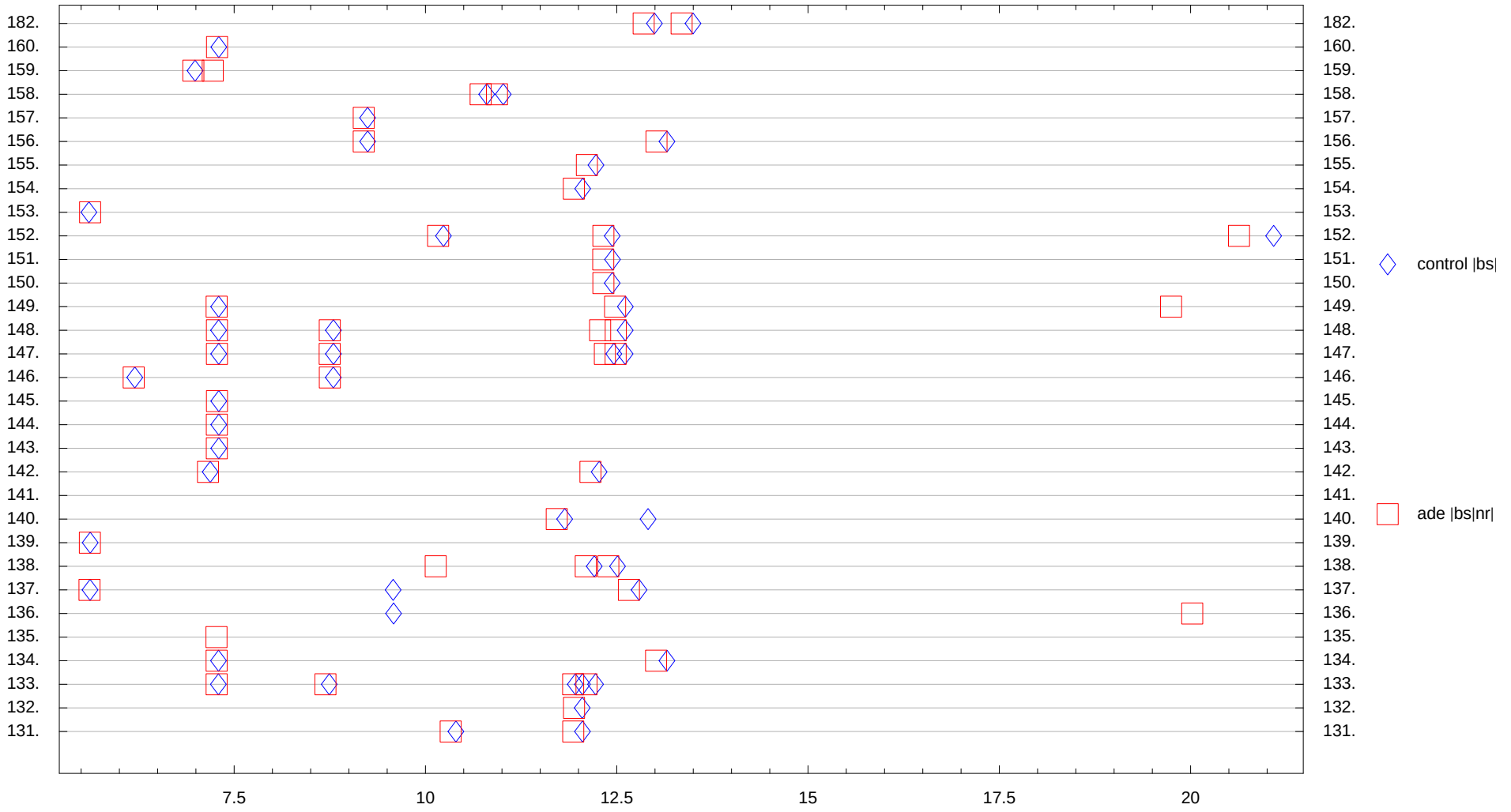
