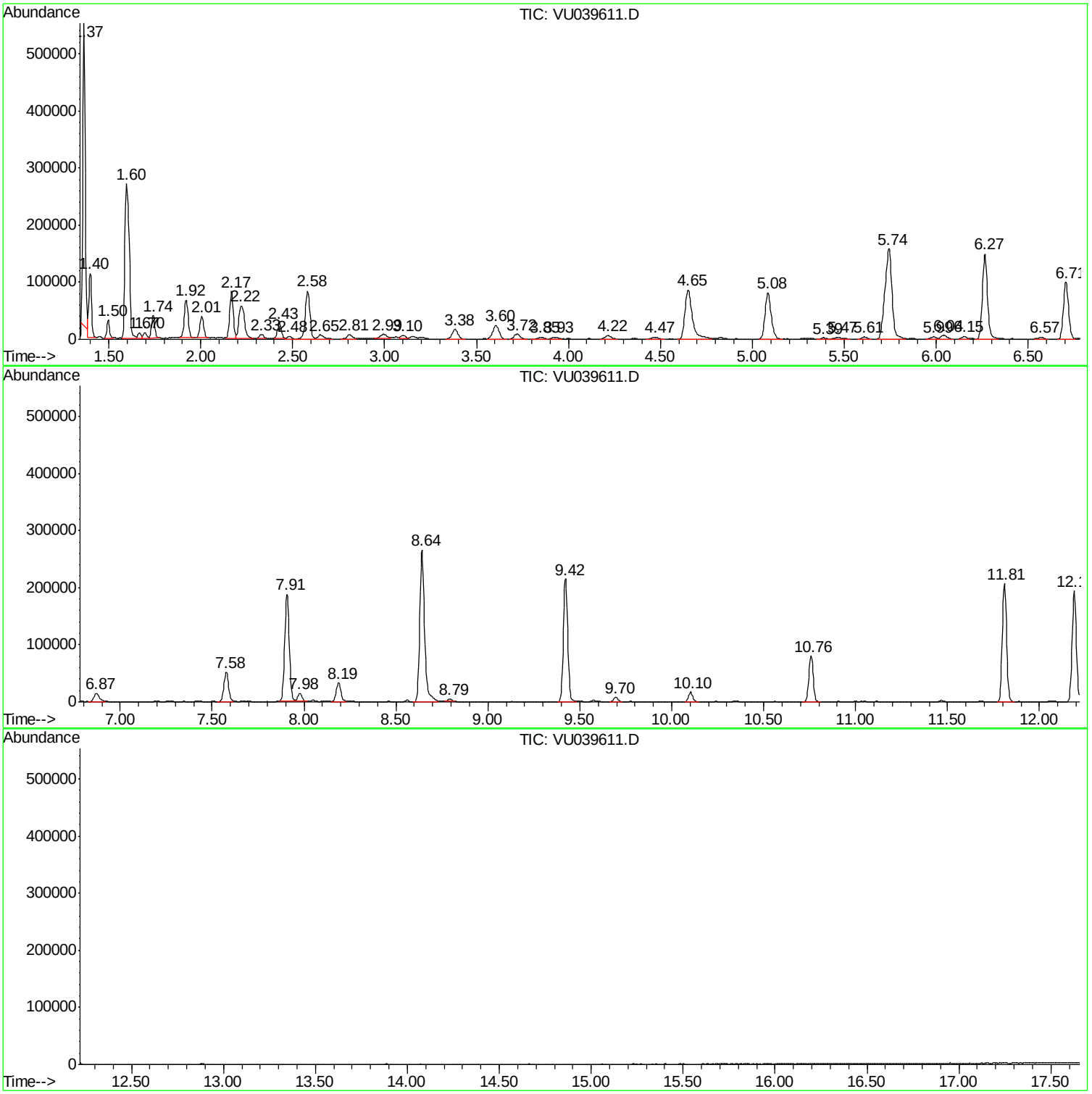
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU072120\
Data File : VU039611.D
Acq On : 21 Jul 2020 20:47
Operator : SY/MD
Sample : L3347-15
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GAY07

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR072120WMA.M
Quant Title : TRACE VOA SOM01.0

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU072120\
Data File : VU039611.D
Acq On : 21 Jul 2020 20:47
Operator : SY/MD
Sample : L3347-15
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GAY07

