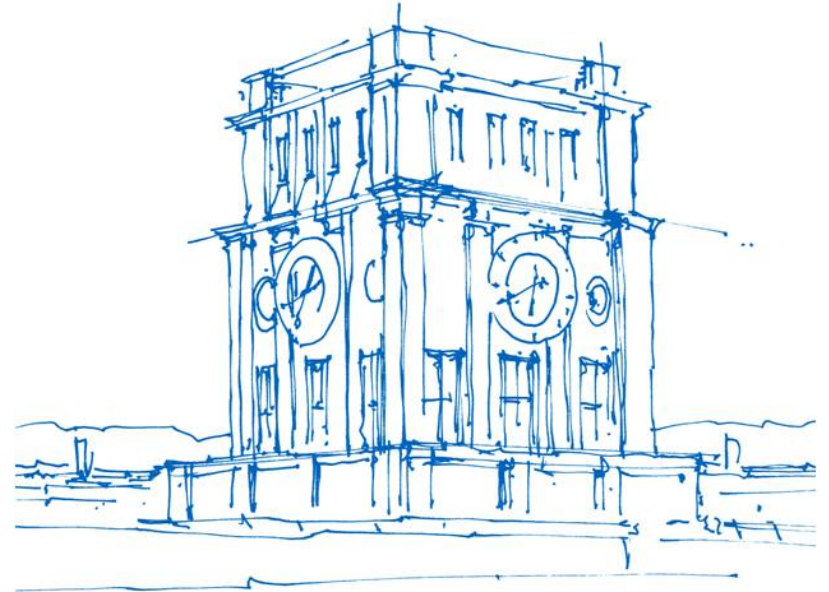


# Real-time spectrum prediction in Skyline via ProteomicsDB's gRPC interface to Prosit

Tobias Schmidt

Technische Universität München



*Uhrenturm der TUM*






# Real-time spectrum prediction in Skyline via ProteomicsDB's gRPC interface to **Prosit**

nature | **methods**

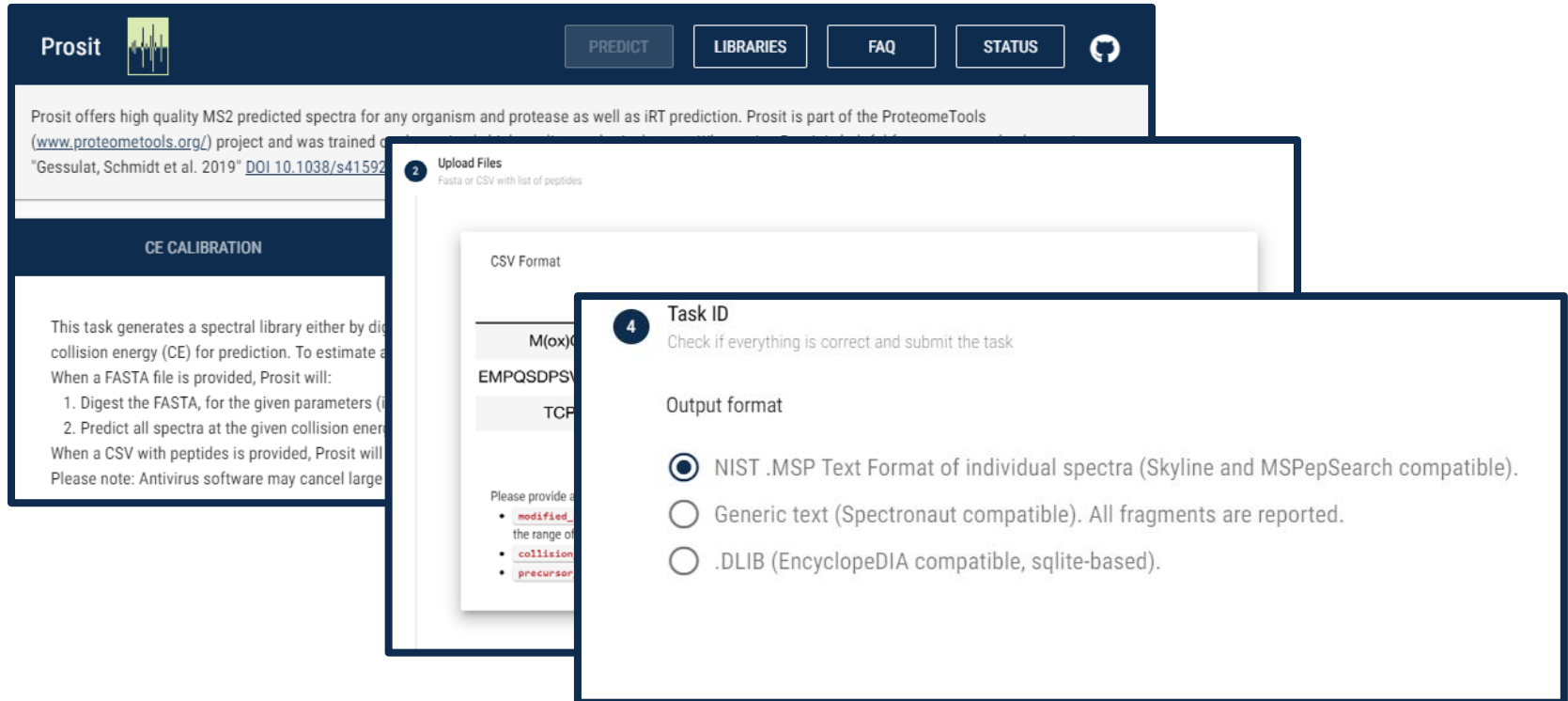
ARTICLES


<https://doi.org/10.1038/s41592-019-0426-7>


## Prosit: proteome-wide prediction of peptide tandem mass spectra by deep learning

Siegfried Gessulat <sup>1,2,7</sup>, Tobias Schmidt<sup>1,7</sup>, Daniel Paul Zolg<sup>1</sup>, Patroklos Samaras <sup>1</sup>,  
Karsten Schnatbaum<sup>3</sup>, Johannes Zerweck<sup>3</sup>, Tobias Knaute<sup>3</sup>, Julia Rechenberger<sup>1</sup>, Bernard Delanghe<sup>4</sup>,  
Andreas Huhmer<sup>5</sup>, Ulf Reimer<sup>3</sup>, Hans-Christian Ehrlich<sup>2</sup>, Stephan Aiche <sup>2</sup>, Bernhard Kuster <sup>1,6\*</sup>  
and Mathias Wilhelm <sup>1\*</sup>

# Spectral libraries are just a click away



**Prosit** 

PREDICT LIBRARIES FAQ STATUS 

Prosit offers high quality MS2 predicted spectra for any organism and protease as well as iRT prediction. Prosit is part of the ProteomeTools ([www.proteometools.org/](http://www.proteometools.org/)) project and was trained on "Gessulat, Schmidt et al. 2019" [DOI 10.1038/s41592-019-0448-4](https://doi.org/10.1038/s41592-019-0448-4)

**CE CALIBRATION**

This task generates a spectral library either by digesting a protein sequence with a given protease and collision energy (CE) for prediction. To estimate a collision energy (CE) for a given protein sequence, Prosit will:

1. Digest the FASTA, for the given parameters (protease, enzyme specificity, etc.)
2. Predict all spectra at the given collision energy (CE) for the given protein sequence.

When a CSV with peptides is provided, Prosit will generate a spectral library for each peptide. Please note: Antivirus software may cancel large files.

**2 Upload Files**  
Fasta or CSV with list of peptides

CSV Format

M(x)K
EMPSQSDPSV
TCF

Please provide a collision energy (CE) in the range of 10-40 eV. If you are using a precursor ion, please provide its m/z.

