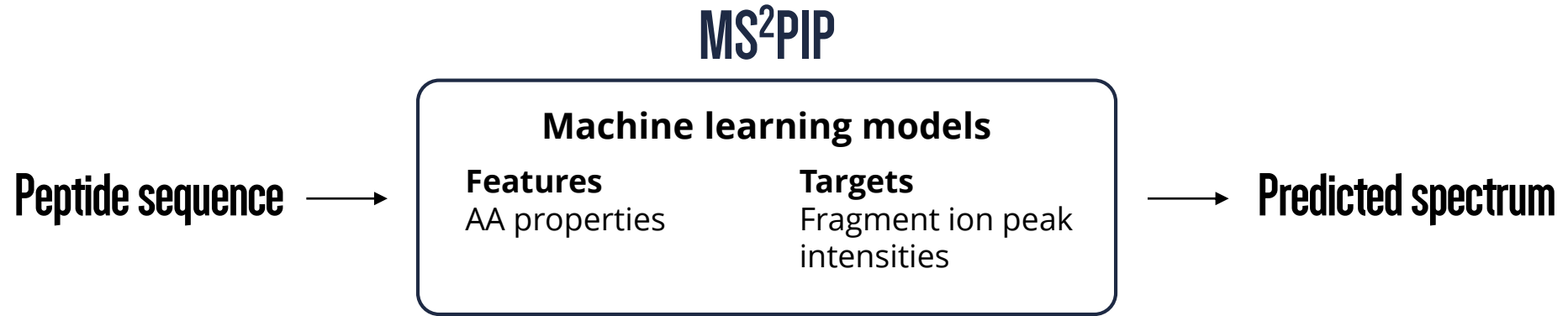


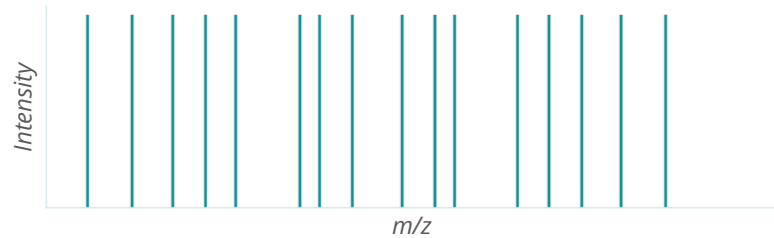
Fast and accurate MS² peak intensity prediction for multiple fragmentation methods, instruments and labeling techniques

Ralf Gabriels

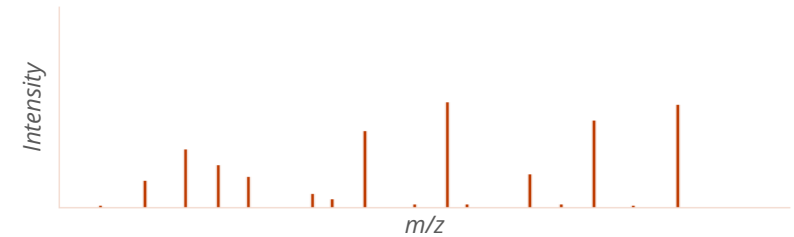
MS²PIP: MS² Peak Intensity Prediction



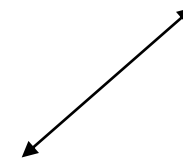
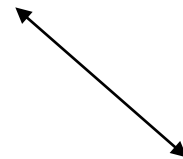
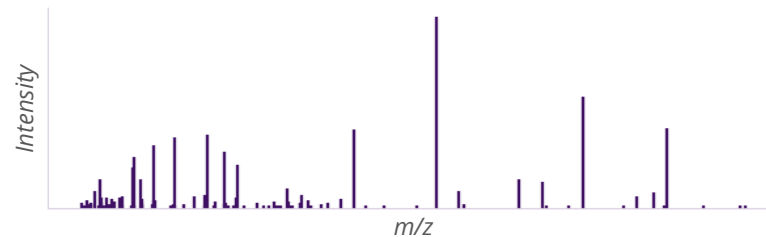
Theoretical spectrum



