SCIENCE MEETS LIFE

MS^2 peak intensity prediction for specific PTMs, fragmentation techniques and instruments

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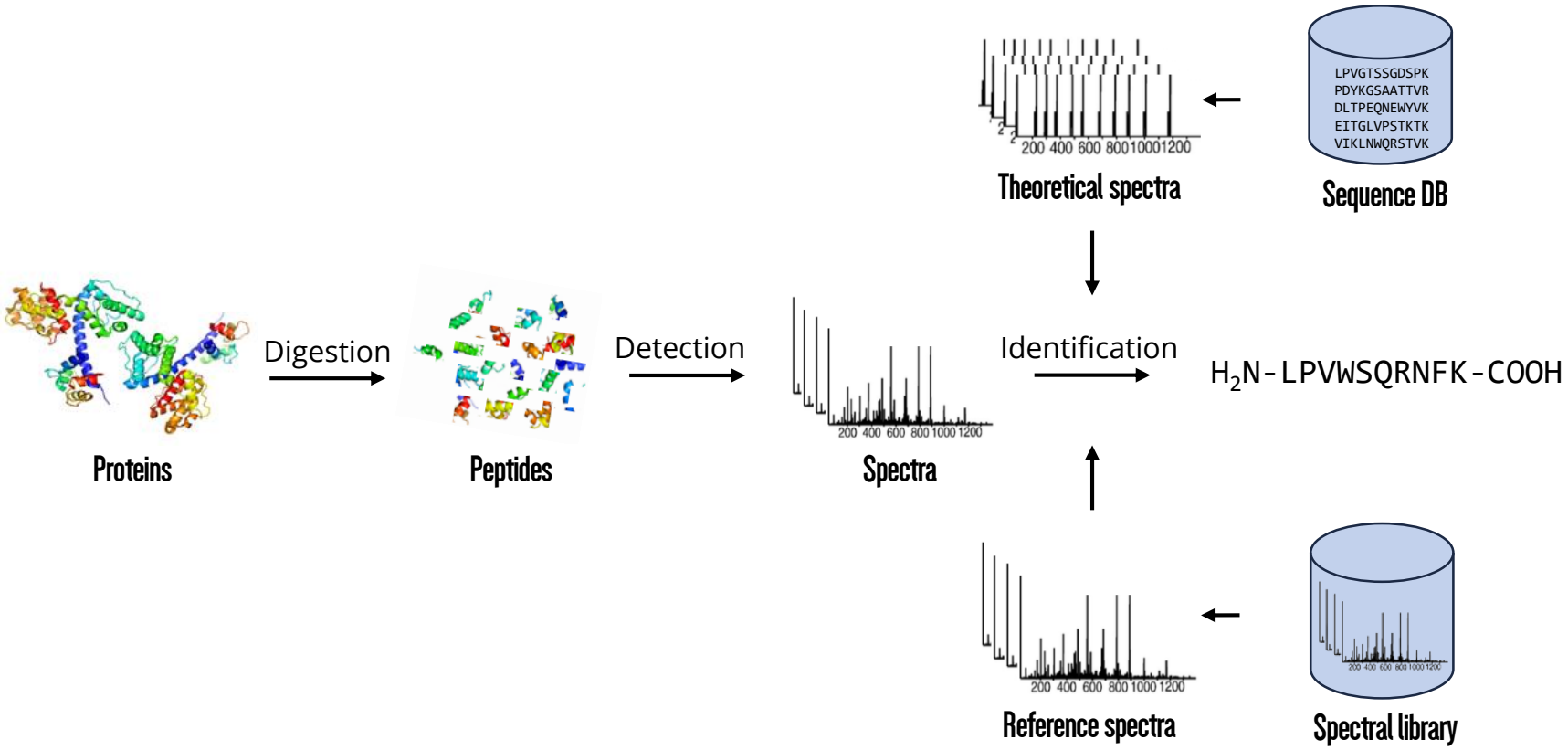
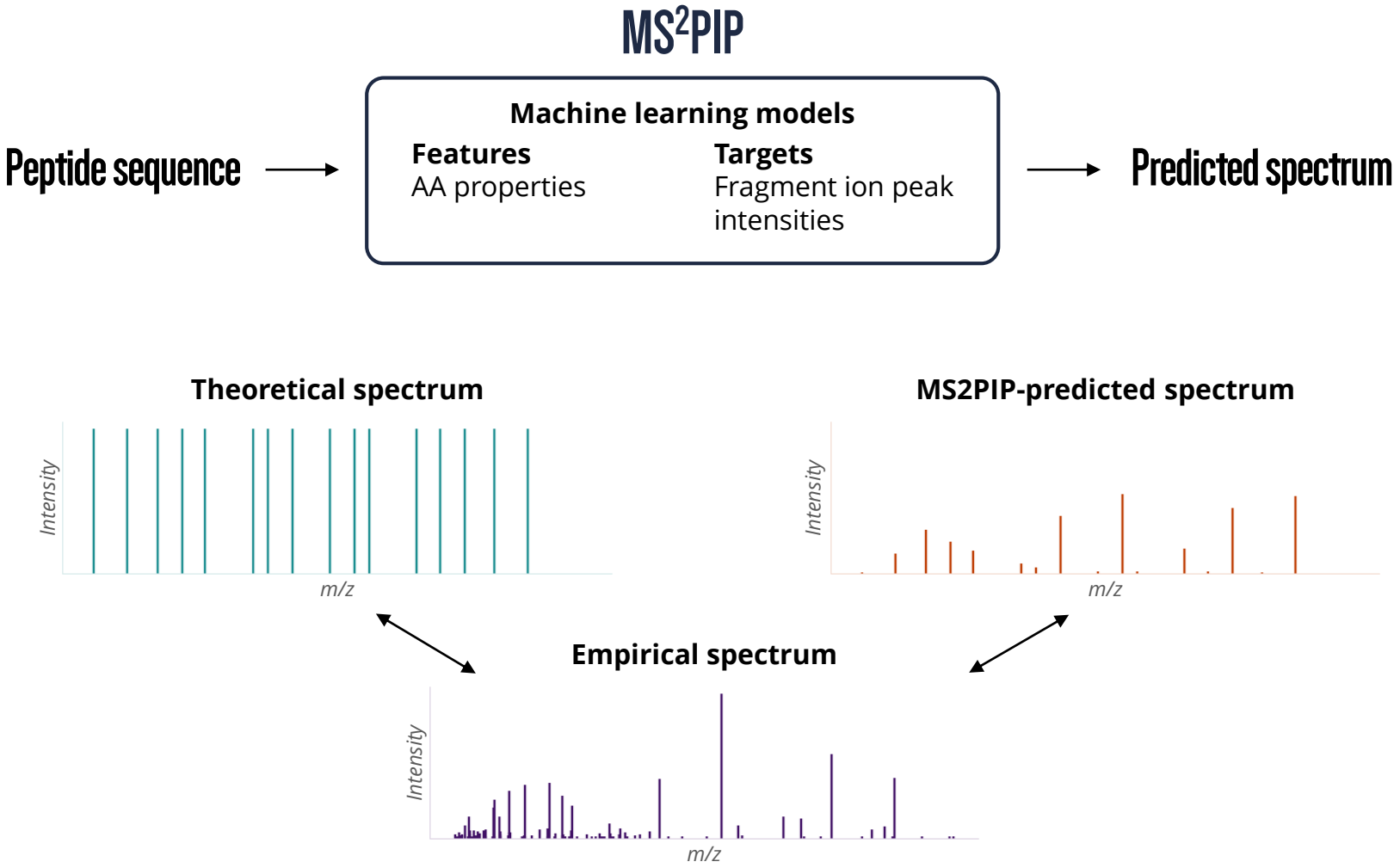
26/09/2018