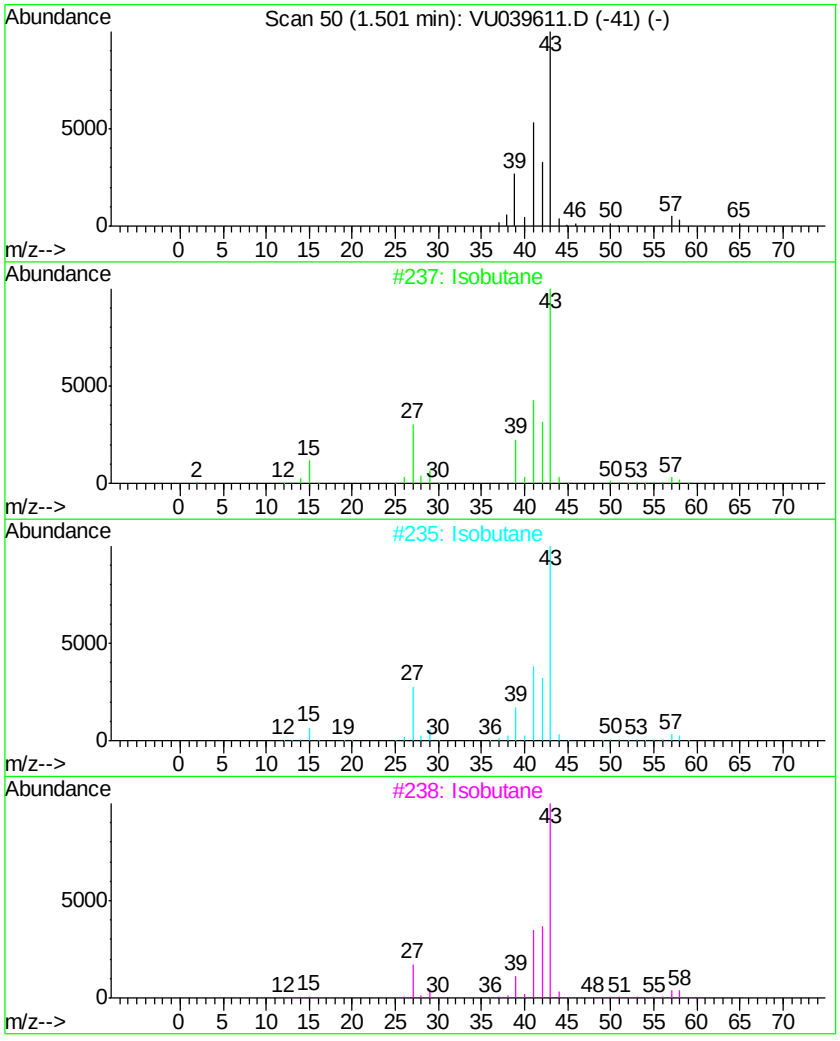
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR072120WMA.M
Quant Title : TRACE VOA SOM01.0

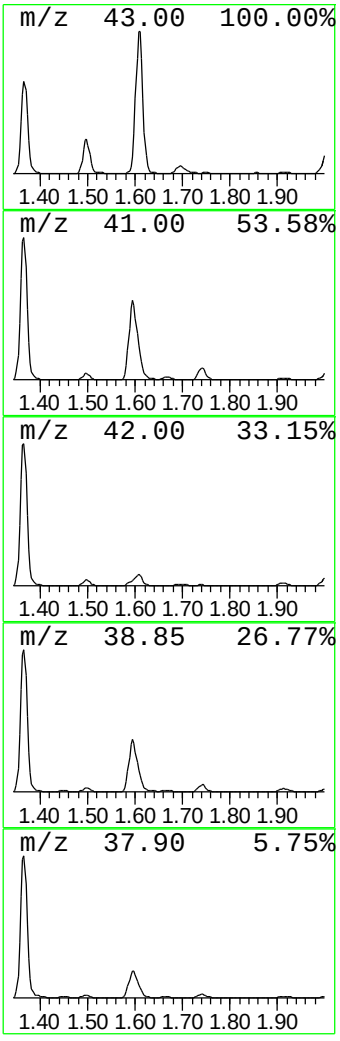
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.50	0.54 ug/L	31399	1,4-Difluorobenzene	6.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutane	58	C4H10	000075-28-5	64
2	Isobutane	58	C4H10	000075-28-5	64
3	Isobutane	58	C4H10	000075-28-5	45
4	Propane, 2-nitro-	89	C3H7NO2	000079-46-9	33
5	Isobutane	58	C4H10	000075-28-5	9





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU072120\
Data File : VU039611.D
Acq On : 21 Jul 2020 20:47
Operator : SY/MD
Sample : L3347-15
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GAY07

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR072120WMA.M
Quant Title : TRACE VOA SOM01.0

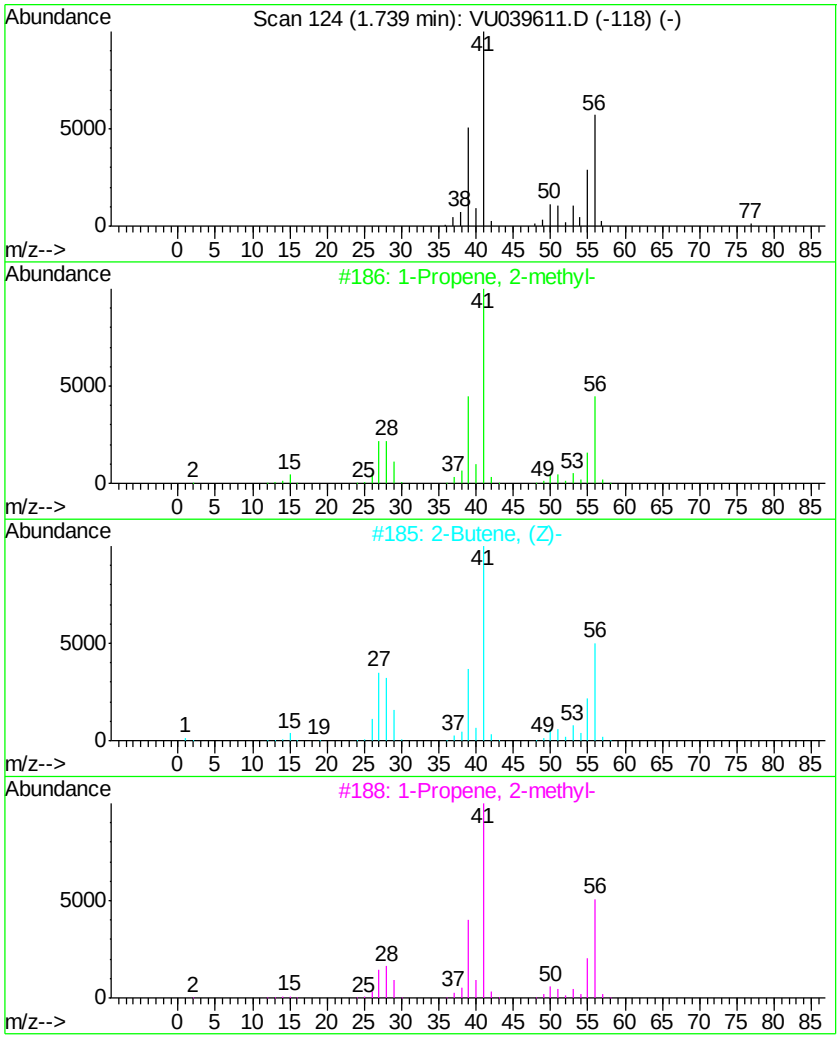
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