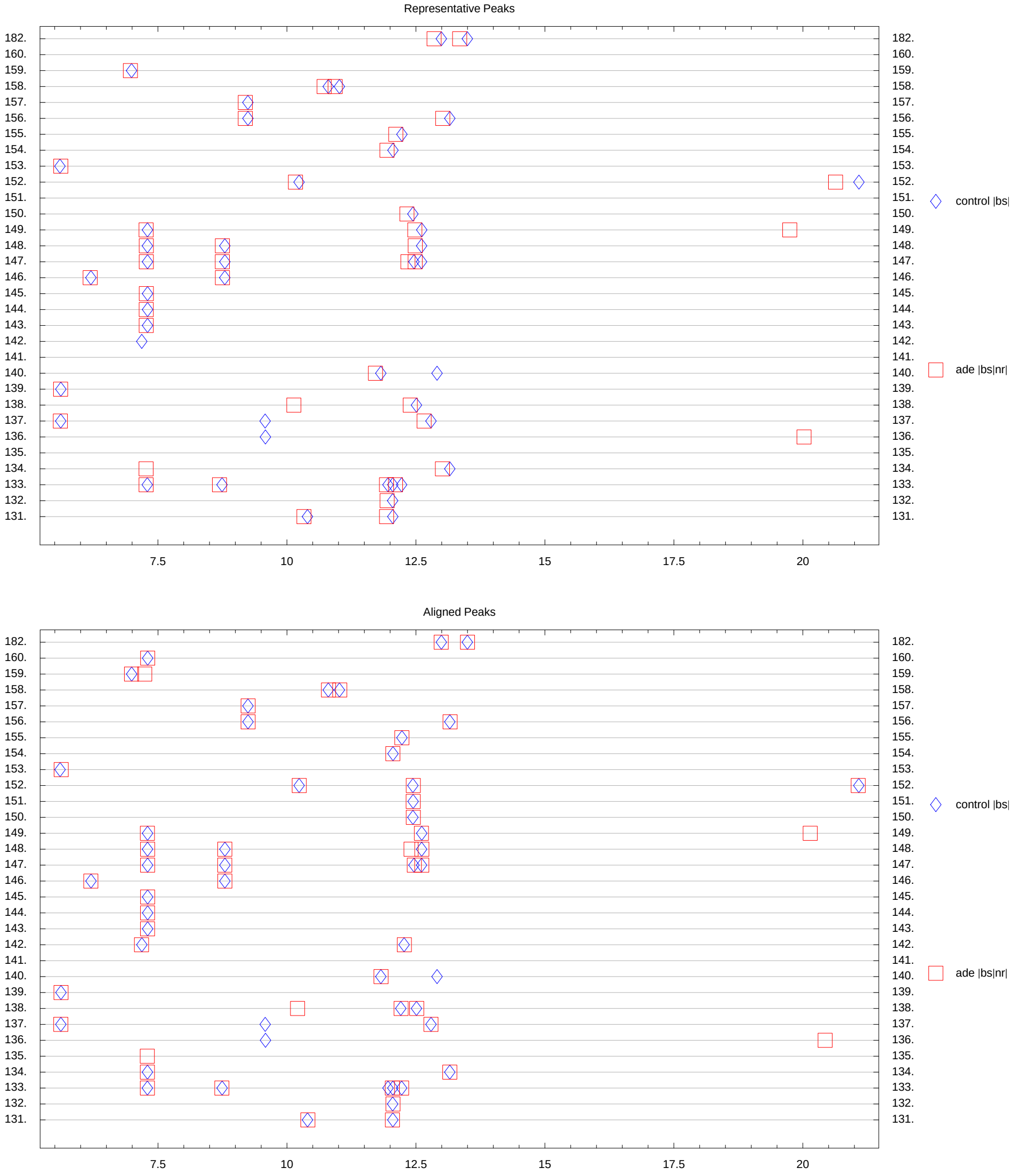
01−MathDAMP−QuickStart

