

Manual for the alignment data

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1. About “alignment”

The term “alignment” represents here the calculation to match the same chemical peak with a similar m/z value and retention time among the multiple samples. The dataset provided here is the alignment results calculated using data from all samples deposited in the database as tables containing sample vs. unique peak information.

Note:

The alignment results may include false results of misalignment. For example, a single chemical that is shared in a large number of samples may be separated into two unique alignments due to subtle fluctuations in retention time.

1.1. Alignment method

The PowerGetBatch software 0.6.5 was used for the alignment. The software is available on the website below.

<https://sakura-kagaku.net/komics/software/PowerGetBatch/>

The parameter settings used for the alignment are available in the file align_parameters.txt. The same setting was used for ESI positive and negative modes.

2. Details of data files

The folders “pos” and “neg” include the results from ESI positive and negative modes, respectively. Each folder contains the following seven files in tab-separated text format.

File name	Description
Adduct.txt	Predicted adduct ion

Charge.txt	Estimated charge
ID.txt	Peak IDs in each sample data
Int.txt	Peak intensity in linear scale
IntLog.txt	Peak intensity in log10 scale (centered by the median of each sample)
Mz.txt	<i>m/z</i> value
Rt.txt	Retention time

Data structure of each file:

Column	Header	Description
1	No	The alignment ID
2	Ave.RT	The averaged retention time (min) of the aligned peak(s)
3	Ave.m/z	The averaged <i>m/z</i> value of the aligned peak(s)
4	Ave.Int	The averaged peak intensity of the aligned peak(s) in linear scale
5-	[Sample ID]_[File name]*	The peak values. A blank represents that the sample does not contain the peak

* The [File name] includes the detection polarity P: positive or N: negative and the shortened sample name, which would help distinguish the samples.