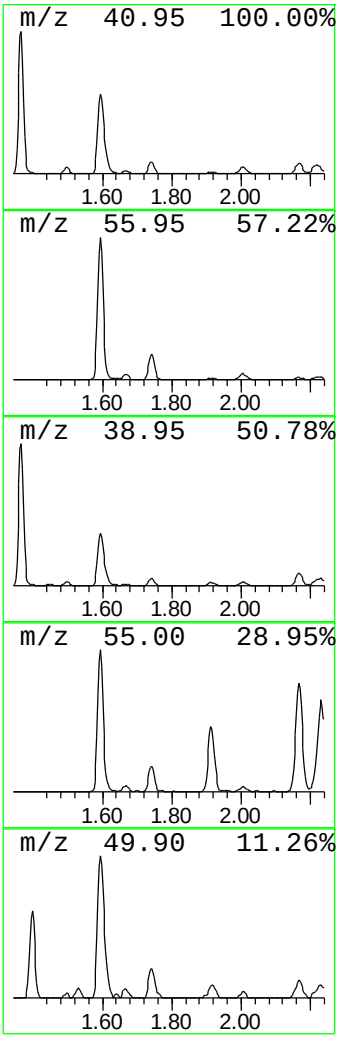
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.74	0.80 ug/L	46398	1,4-Difluorobenzene	6.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene, 2-methyl-	56	C4H8	000115-11-7	72
2	2-Butene, (Z)-	56	C4H8	000590-18-1	64
3	1-Propene, 2-methyl-	56	C4H8	000115-11-7	64
4	2-Butene, (Z)-	56	C4H8	000590-18-1	58
5	2-Butene, (E)-	56	C4H8	000624-64-6	58





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU072120\
Data File : VU039611.D
Acq On : 21 Jul 2020 20:47
Operator : SY/MD
Sample : L3347-15
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GAY07

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR072120WMA.M
Quant Title : TRACE VOA SOM01.0

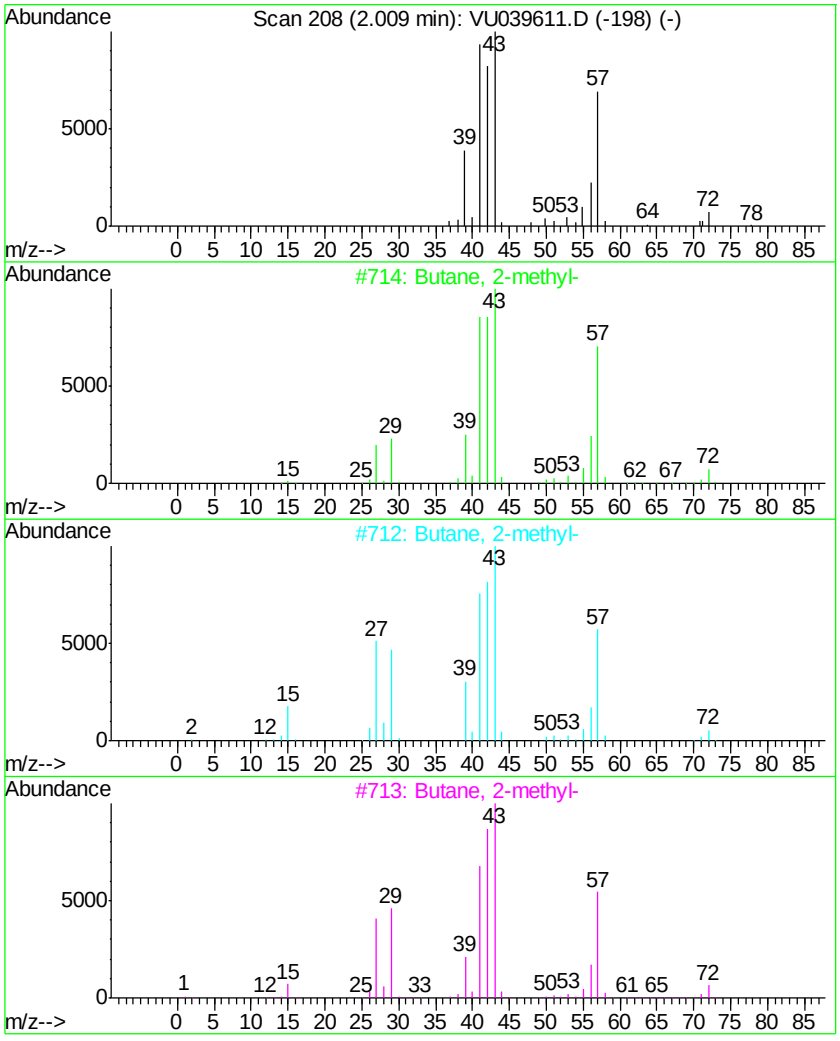
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