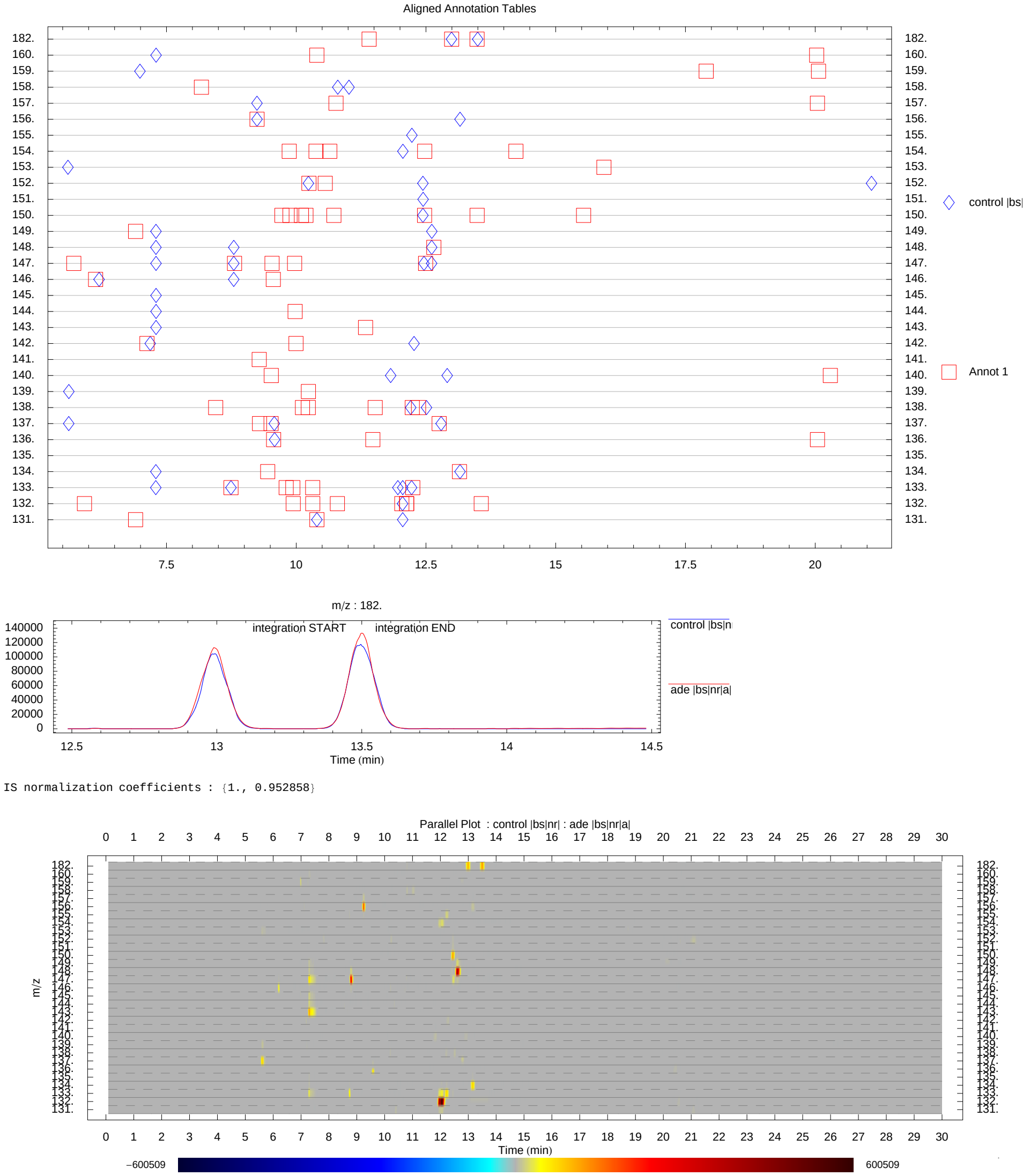
This notebook demonstrates the differential analysis of two datasets acquired by capillary electrophoresis coupled to a quadrupole mass spectrometer (CE−QMS) operated in selected ion monitoring (SIM) mode. The datafiles are part of the *Math*DAMP package. A parallel density plot of the two normalized datasets is shown along with a density plot representing the absolute×relative difference. Overlaid electropherograms in the vicinities of the most significant differences from the absolute×relative result are plotted as well. For a more in−depth step−by−step description of the procedure, please refer to the 03−MathDAMP−TwoDatasets.nb notebook.
Please assign the path leading to the *Math*DAMP files to the `MathDAMPPath` variable.

```
MathDAMPPath = "/home/baran/math/ms/MathDAMP.1.0.0/";
<< (MathDAMPPath <> "MathDAMP.m")
{ctrl, smpl} = DAMPImportMS[MathDAMPPath <> "/data/" <> #] & /@ {"control.ms", "sample.ms"};
{ppctrl, ppsmpl} = DAMPRemoveNoise[DAMPSubtractBaselines[#]] & /@ {ctrl, smpl};
rslt = DAMPTwoDatasets[ppctrl, ppsmpl, NormalizeGroupOptions → {InternalStandard → 363, AutoISIntegrationVicinity → {-.2, .2},
     AnnotationTables → {Select[DAMPLoadAnnotationTable[MathDAMPPath <> "/iab_cems_cation.csv"], MemberQ[ppctrl[[2]], 1. Round[#[[1]]] &]}}];
DAMPParallelPlot[NormalizedDatasets /. rslt];
DAMPDensityPlot[AbsoluteRelative /. rslt];
DAMPPlotCandidates[NormalizedDatasets /. rslt, AbsoluteRelative /. rslt,
  PlotCount → 12, PlotChromatogramOptions → {AnnotationTable → (AlignedAnnotationTables /. rslt)[[1]]}];
```

