LectinOracle@glycowork
Lectin binding predictions &
glycan sequence analysis in Python

JON LUNDSTRØM | BOJAR LAB | GLIC SEMINAR SERIES | 2023-03-27

Overview

The Bojar Lab   Intersection of computational and experimental glycobiology

glycowork   Glycan analysis codebase & database

LectinOracle   Deep Learning approach to predict glycan-binding specificity of a protein

glycowork

GlycoDraw   evolution

MS/MS   m/z values

compositions → structures

motifs

models

AI

enrichment

biosynthesis networks
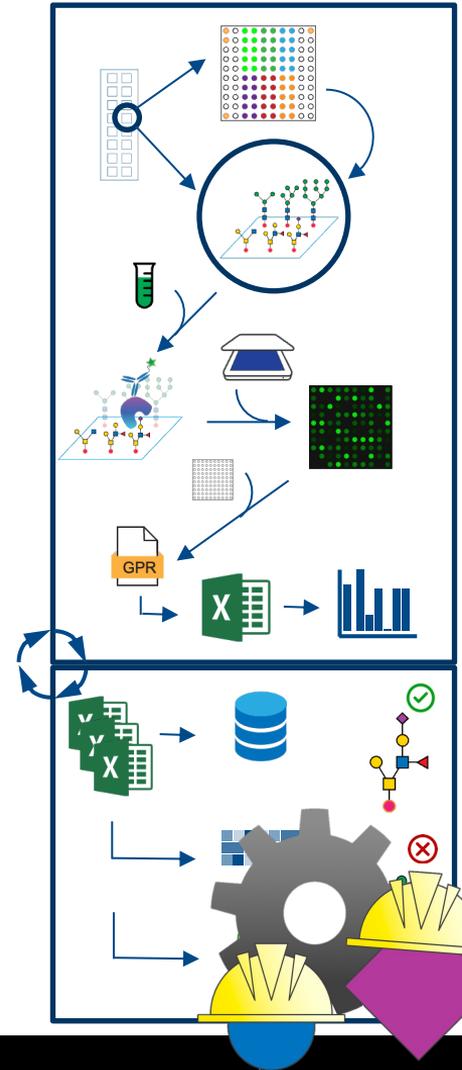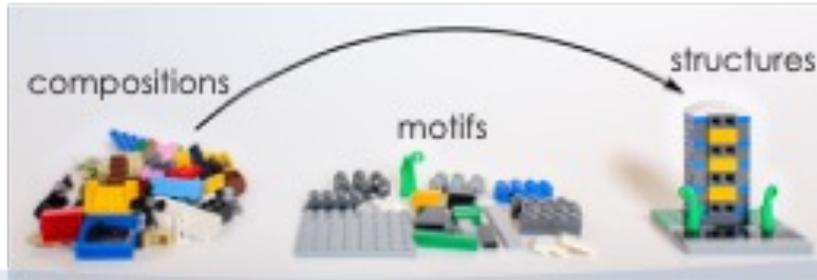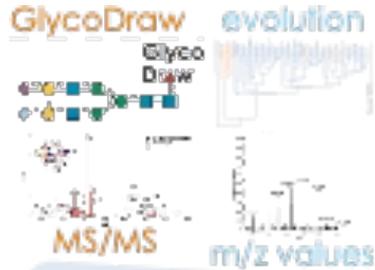
>52,500
>35,000
>13,000

glycowork

>51,500 unique glycan sequences
>33,000 species labels
>9,500 tissue labels
>500 disease labels
>600,000 protein-glycan interactions