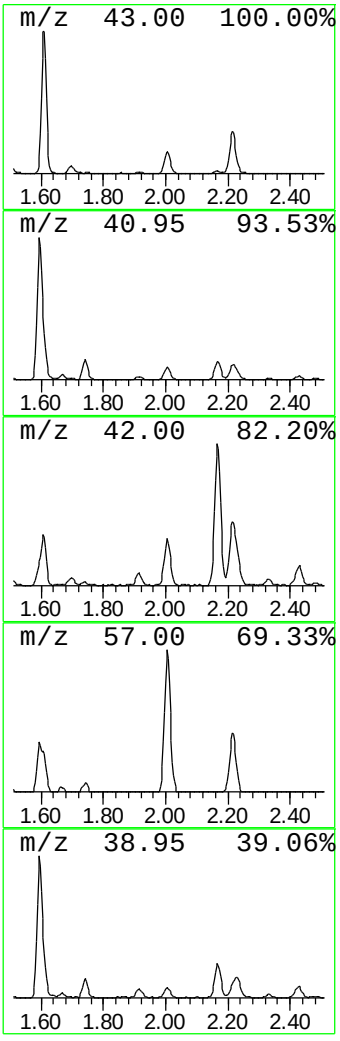
****

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.01	0.89 ug/L	51730	1,4-Difluorobenzene	6.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	81
2	Butane, 2-methyl-	72	C5H12	000078-78-4	64
3	Butane, 2-methyl-	72	C5H12	000078-78-4	64
4	Pentane	72	C5H12	000109-66-0	38
5	3-Buten-1-ol	72	C4H8O	000627-27-0	36





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU072120\
Data File : VU039611.D
Acq On : 21 Jul 2020 20:47
Operator : SY/MD
Sample : L3347-15
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GAY07

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR072120WMA.M
Quant Title : TRACE VOA SOM01.0

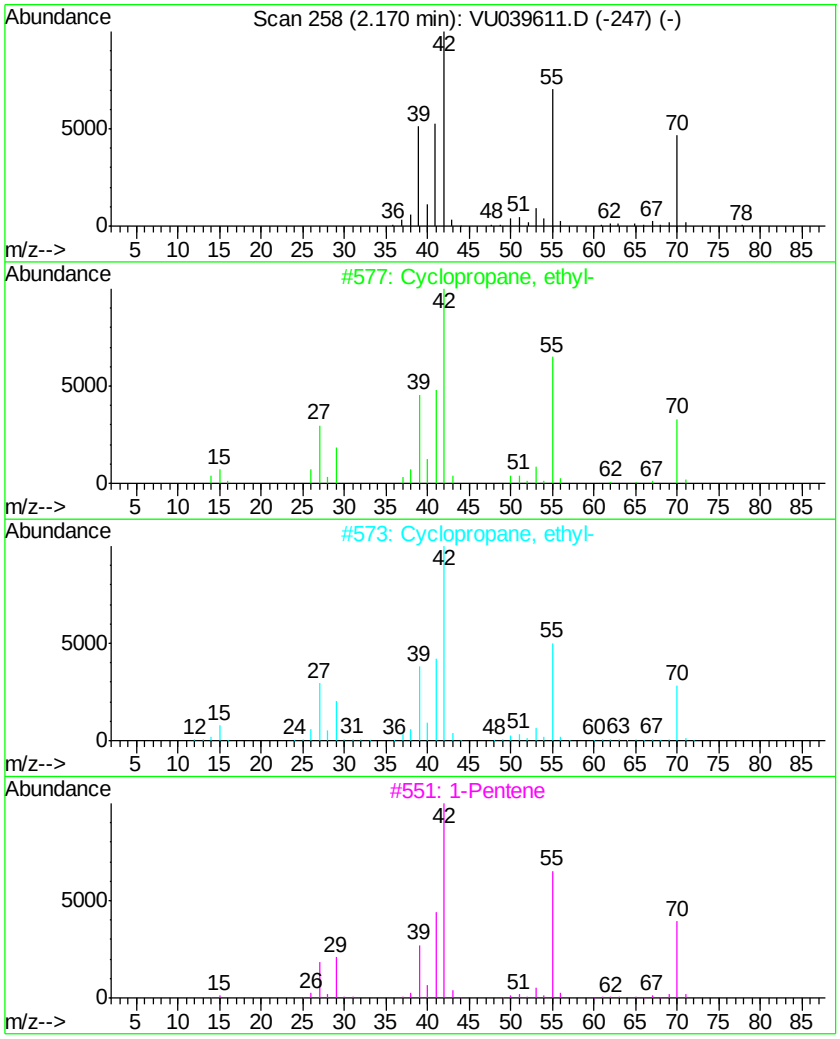
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