MS²PIP-predicted spectrum



Empirical spectrum



We are all trained to recognize people



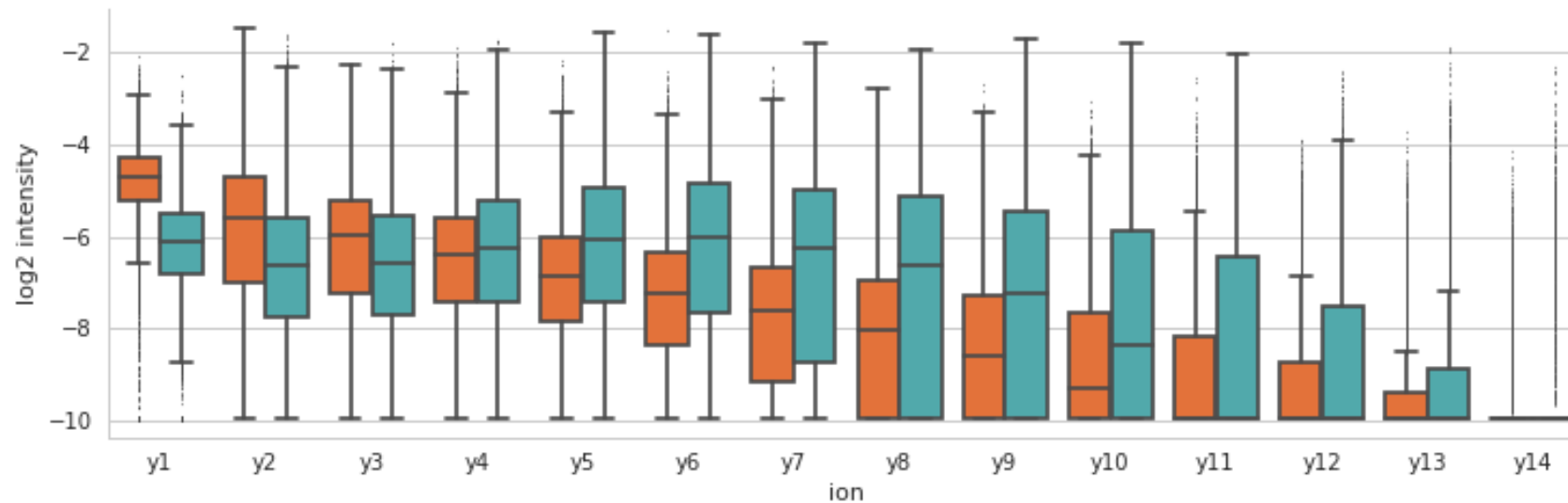
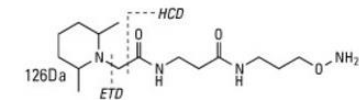
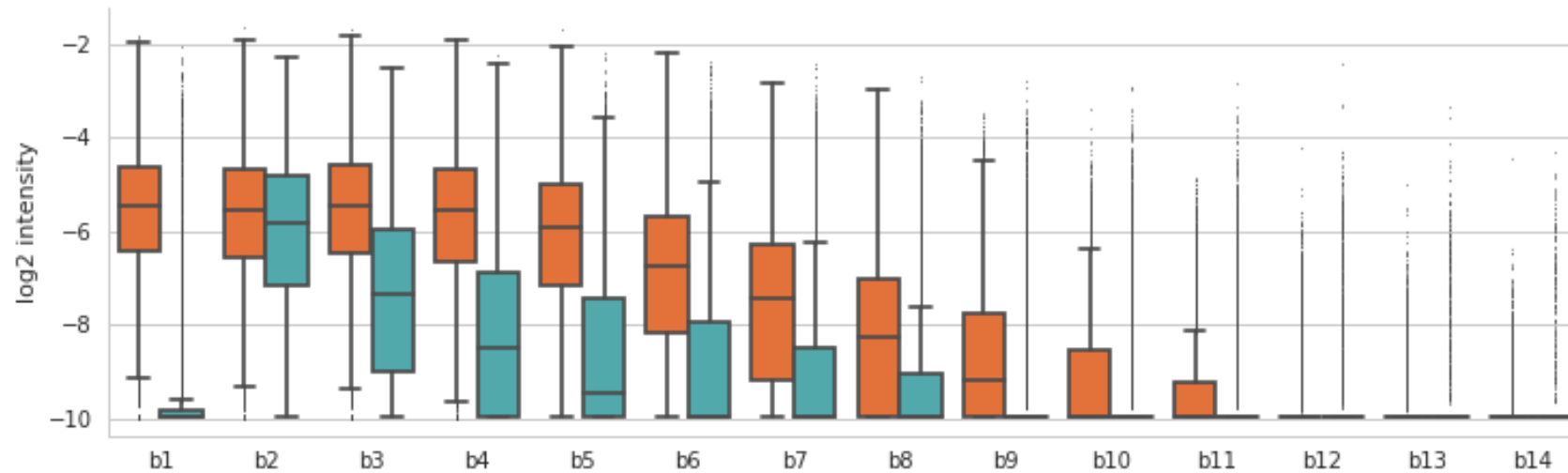
However, recognizing penguins is not as easy