f-TALES - Big Data in Life Sciences and Biomedicine

MS² peptide spectra are identified using sequence databases or spectral libraries



MS²PIP combines the best of both worlds



We are all trained to recognize people

Image adapted from www.freepik.com/free-vector/casual-characters_774641.htm

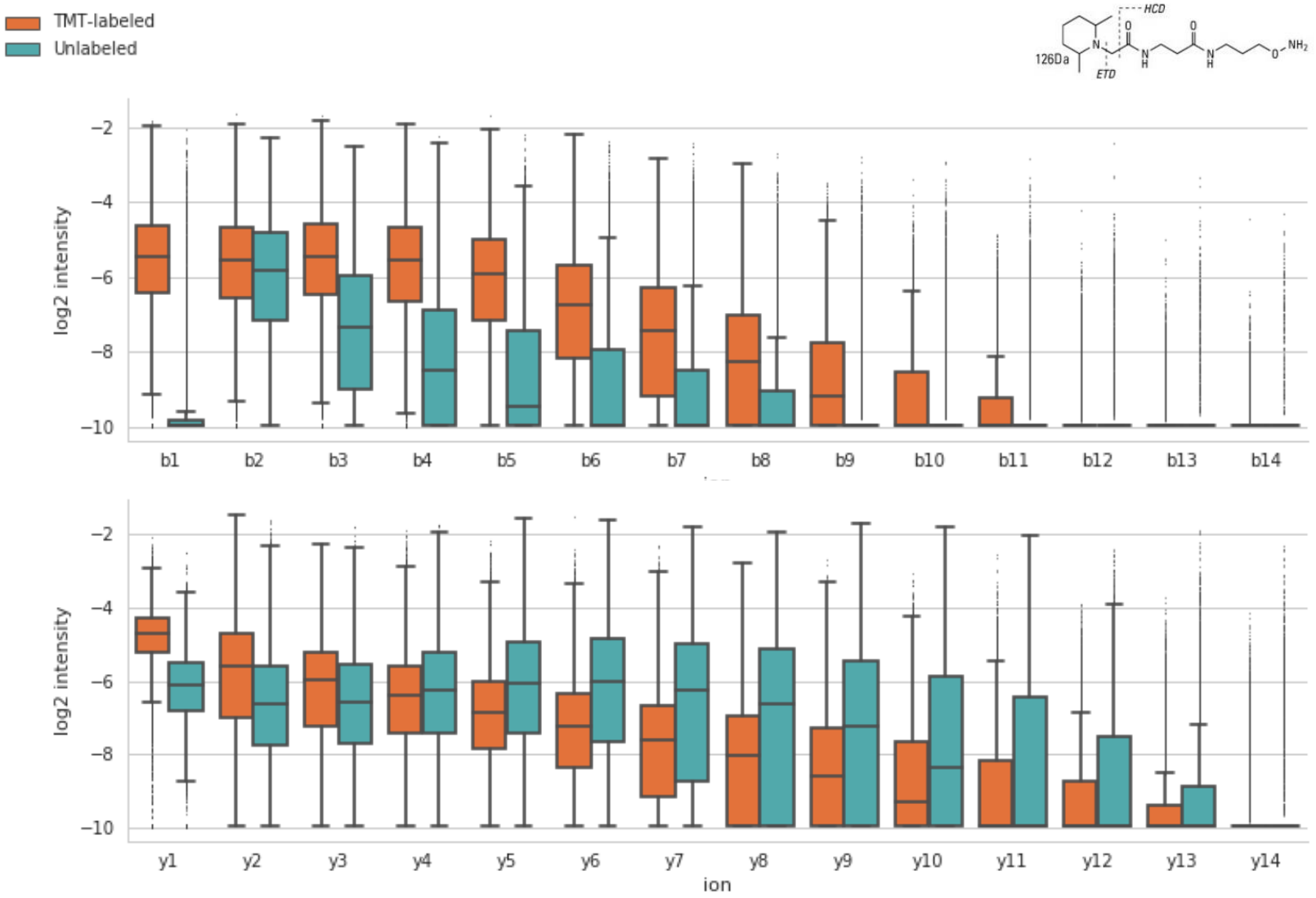
However, recognizing penguins is not as easy