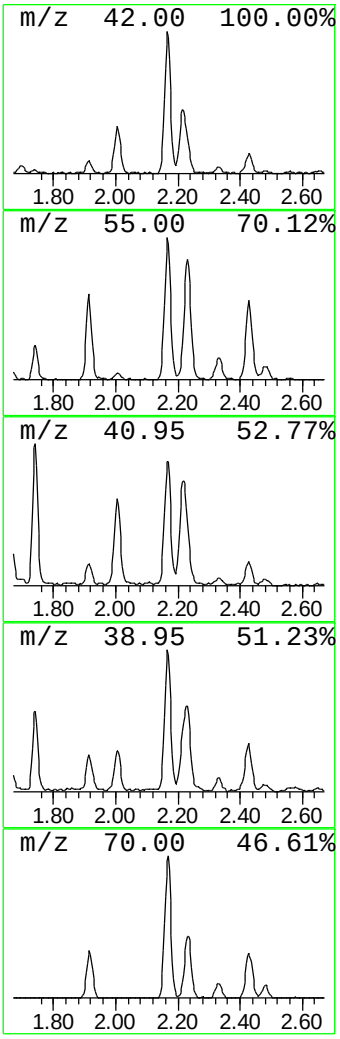
****

Peak Number 4 (DEL) Alkane: Cyclic2.17 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	1.96 ug/L	113968	1,4-Difluorobenzene	6.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, ethyl-	70	C5H10	001191-96-4	87
2	Cyclopropane, ethyl-	70	C5H10	001191-96-4	68
3	1-Pentene	70	C5H10	000109-67-1	64
4	Cyclobutane, methyl-	70	C5H10	000598-61-8	64
5	Cyclopropane, ethyl-	70	C5H10	001191-96-4	59





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU072120\
Data File : VU039611.D
Acq On : 21 Jul 2020 20:47
Operator : SY/MD
Sample : L3347-15
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GAY07

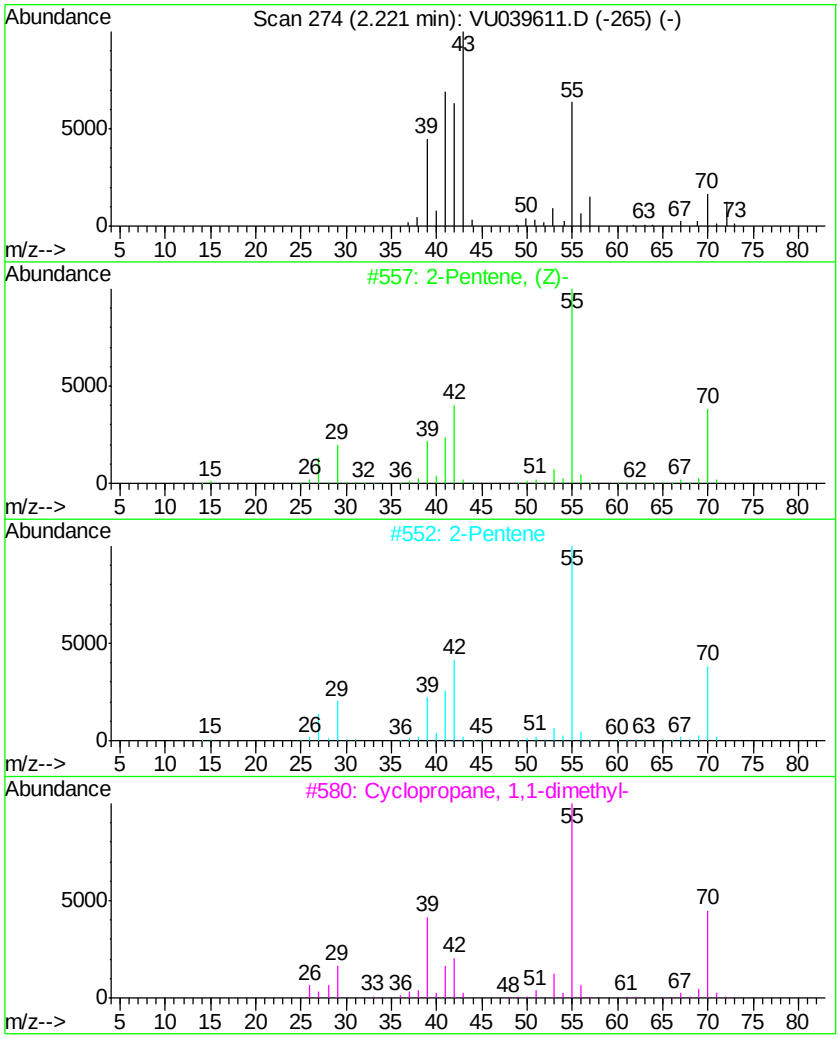
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR072120WMA.M
Quant Title : TRACE VOA SOM01.0