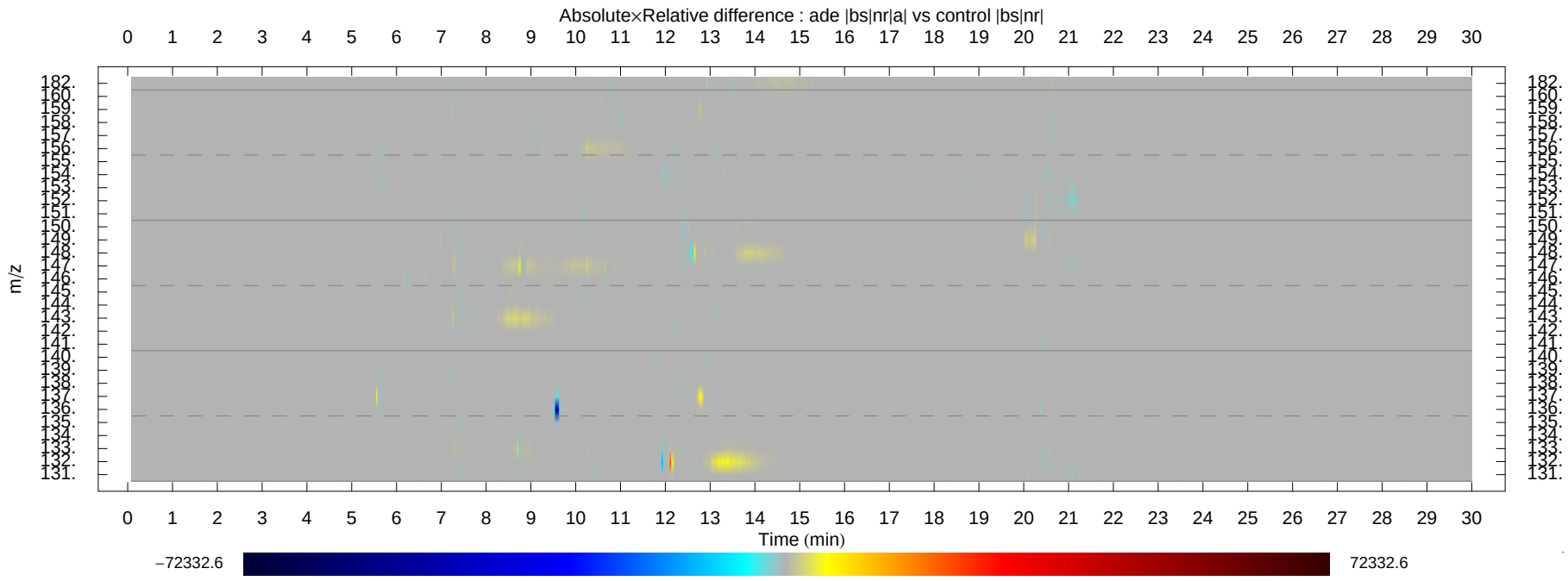
```
MathDAMP version 1.0.0 loaded (2006/04/26)

This program is distributed in the hope that it will be useful, but WITHOUT
  ANY WARRANTY; without even the implied warranty of MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE.
```