Unless you are a trained zookeeper

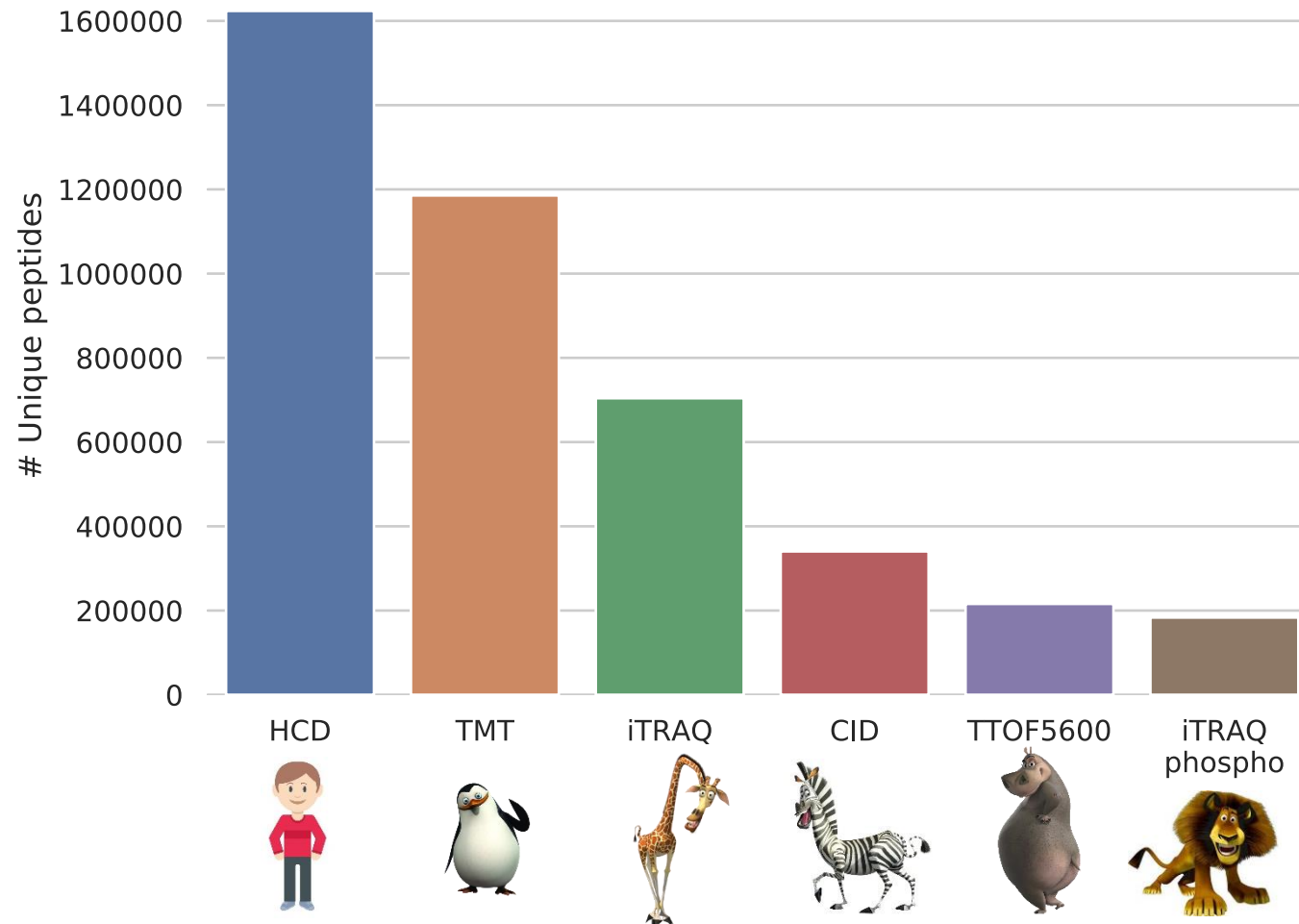


Specific fragmentation methods, instruments and labeling techniques are the proverbial penguins



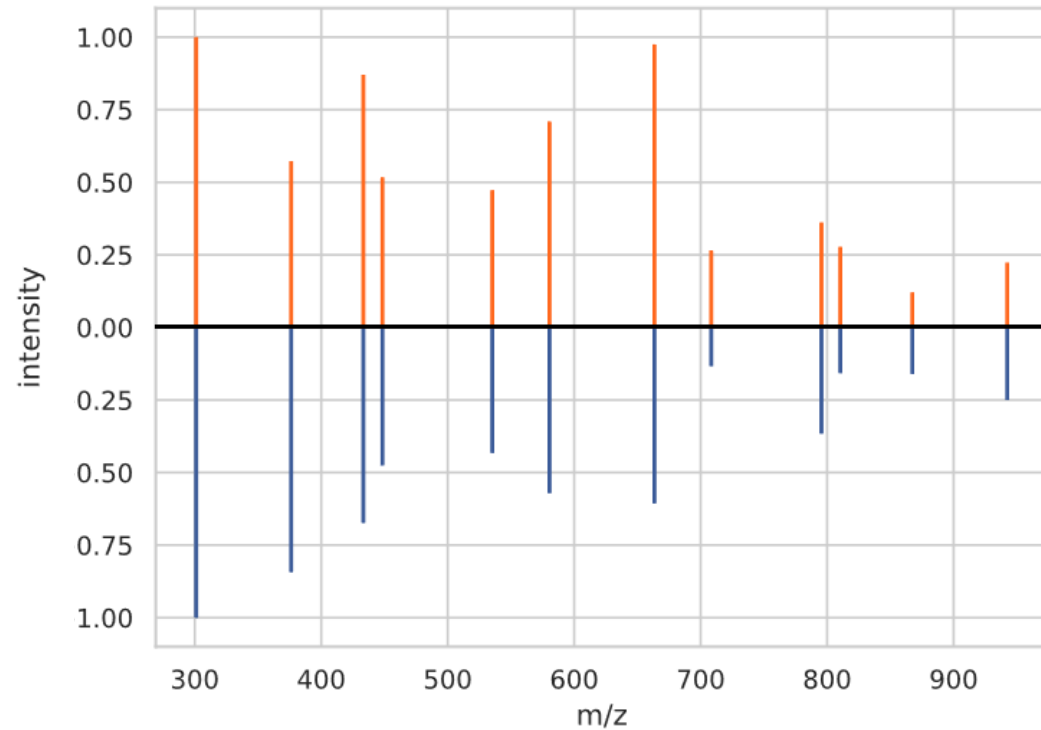
Legend:
TMT-labeled (orange)
Unlabeled (teal)

We retrained MS²PIP for these specific cases using publicly available datasets



Model performance is measured by calculating the Pearson correlations with empirical spectra