v0.7   v0.6
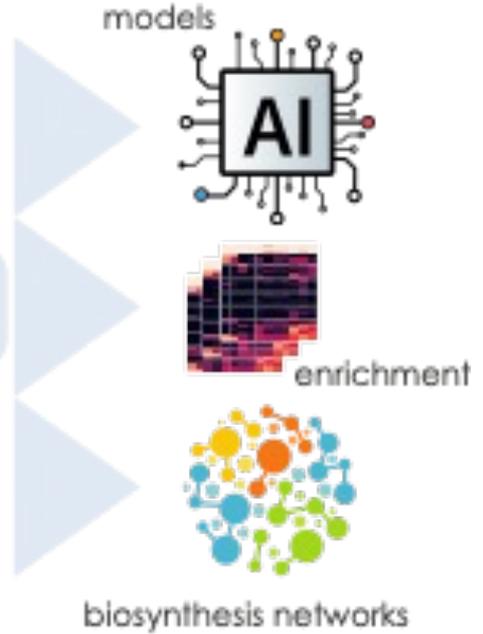
Thomès et al., Glycowork: A Python package for glycan data science and machine learning. *Glycobiology* (2021)

glycowork

| glycan_data	ml	motif	network
loader data_entry	model_training models processing inference train_test_split	analysis annotate graph processing query tokenization	biosynthesis evolution
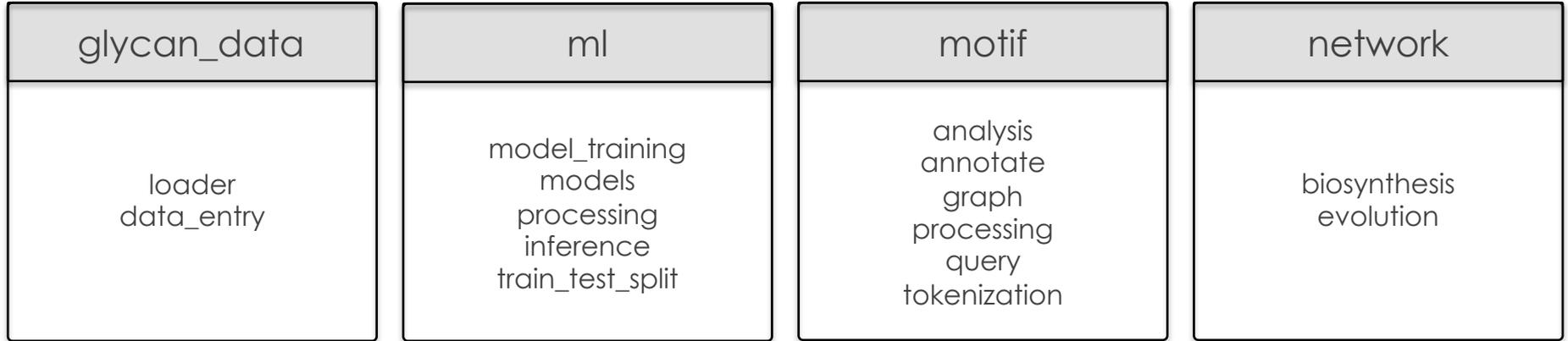
Demo:

(i) Analyzing glycan array data using glycowork
(ii) Predicting lectin binding specificity with LectinOracle

LectinOracle

3,328 array experiments

564,647 unique lectin-glycan interactions

1,392 Lectins
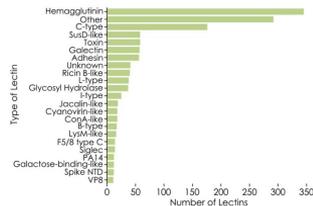
927 Glycans
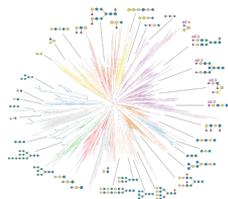
MRLVAKLLYLAVLAI...

MAKMITNYVGKRI...

MSDSKEPRLQQLGL...

MATSNSKPTQVLLATFLT...

MKPFCVFLTFFL...

MTPQNITDLCA...