Image adapted from www.sciencing.com

Unless you are a trained zookeeper

Image adapted from www.kisspng.com/png-rico-kowalski-skipper-penguin-madagascar-penguins-819595

TMT-spectra are the proverbial penguins

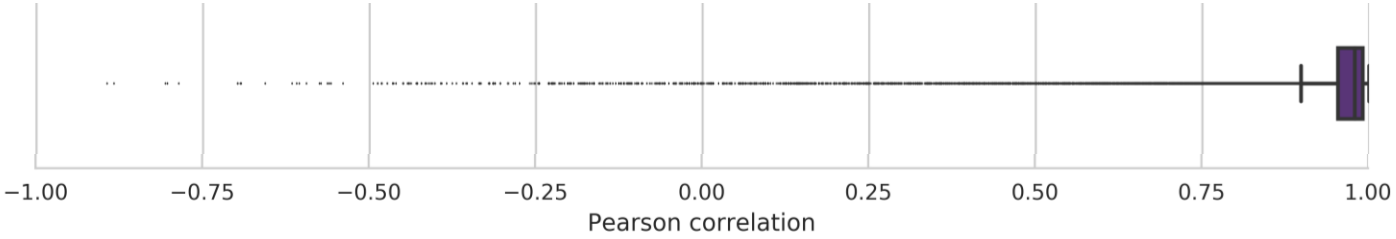


TMT structure adapted from www.thermofisher.com/order/catalog/product/90401

The solution is to retrain MS²PIP on the appropriate MS² spectra

Dataset	Source	Reference	# Peptides
Train data	TMT Spectral library (90%)	Shen J. et al. Journal of Proteome Research (2018)	492 083
External unseen TMT data	TMT experiment	Kris Gevaert Lab, VIB-UGent	45 015
Unlabeled reference dataset	Unlabeled experiment	Chick J.M. et al. Nature Biotechnology (2015)	14 256

TMT model performance is only limited by the technical variation



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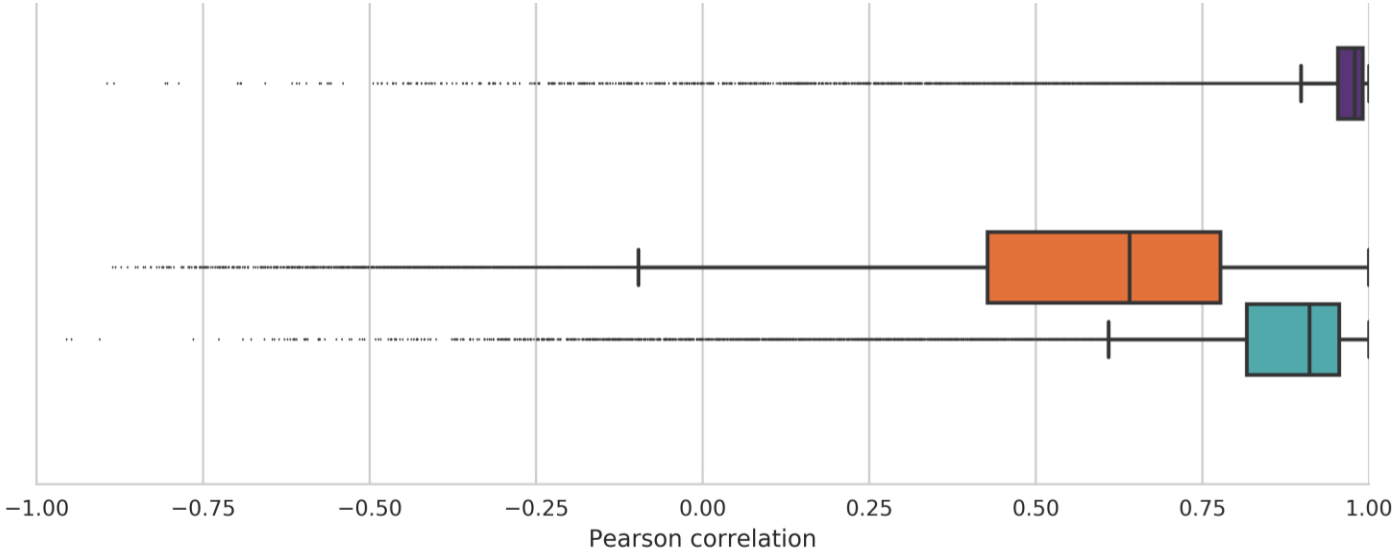