**4 Task ID**  
Check if everything is correct and submit the task

Output format

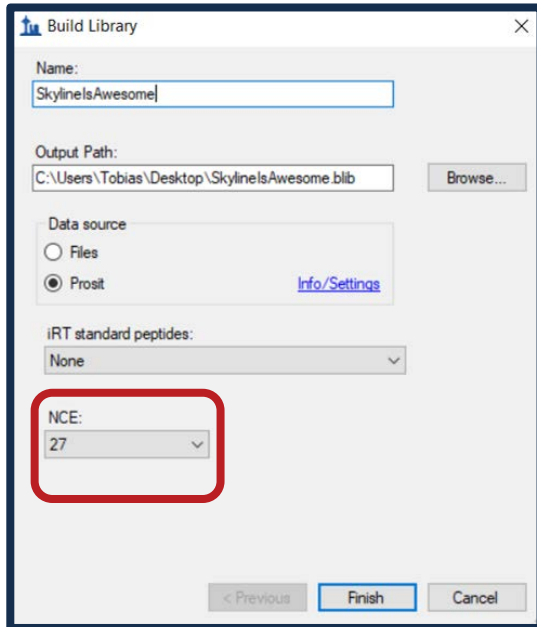
- NIST .MSP Text Format of individual spectra (Skyline and MSPepSearch compatible).
- Generic text (Spectronaut compatible). All fragments are reported.
- .DLIB (EncyclopeDIA compatible, sqlite-based).

# Real-time spectrum prediction in Skyline via **ProteomicsDB's gRPC interface** to Prosit

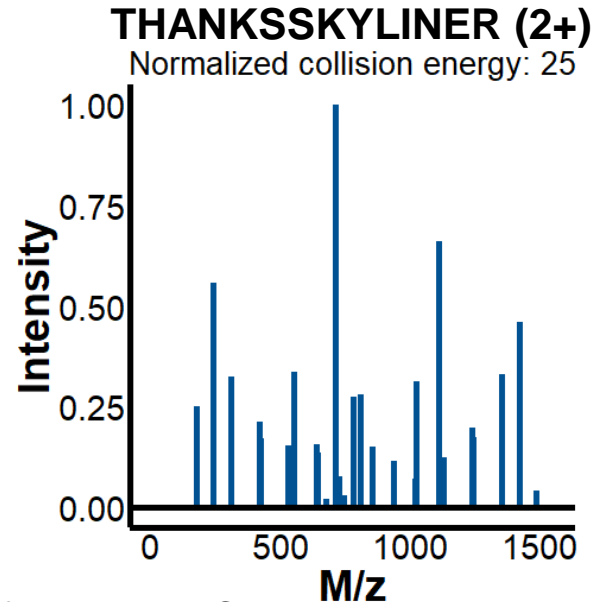
Tobias Rhode (a student at the MacCoss lab) was sent to our lab to evaluate with us how to become “real-time”