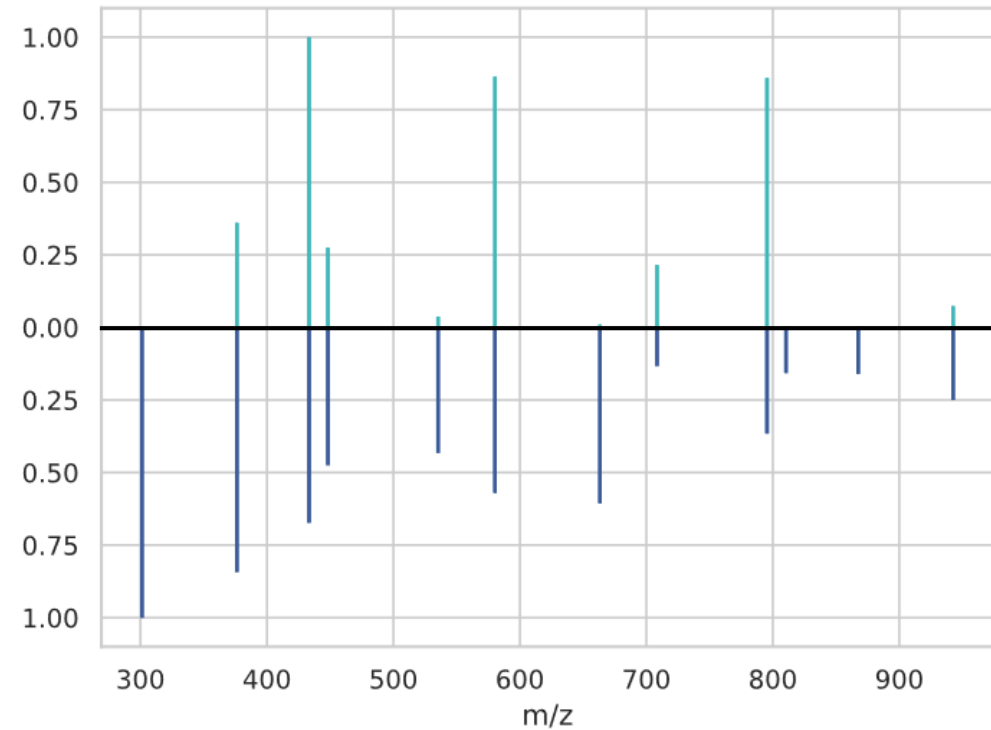
Prediction TMT model



Empirical TMT spectrum