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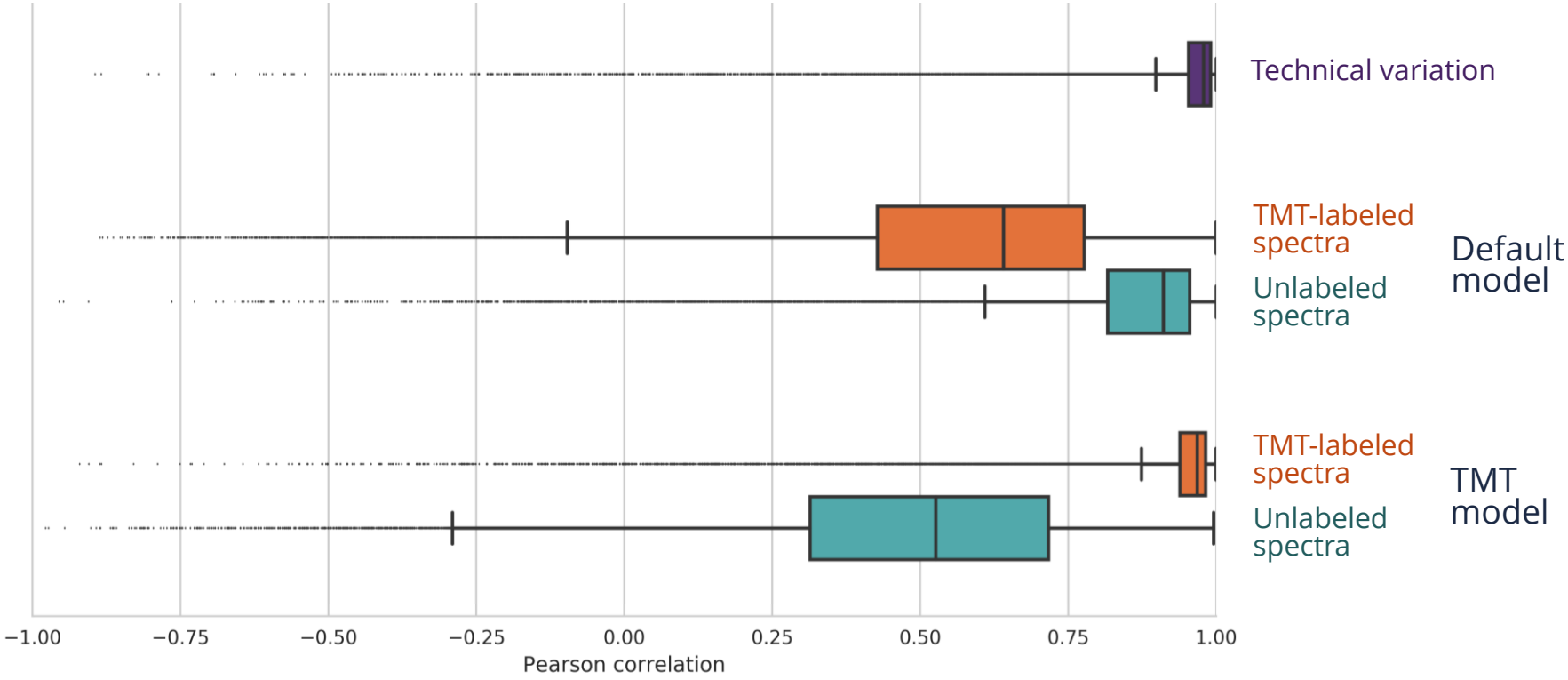
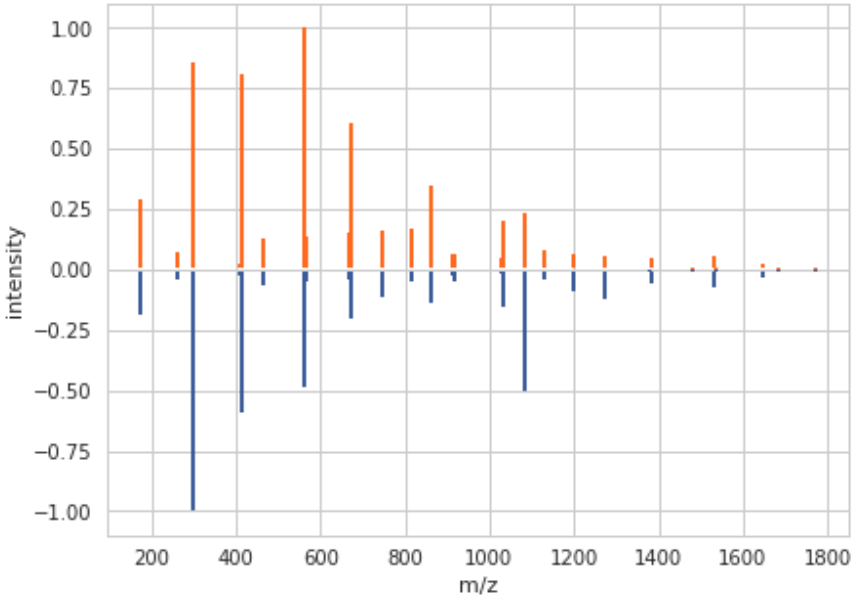