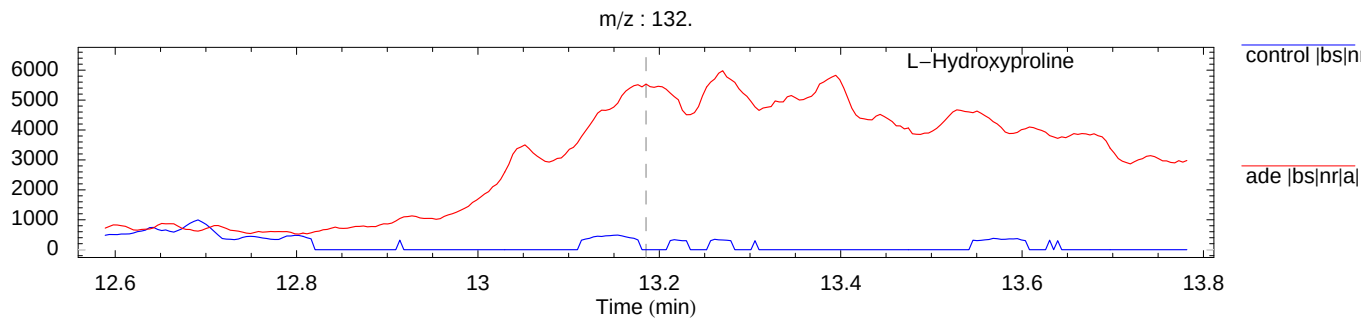

Representative Peaks
182.
160.
159.
158.
157.
156.
155.
154.
153.
152.
151.
150.
149.
148.
147.
146.
145.
144.
143.
142.
141.
140.
139.
138.
137.
136.
135.
134.
133.
132.
131.
7.5
10
12.5
15
17.5
20
control |bs|
ade |bs|nr|
Aligned Peaks
182.
160.
159.
158.
157.
156.
155.
154.
153.
152.
151.
150.
149.
148.
147.
146.
145.
144.
143.
142.
141.
140.
139.
138.
137.
136.
135.
134.
133.
132.
131.
7.5
10
12.5
15
17.5
20
control |bs|
ade |bs|nr|