# Real-time spectrum prediction in Skyline via ProteomicsDB's gRPC interface to Prosit

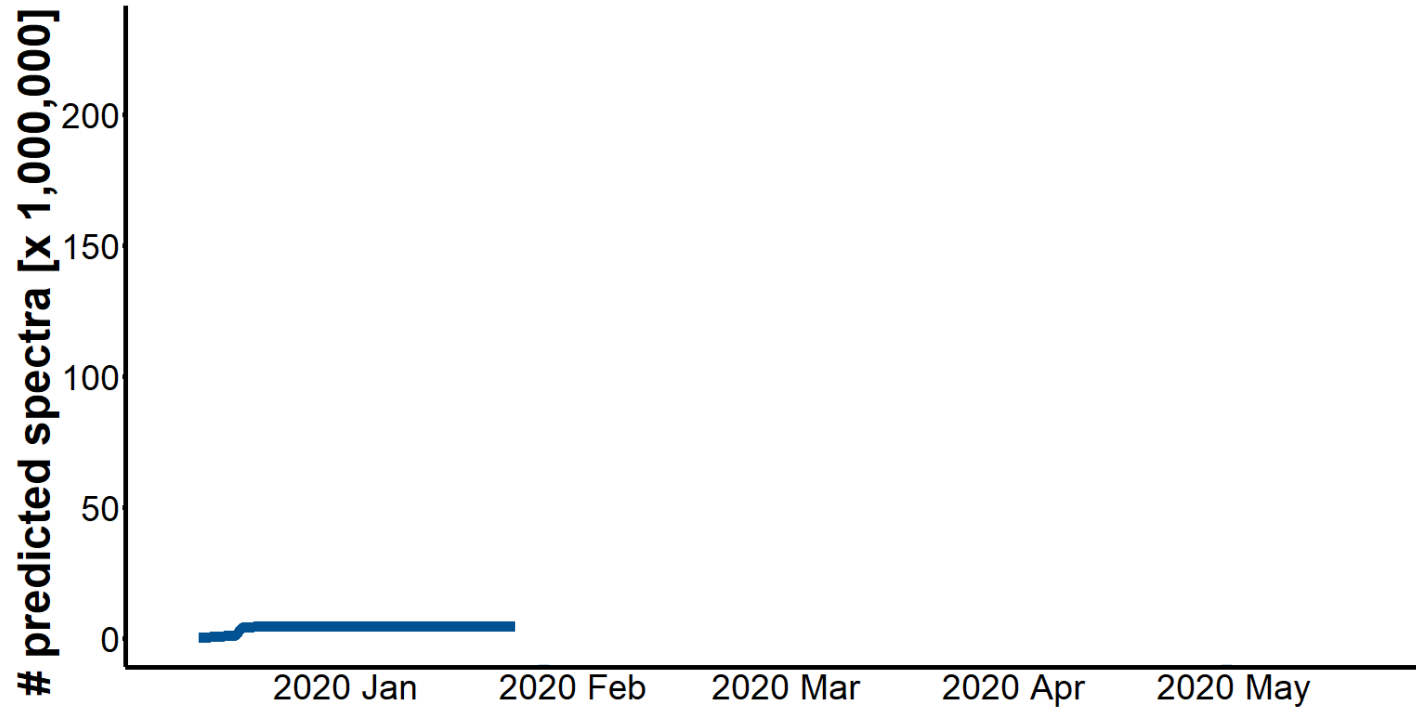


\* Predicting the human Swiss-Prot database takes as long as listening to this slide (~30s)