ESM-1b

Node Embedding

SweetNet

Binding Prediction
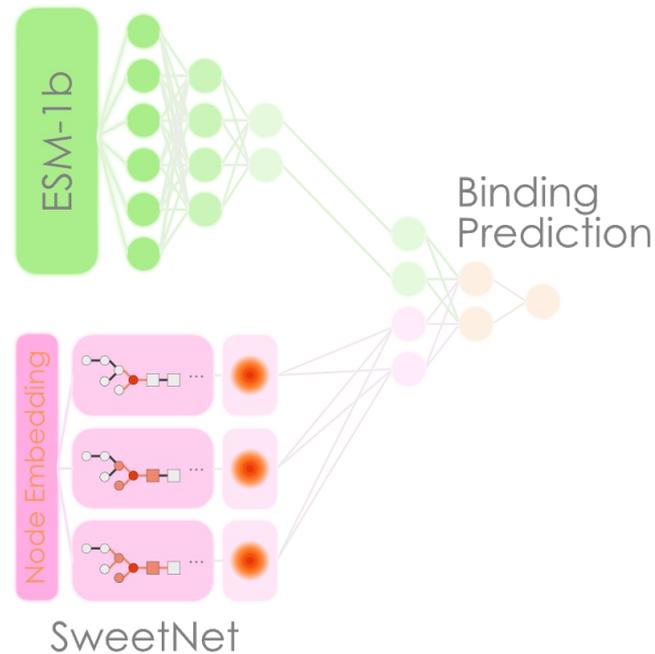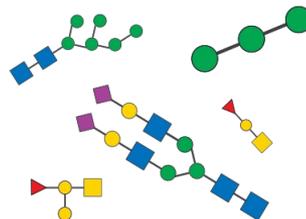
# Qualitative Predictions
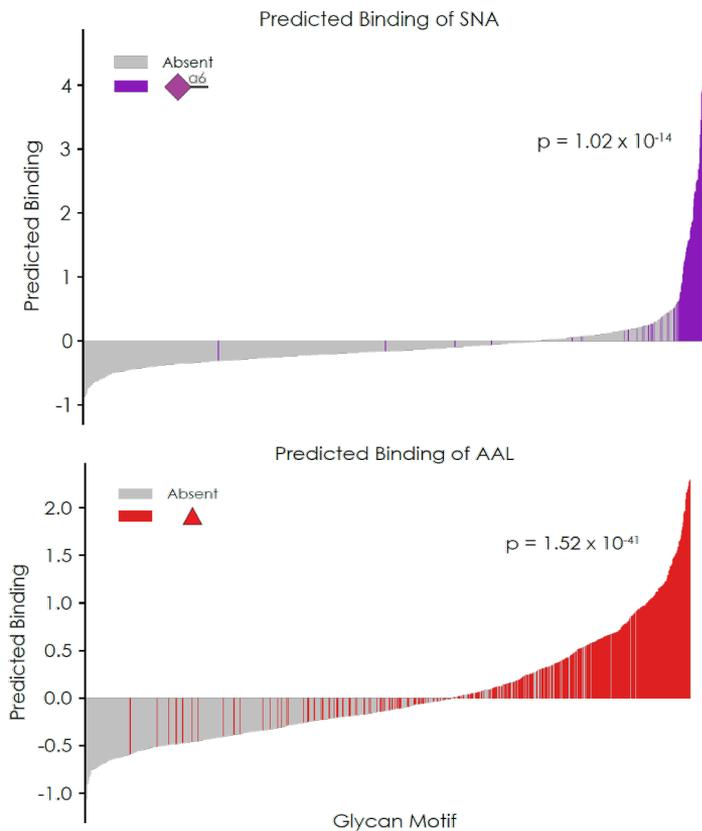
# Qualitative & Generalizable Predictions
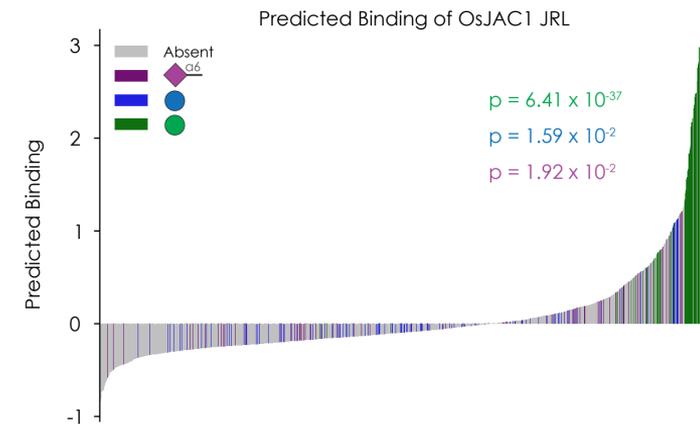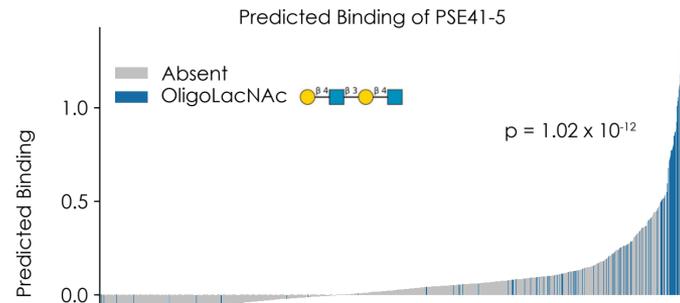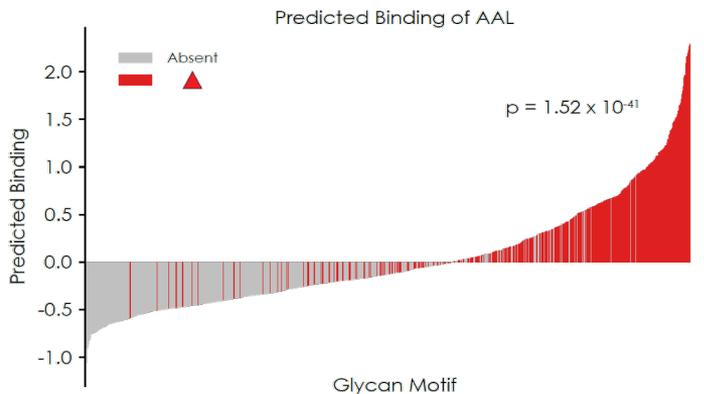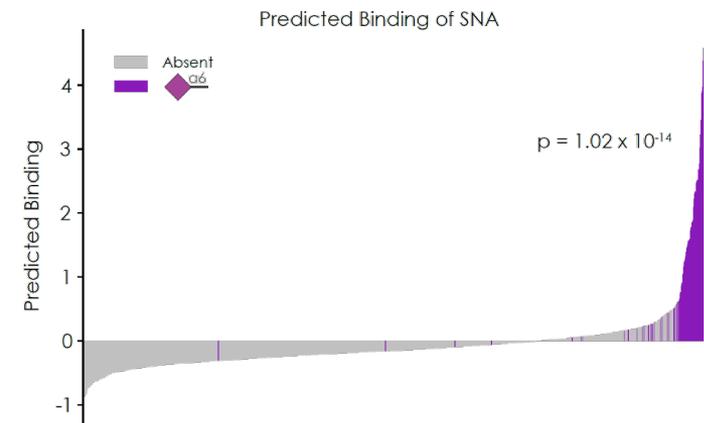
Quantitative Predictions