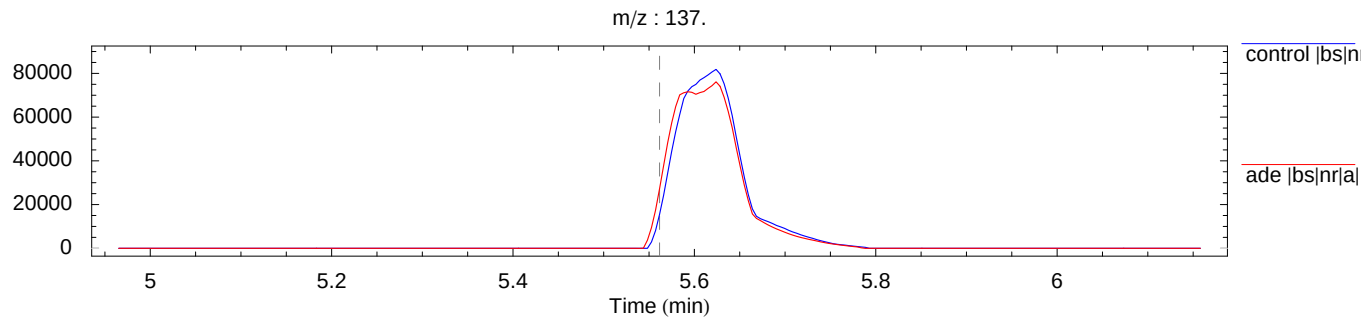


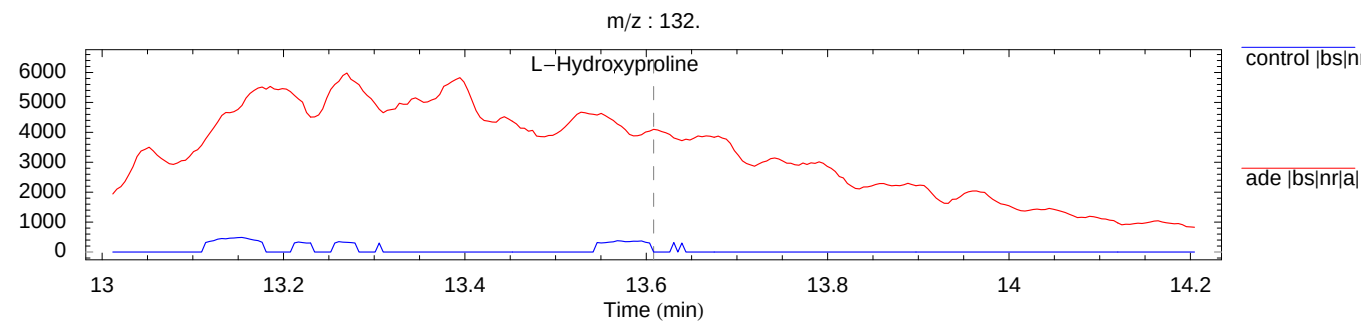
IS normalization coefficients : {1., 0.952858}

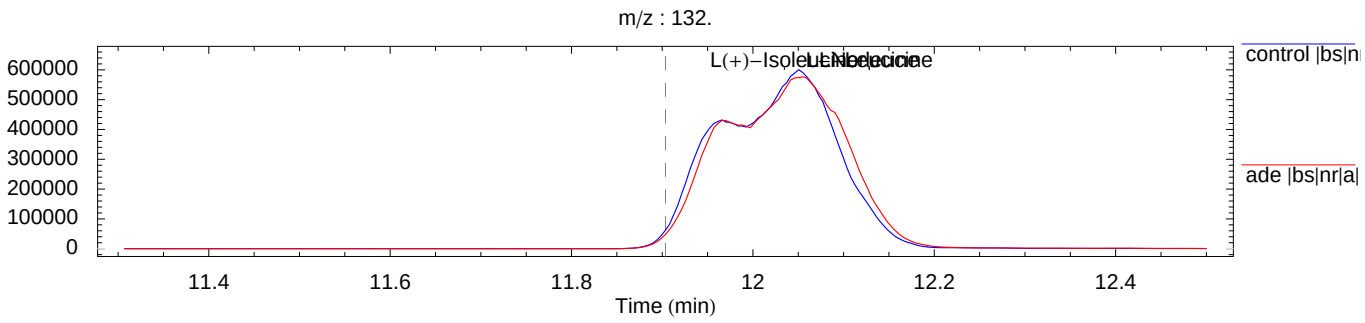

Absolute×Relative difference : ade |bs|nr|a| vs control |bs|nr|
m/z
Time (min)
−72332.6
72332.6

