SCIENCE MEETS LIFE

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

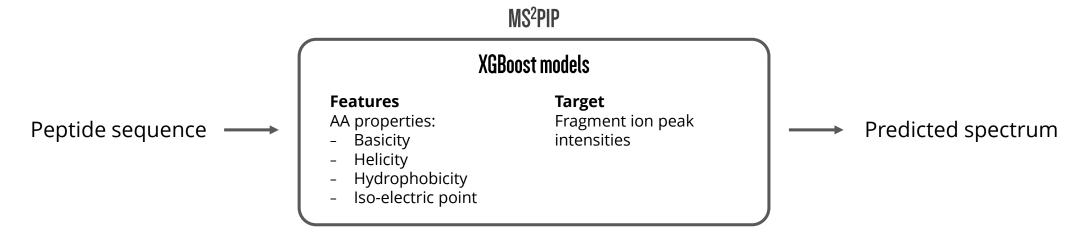
Ralf Gabriels

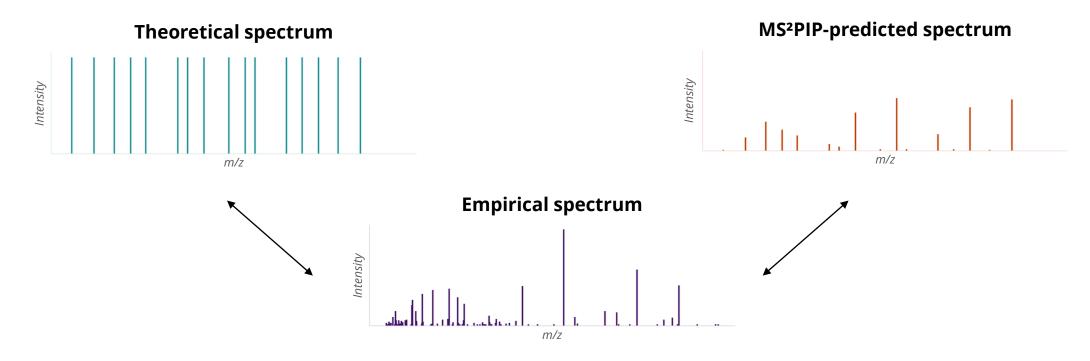




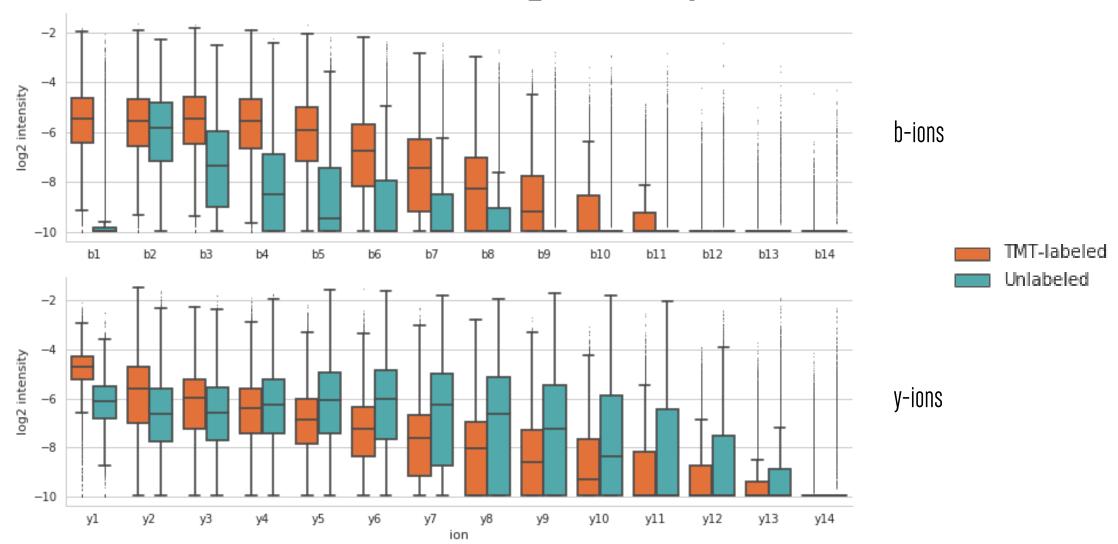


MS²PIP: MS² Peak Intensity Prediction

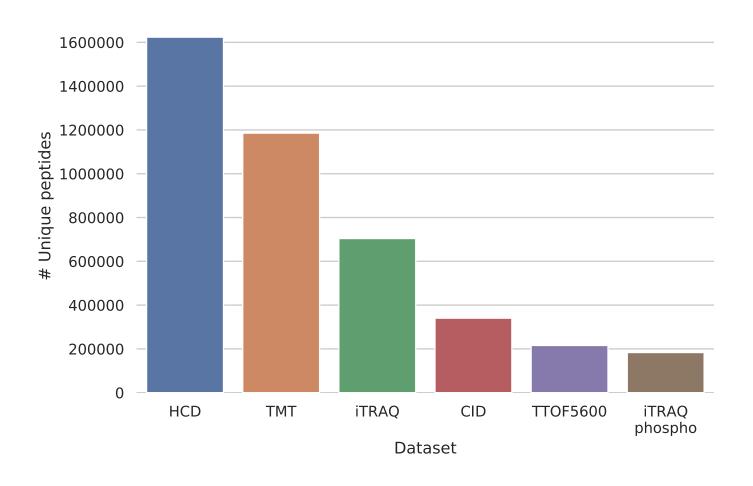




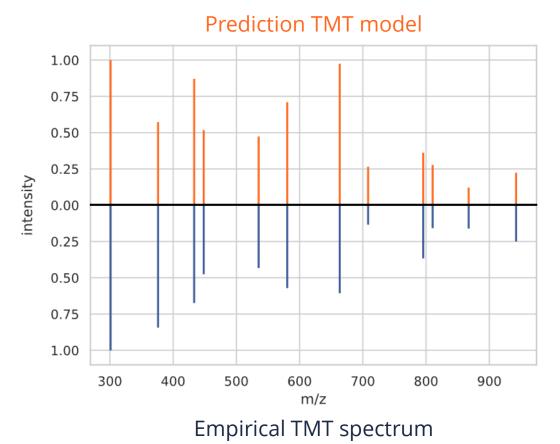
Peak intensity patterns are influenced by fragmentation method, instrument, labeling technique...