Oligomannose glycans
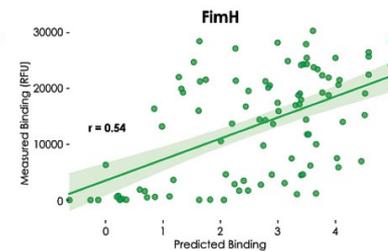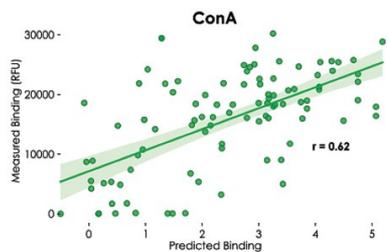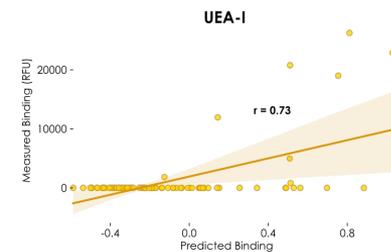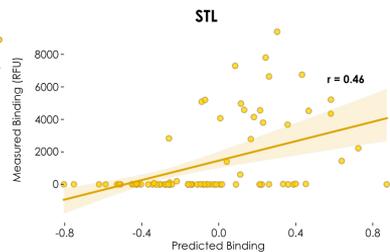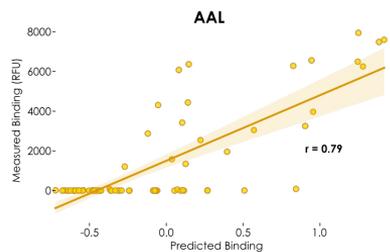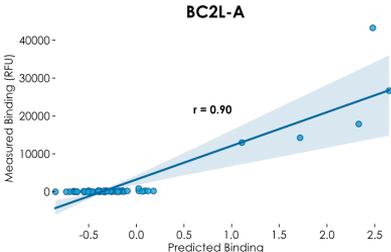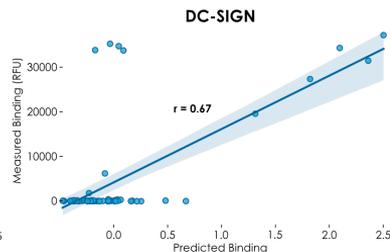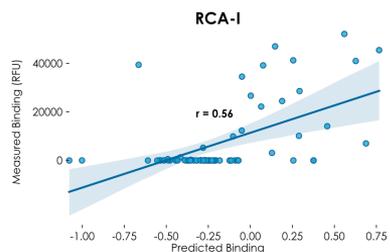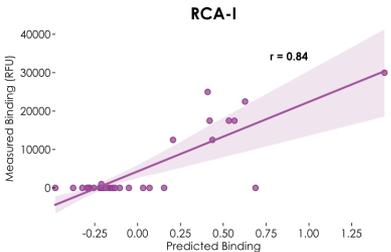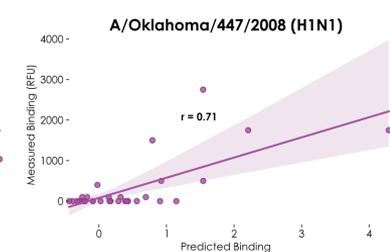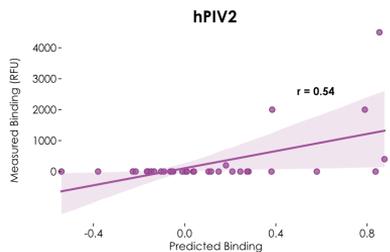
Example Applications