→ Pearson correlation = 0.85

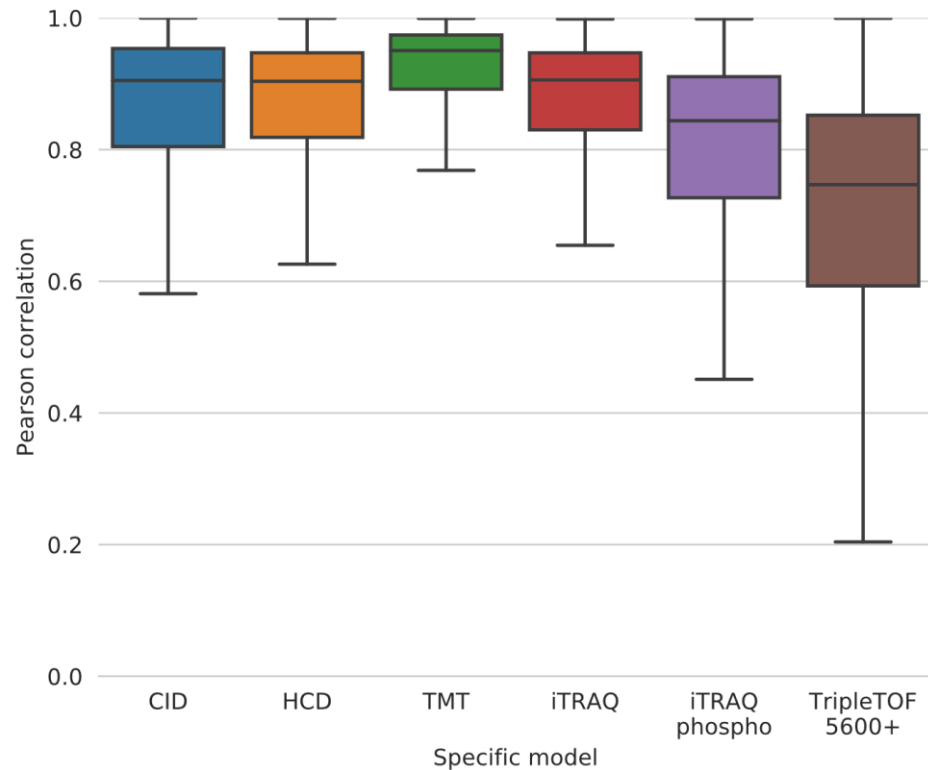
Prediction HCD model



