`idpp.msms`

subpackage for code related to MS/MS stuff

Module Reference

Spectra

module with functions for comparing or combining spectra

`spec_norm`

`idpp.msms.spectra.spec_norm`(*spectrum*)

normalize spectrum such that all intensities sum to 1

Parameters: spectrum : `list(list(float))`

MS/MS spectrum as list of [[m/z values...], [intensities...]]

Returns: spectrum : `numpy.ndarray()`

normalized MS/MS spectrum with same shape as input

`spec_entropy`

`idpp.msms.spectra.spec_entropy`(*spectrum*)

compute spectral entropy for single spectrum

Parameters: spectrum : `list(list(float))`

MS/MS spectrum as list of [[m/z values...], [intensities...]]

Returns: entropy : `float`

spectral entropy

`spec_entropy_similarity`

`idpp.msms.spectra.spec_entropy_similarity`(*spectrum_A, spectrum_B*)

pairwise spectral entropy based similarity as defined in the paper:

https://www.nature.com/articles/s41592-021-01331-z

Parameters: spectrum_A, spectrum_B : `numpy.ndarray()`

input MS/MS spectra (2D arrays with shape (2, n_points)) to compare

Returns: similarity : `float`

spectral entropy similarity score

`spec_combine`

`idpp.msms.spectra.spec_combine`(*spectra: List[ndarray[Any, dtype[_ScalarType_co]]], weights: List[float], mztol: float = 0.05*)→ ndarray[Any, dtype[_ScalarType_co]]

combine multiple spectra into a single spectrum

Parameters:

spectra : `list(numpy.ndarray())`

list of MS/MS spectra (2D arrays with shape (2, n_points)) to combine

weights : `list(float)`

weights for each spectrum

mztol : `float`, default=0.05

m/z tolerance for combining m/z peaks from different spectra

Returns:

comb_spectrum : `numpy.ndarray()`

combined MS/MS spectrum (shape: (2, n_points))