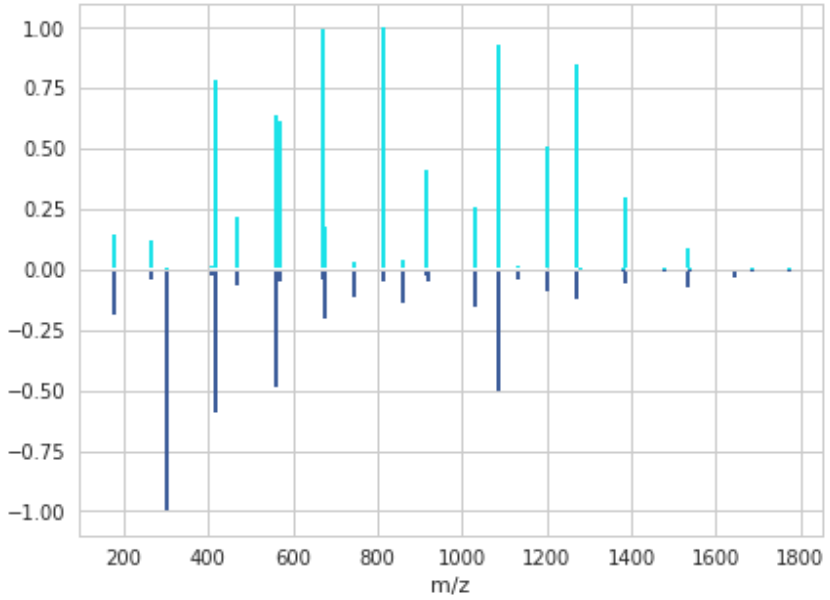
Some example spectra

TMT model prediction



Empirical TMT spectrum

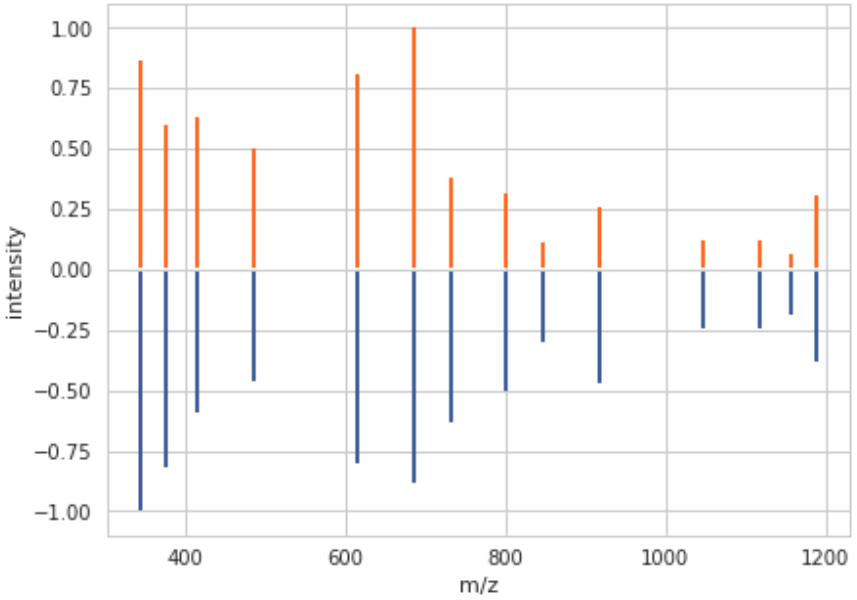
Default MS²PIP prediction



Empirical TMT spectrum

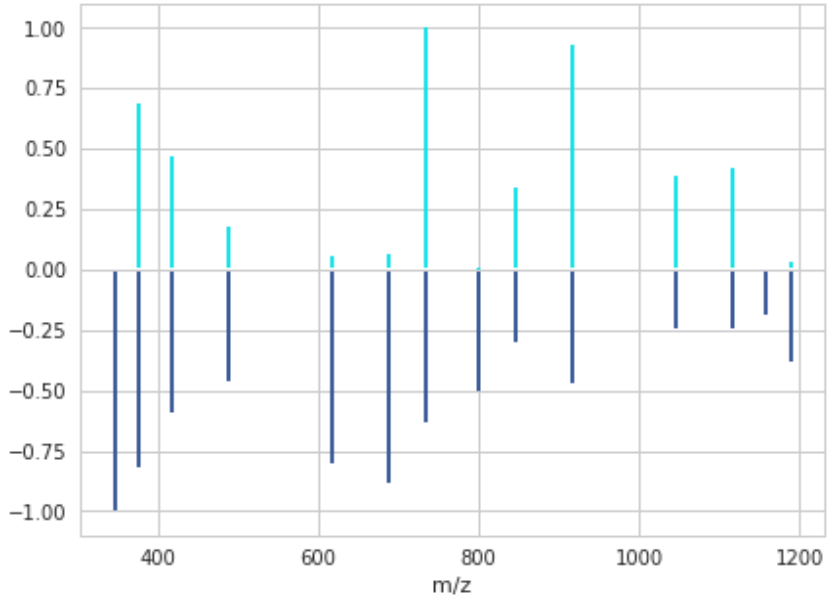
Some example spectra

TMT model prediction



Empirical TMT spectrum

Default MS²PIP prediction



Empirical TMT spectrum

Many other specific models can be trained

TTOF5600 instruments

ET(hc)D fragmentation

Phosphorylation

Non-tryptic (immuno-) peptides

All models are (or will be) available on the user-friendly MS²PIP Server

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iomics.ugent.be/ms2pip

MS²PIP SERVER

MS² Peak Intensity Prediction

MS²PIP is a tool to predict MS² signal peak intensities from peptide sequences. It employs the XGBoost machine learning algorithm and is written in Python.

You can install MS²PIP on your machine by following our extended install instructions found on the MS²PIP GitHub repository. For a more user friendly experience, we created this web server. Below, you can easily upload a list of peptide sequences, after which the corresponding predicted MS² spectra can be downloaded in a CSV or MGF file format.

More advanced users can also access MS²PIP Server through our RESTful API. Swagger-generated documentation can be found here and an example Python script to access the API can be found here.

If you use MS²PIP for your research, please cite the following papers:

- Degroeve, S., Maddelein, D., & Martens, L. (2015). MS²PIP prediction server: compute and visualize MS2 peak intensity predictions for CID and HCD fragmentation. *Nucleic Acids Research*, *43*(W1), W326–W330.

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