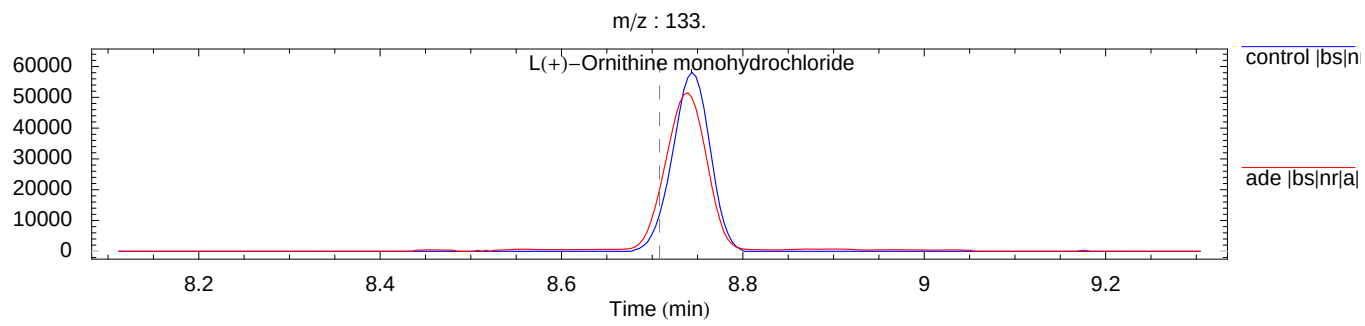
m/z : 136.
Adenine
Time (min)
control |bs|n
ade |bs|nr|a|
m/z : 132.
L(+)−Isoleucine
L−Leucine
Time (min)
m/z : 147.
L−Lysine
Time (min)
m/z : 137.
Hypoxanthine
Time (min)
m/z : 148.
L−Glutamate
Time (min)
m/z : 132.
L−Hydroxyproline
Time (min)

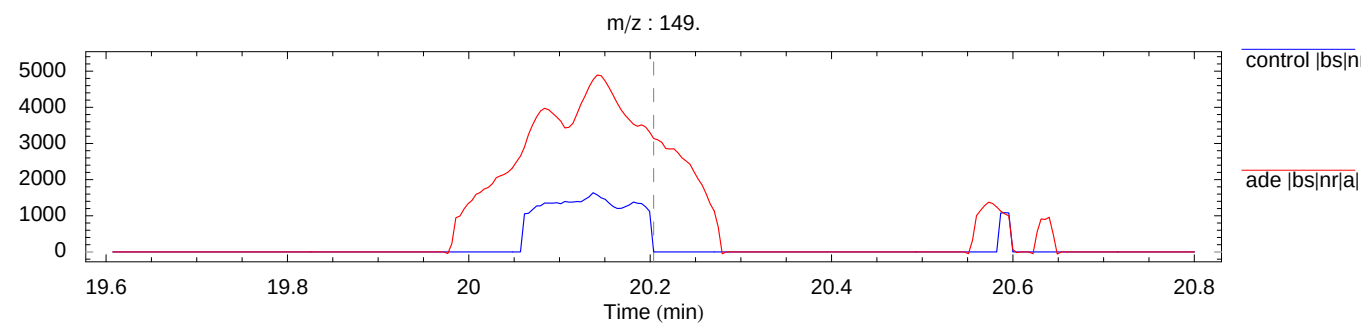

m/z : 132.
L−Hydroxyproline
6000
5000
4000
3000
2000
1000
0
12.6
12.8
13
13.2
13.4
13.6
13.8
Time (min)
control |bs|n
ade |bs|nr|a|


m/z : 137.
80000
60000
40000
20000
0
5
5.2
5.4
5.6
5.8
6
Time (min)
control |bs|n
ade |bs|nr|a|


m/z : 132.
L−Hydroxyproline
6000
5000
4000
3000
2000
1000
0
13
13.2
13.4
13.6
13.8
14
14.2
Time (min)
control |bs|n
ade |bs|nr|a|


m/z : 132.
600000
500000
400000
300000
200000
100000
0
11.4
11.6
11.8
12
12.2
12.4
Time (min)
control |bs|n
ade |bs|nr|a|


m/z : 133.
L(+)−Ornithine monohydrochloride
60000
50000
40000
30000
20000
10000
0
8.2
8.4
8.6
8.8
9
9.2
Time (min)
control |bs|n
ade |bs|nr|a|


m/z : 149.
5000
4000
3000
2000
1000
0
19.6
19.8
20
20.2
20.4
20.6
20.8
Time (min)
control |bs|n
ade |bs|nr|a|