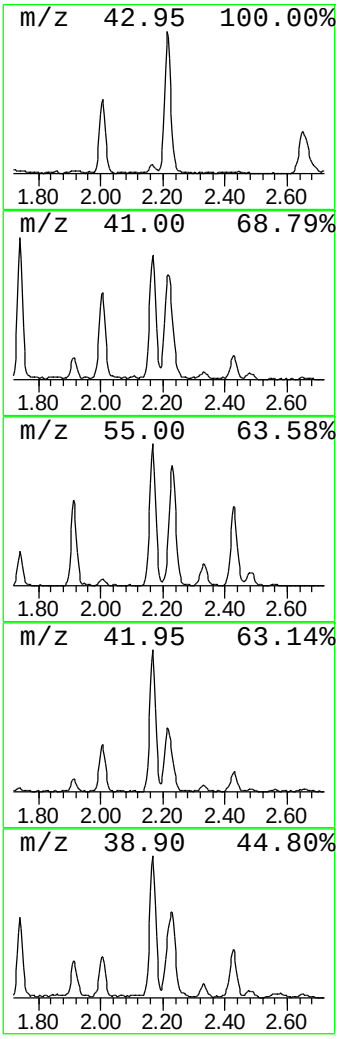
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.22	2.06 ug/L	119726	1,4-Difluorobenzene	6.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, (Z)-	70	C5H10	000627-20-3	50
2	2-Pentene	70	C5H10	000109-68-2	50
3	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	47
4	Pentane	72	C5H12	000109-66-0	47
5	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	43





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU072120\
Data File : VU039611.D
Acq On : 21 Jul 2020 20:47
Operator : SY/MD
Sample : L3347-15
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GAY07

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR072120WMA.M
Quant Title : TRACE VOA SOM01.0

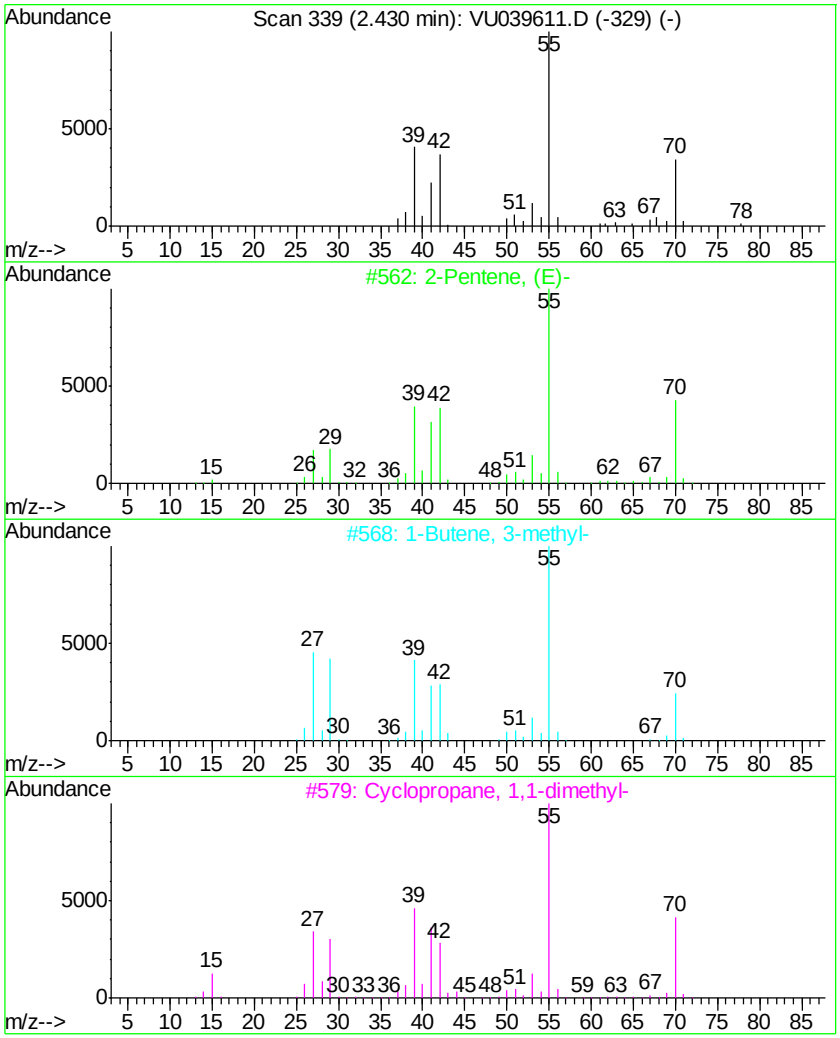
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

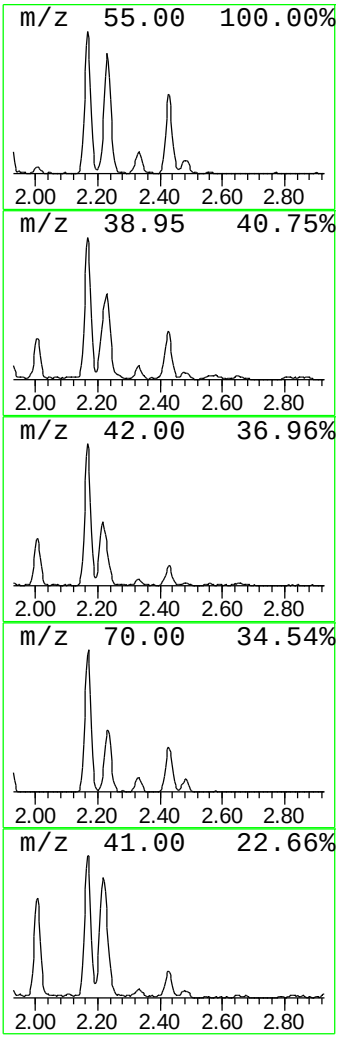
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.43	0.68 ug/L	39315	1,4-Difluorobenzene	6.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, (E)-	70	C5H10	000646-04-8	91
2	1-Butene, 3-methyl-	70	C5H10	000563-45-1	87
3	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	87
4	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	86
5	2-Butene, 2-methyl-	70	C5H10	000513-35-9	78