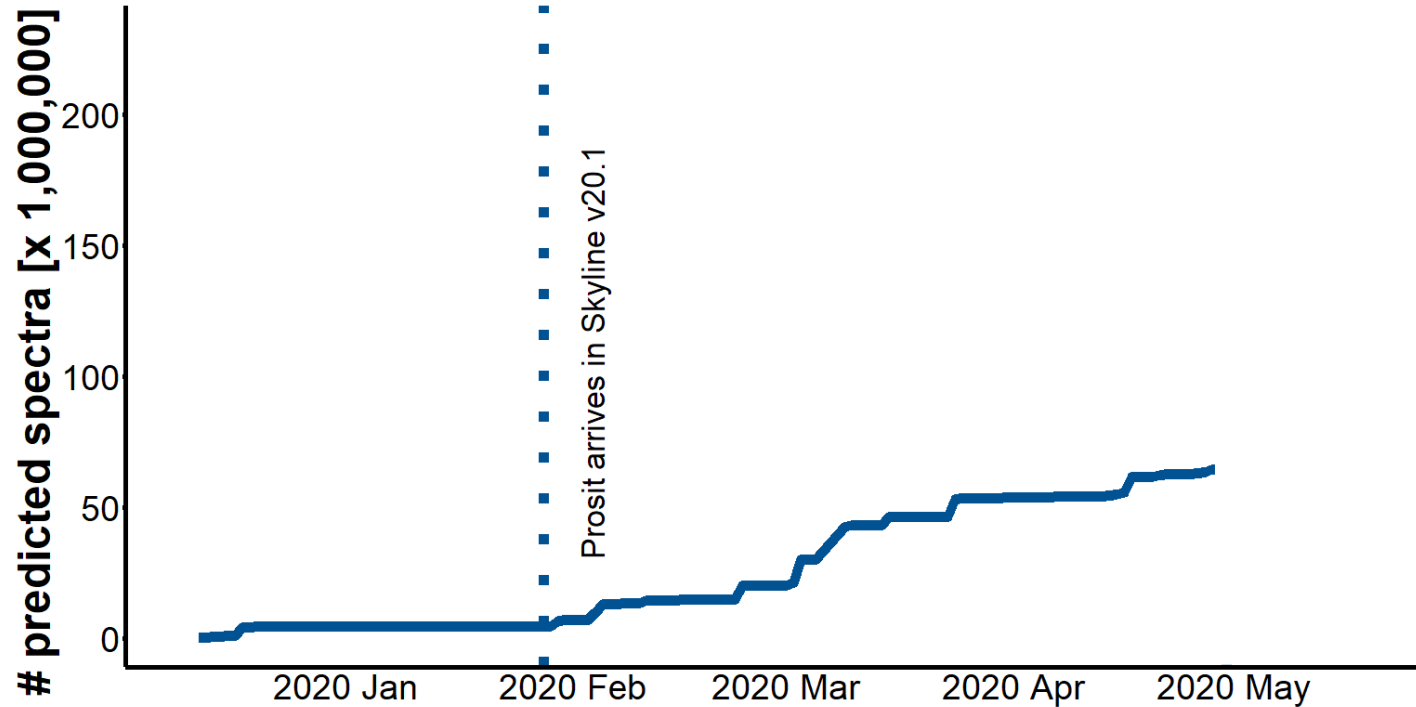


Word of caution: for optimal NCE, please use our CE alignment tool at [proteomicsdb.org/prosit](http://proteomicsdb.org/prosit)

