Columns

D MZ

Meta information

Num ID of the detected feature pair. Arbitrary. Only

valid in this column and cannot be used to reference the feature pair in the different

chromatograms

MZ The m/z value of the monoisotopic, native feature L MZ The m/z value of the labeled feature. Theoretical

The m/z difference between MZ and L_MZ.

Theoretical

RT The retention time of the feature pair. It is

determined as the most abundant scan for the chromatographic peak of the monoisotopic, native

feature

Xn The number of labeling atoms

Charge The number of charges of this feature pair.

Determined by the difference between the native

and the labeled feature

ScanEvent The HRMS scan event in which this feature pair

was detected

Ionisation Mode The ionization mode this feature pair was detected

in

Tracer The tracer used for the experiment.

OGroup ID of the feature group this feature pairs was

assigned to. All rows (i.e. feature pairs) with the same ID in the column OGroup are ions of the

same metabolite.

Sample information For each sample the following 4 columns are saved

<SampleName>_Area_N
The peak area of the monoisotopic, native feature

<SampleName>_Area_L
The peak area of the labeled feature

<SampleName>_FID
The ID of the feature pair in the respective file.

They are only unique in this file and cannot be referenced to the Num column in the meta

information

<SampleName>_GroupID
The feature group ID of the feature pair in the

respective file. They are only unique in this file and cannot be referenced to the OGroup column in the

meta information

At the bottom of the list of the detected feature pairs the most important data processing parameters are saved as comments starting in the column Num with a #-symbol.