Columns

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| --- | --- |
| 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 |
| D\_MZ | 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.