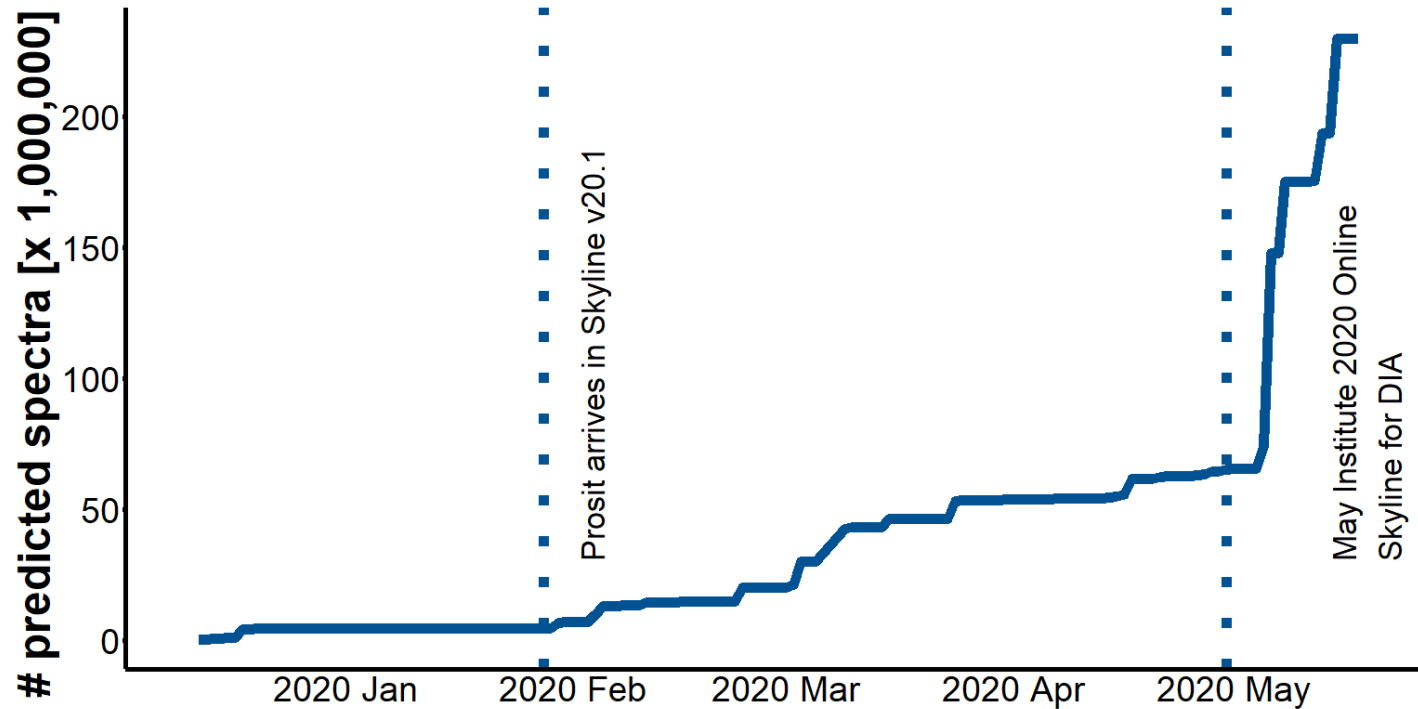
# Skyline user ♥ Prosit



# Skyline user ♥ Prosit

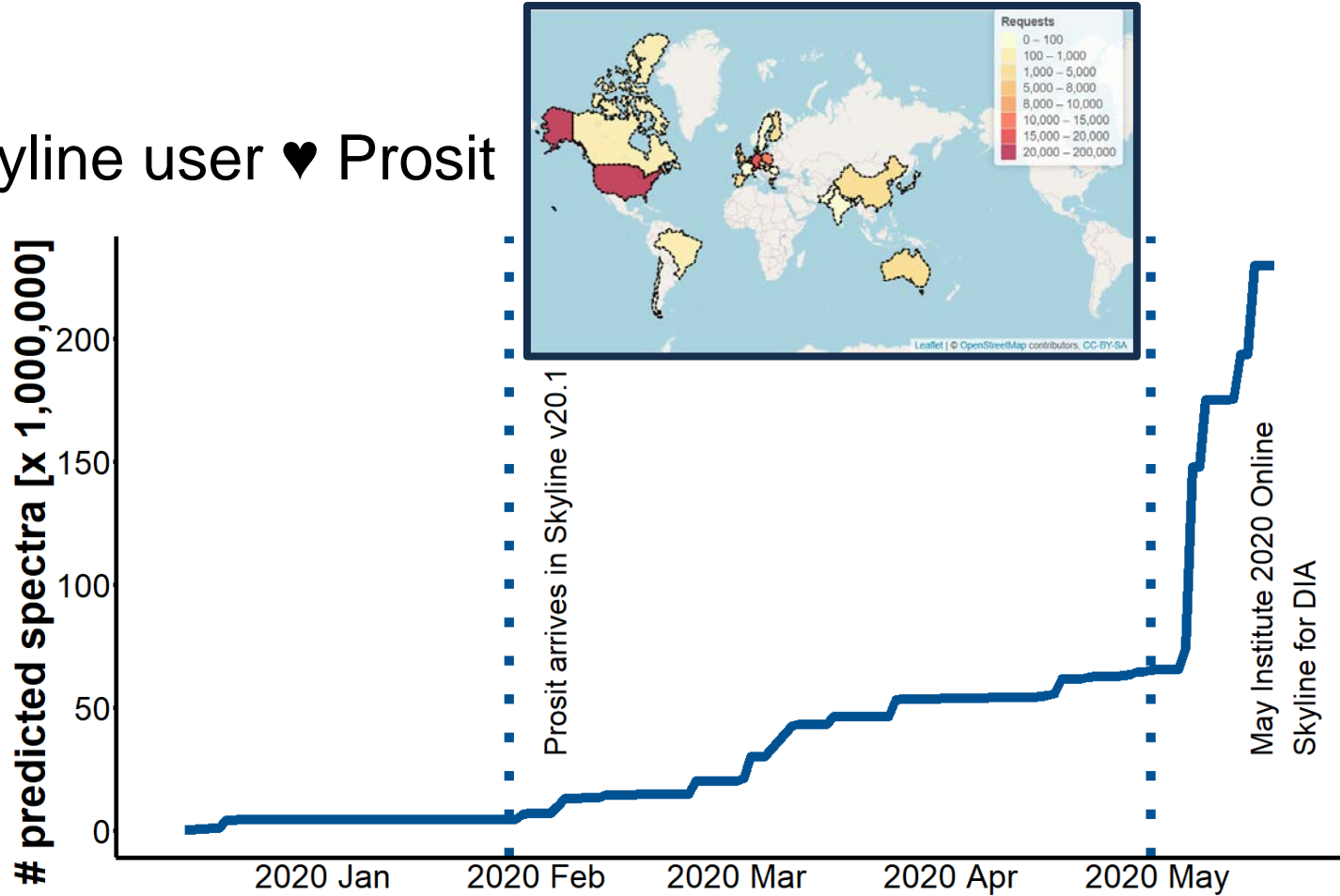


# Skyline user ♥ Prosit





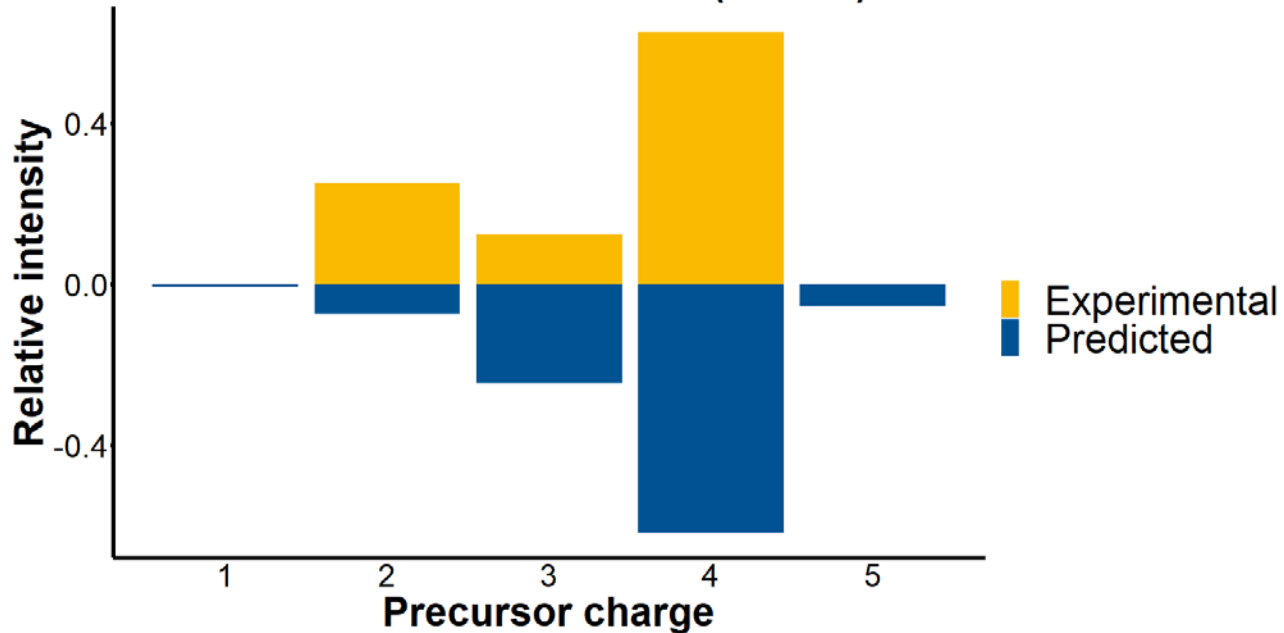
# Skyline user ♥ Prosit



# Outlook for more Prosit features in Skyline

Prosit keeps a common interface => new models will need minimal work for Skyline developers

**GHYRGDPNWFMKKAQE (R=0.91)**





Bernhard Kuster  
Siegfried Gessulat  
Patroklos Samaras  
Miriam Abele  
And all lab members



Johannes Rank  
Marwin Shraideh  
Helmut Krcmar



Brendan McLean  
Tobias Rhode  
Brian Connolly

## Want to learn more?

Brendan MacLean @ WOD am 09:30  
**Prosit meets Skyline**

Mathias Wilhelm @ MOD am 10:10  
**Extending Prosit's predictions to proteotypicity, precursor ion charge and ion mobility collisional cross sections**