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

Instrument : MSVOA_U
ClientSampleId : GAY07

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR072120WMA.M
Quant Title : TRACE VOA SOM01.0

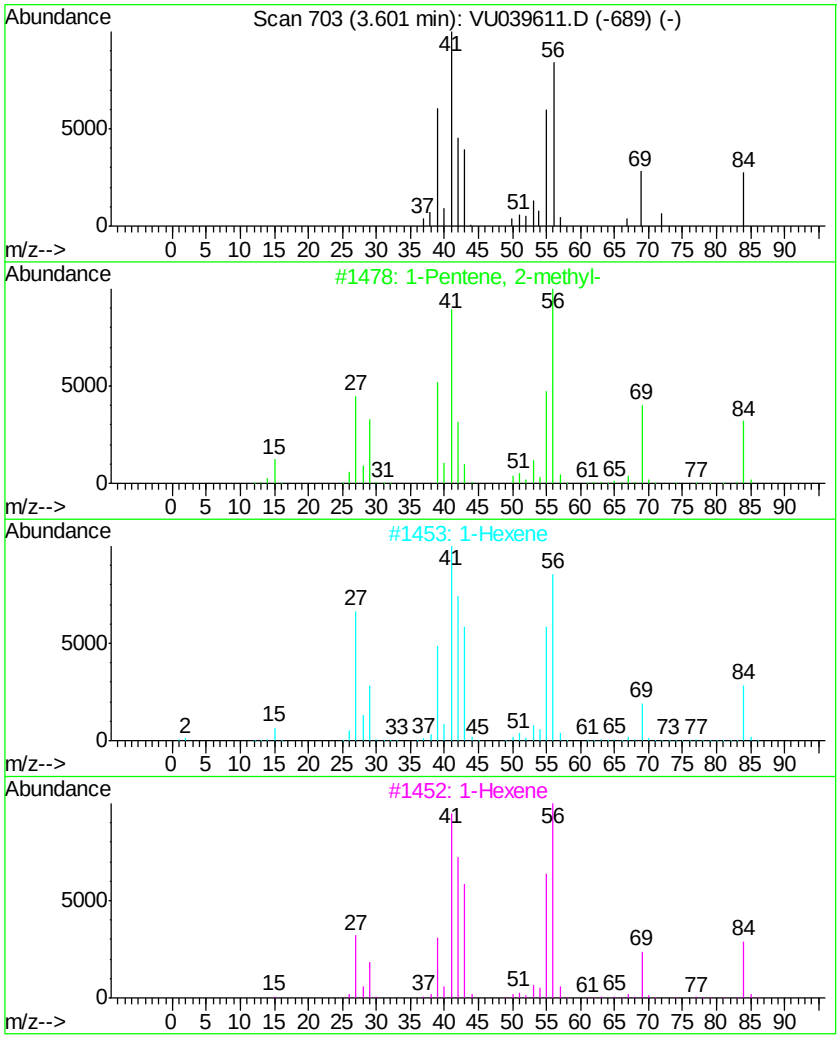
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

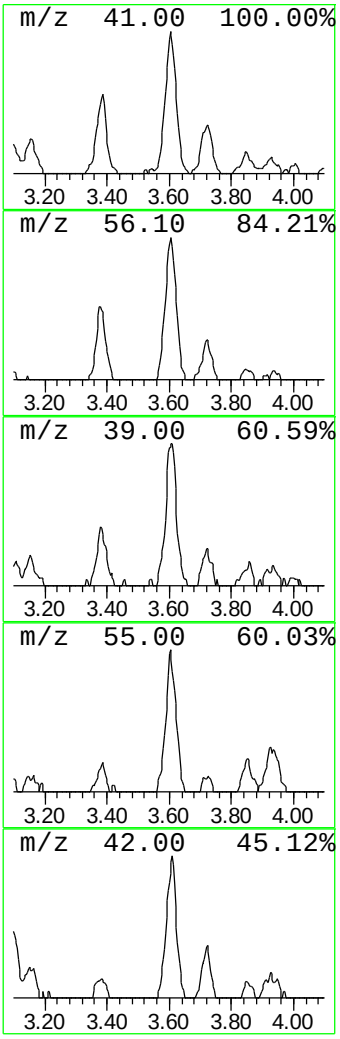
****

Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.60	1.01 ug/L	58989	1,4-Difluorobenzene	6.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	83
2	1-Hexene	84	C6H12	000592-41-6	76
3	1-Hexene	84	C6H12	000592-41-6	64
4	1-Hexene, 3,4-dimethyl-	112	C8H16	016745-94-1	47
5	1-Propene, 2-methyl-	56	C4H8	000115-11-7	43





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU072120\
Data File : VU039611.D
Acq On : 21 Jul 2020 20:47
Operator : SY/MD
Sample : L3347-15
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GAY07

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR072120WMA.M
Quant Title : TRACE VOA SOM01.0