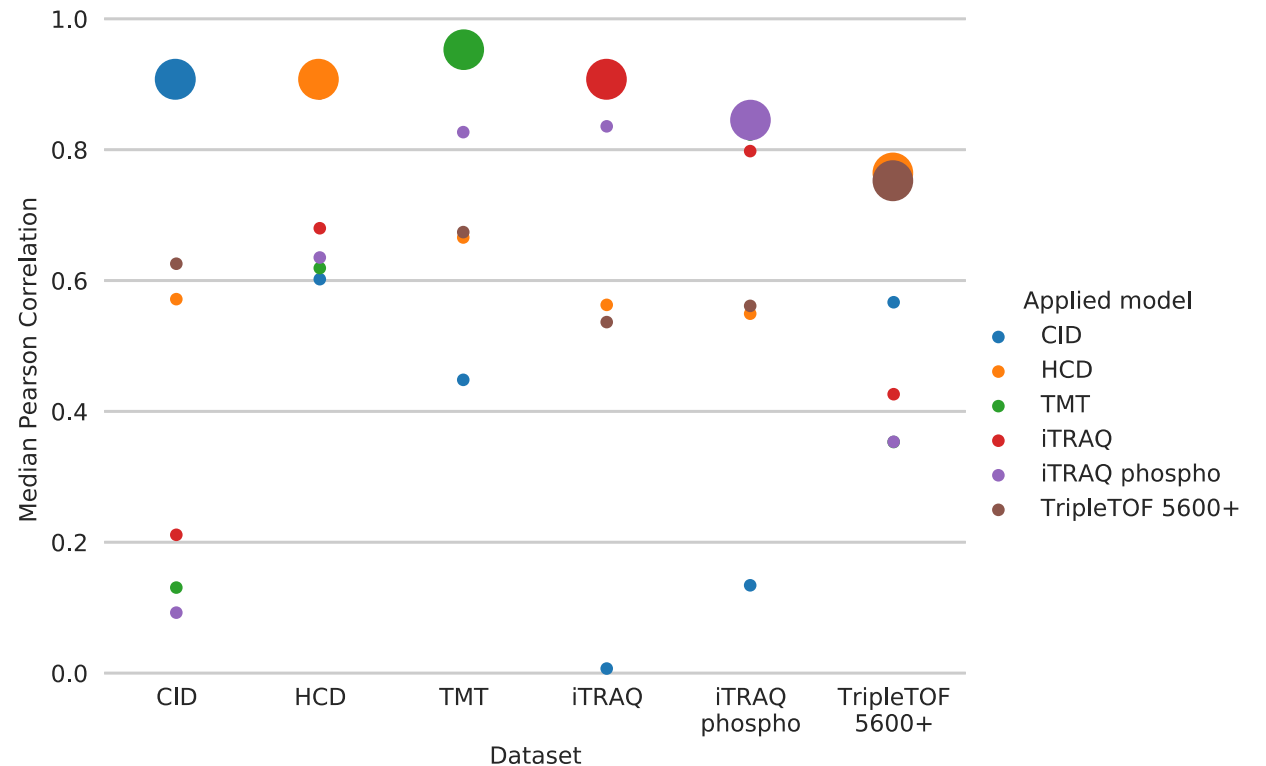
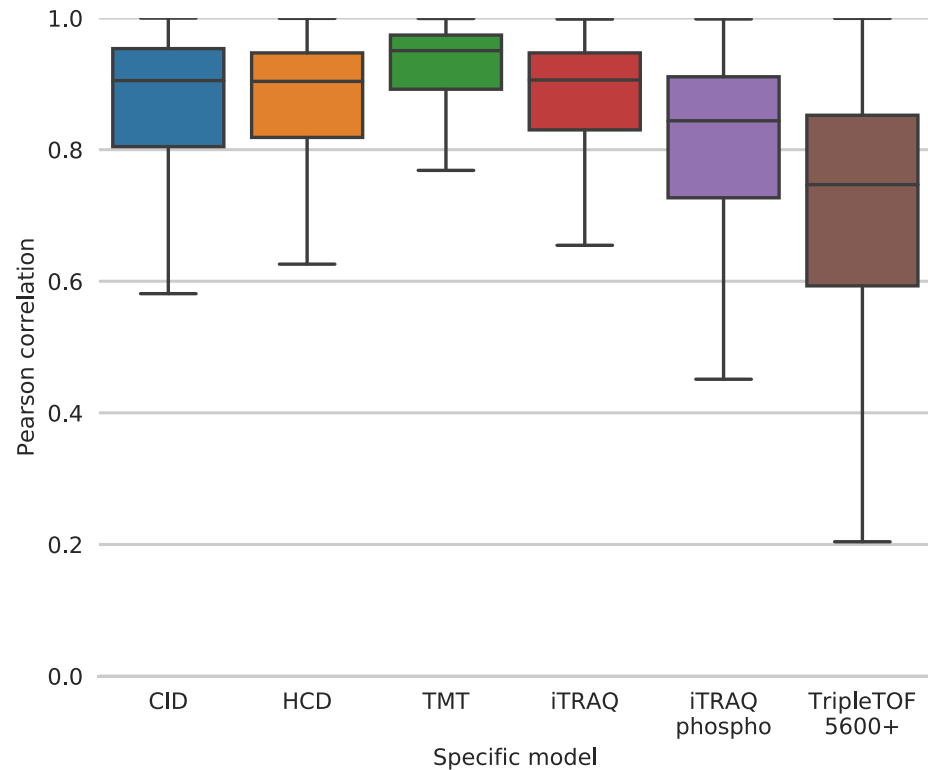
Empirical TMT spectrum