We retrained MS²PIP for these specific cases using publicly available datasets



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



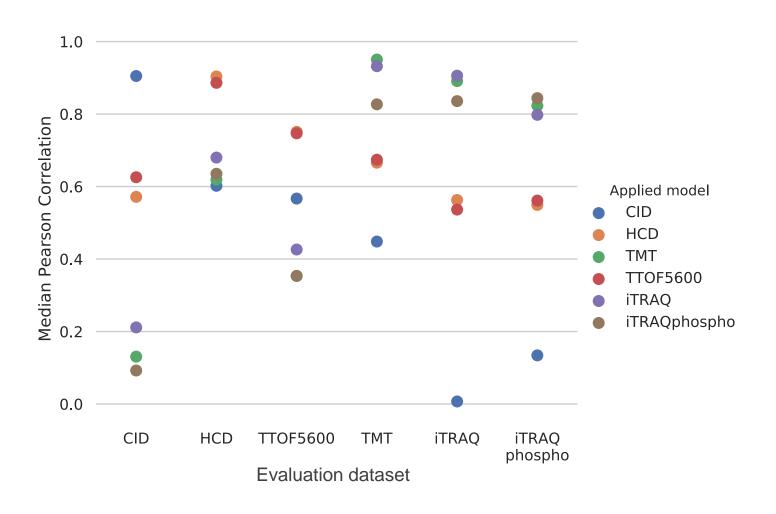
Prediction HCD model 1.00 0.75 0.50 0.25 0.00 0.25 0.50 0.75 1.00 300 400 500 600 700 800 900 m/z

Empirical TMT spectrum

 \rightarrow Pearson correlation = 0.85

 \rightarrow Pearson correlation = 0.20

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



TRY OUT MS²PIP YOURSELF AT IOMICS.UGENT.BE/MS2PIP

