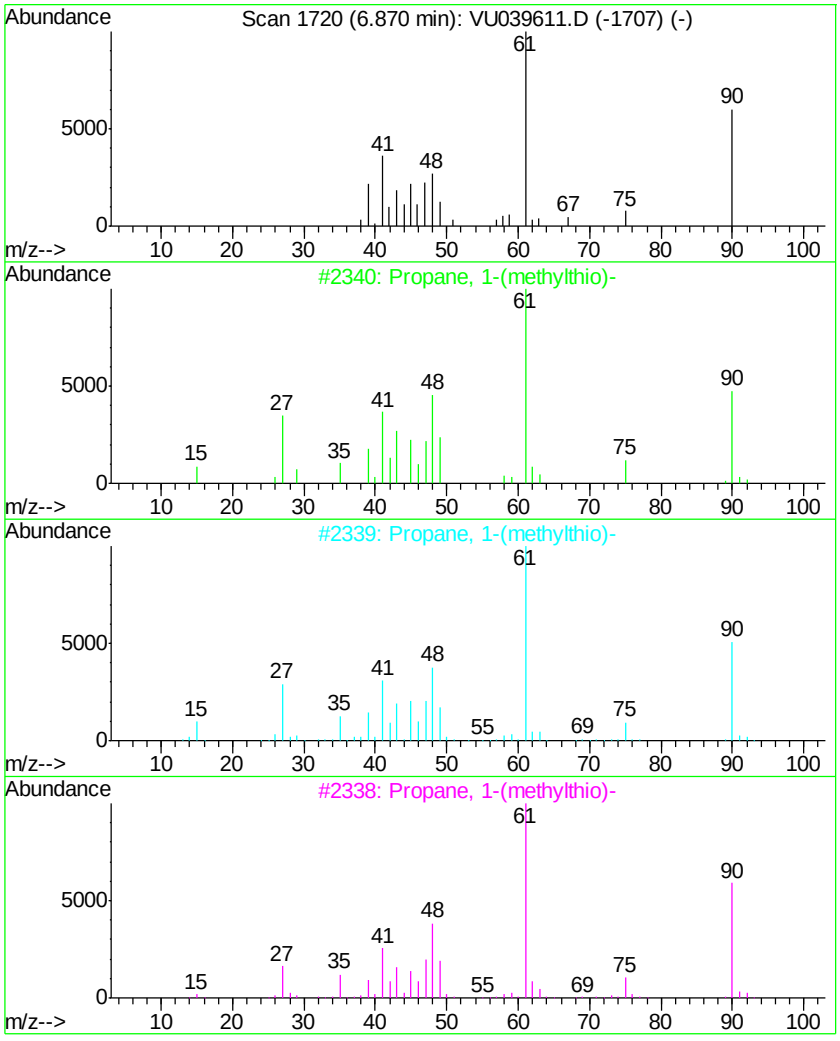
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

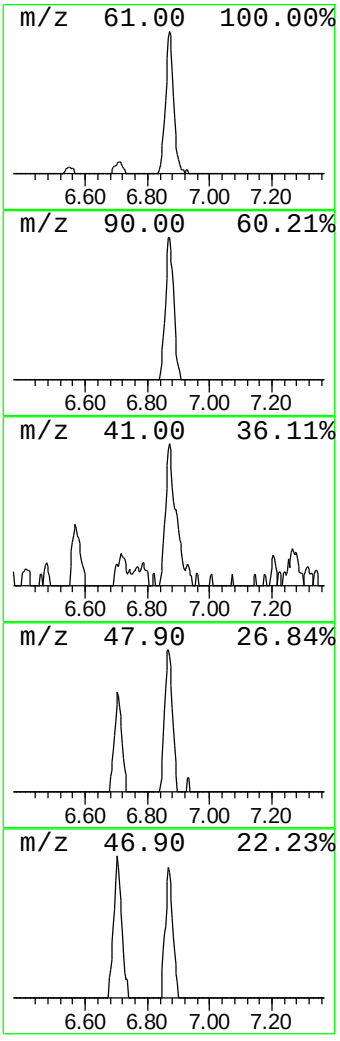
****

Peak Number 8 Propane, 1-(methylthio)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.87	0.52 ug/L	30341	1,4-Difluorobenzene	6.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1-(methylthio)-	90	C4H10S	003877-15-4	64
2	Propane, 1-(methylthio)-	90	C4H10S	003877-15-4	64
3	Propane, 1-(methylthio)-	90	C4H10S	003877-15-4	59
4	3-Thietanol	90	C3H6OS	010304-16-2	53
5	Propane, 1-(methylthio)-	90	C4H10S	003877-15-4	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU072120\
Data File : VU039611.D
Acq On : 21 Jul 2020 20:47
Operator : SY/MD
Sample : L3347-15
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GAY07

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR072120WMA.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...	1.50	0.5	ug/L	31399	1	6.27	290737	5.0
(DEL) Alkane: Str...	1.74	0.8	ug/L	46398	1	6.27	290737	5.0
(DEL) Alkane: Str...	2.01	0.9	ug/L	51730	1	6.27	290737	5.0
(DEL) Alkane: Cyc...	2.17	2.0	ug/L	113968	1	6.27	290737	5.0
(DEL) Alkane: Str...	2.22	2.1	ug/L	119726	1	6.27	290737	5.0
(DEL) Alkane: Str...	2.43	0.7	ug/L	39315	1	6.27	290737	5.0
(DEL) Alkane: Str...	3.60	1.0	ug/L	58989	1	6.27	290737	5.0
Propane, 1-(methy...	6.87	0.5	ug/L	30341	1	6.27	290737	5.0