→ Pearson correlation = 0.20

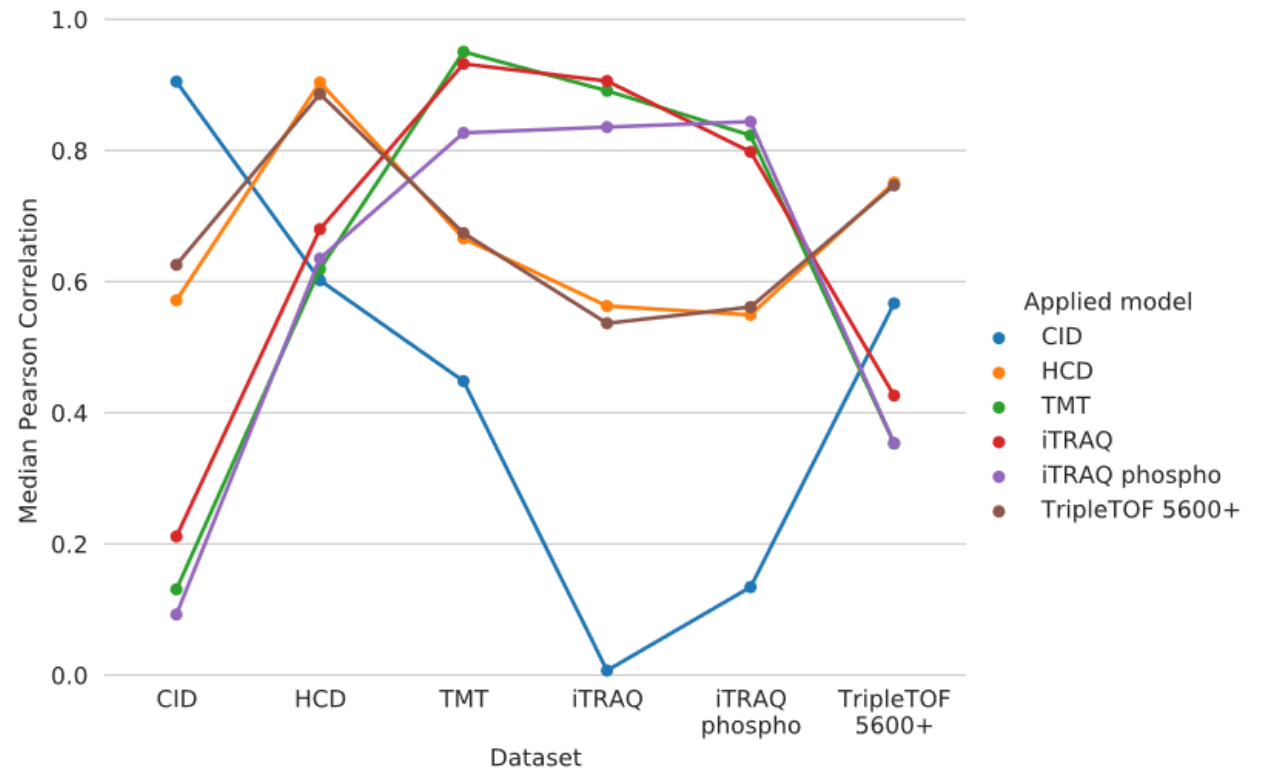
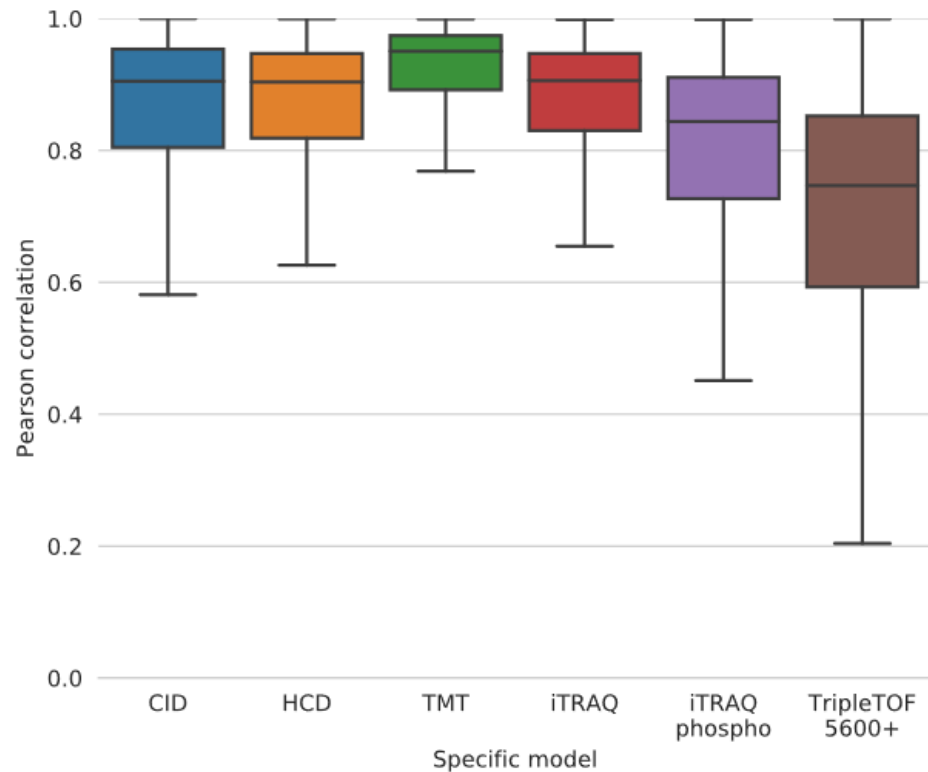
As expected, training data-specific models substantially improves the predictions



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All models are available on iomics.ugent.be/ms2pip

MS²PIP SERVER

HOW TO

RUN MS²PIP

CONTACT

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. [DOI: 10.1093/nar/nkv104](#)

Try out MS²PIP yourself at iomics.ugent.be/ms2pip