Lectin Engineering

Epidemiological outcomes
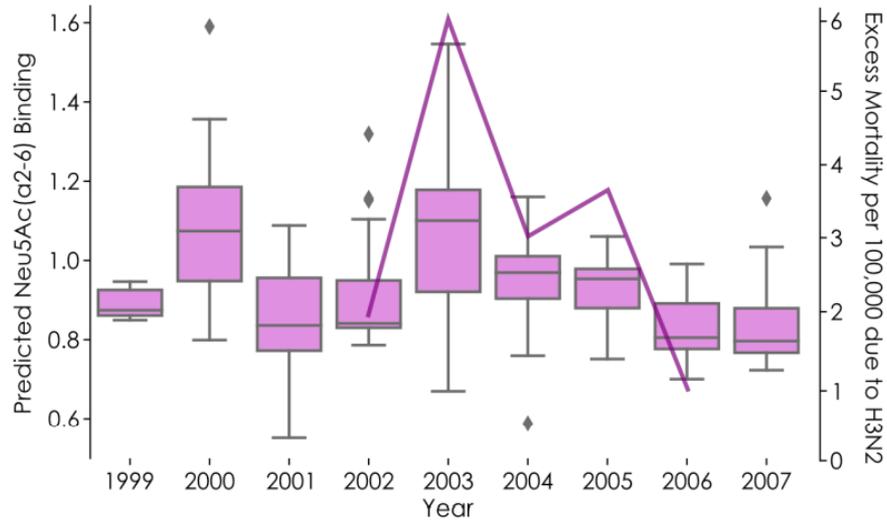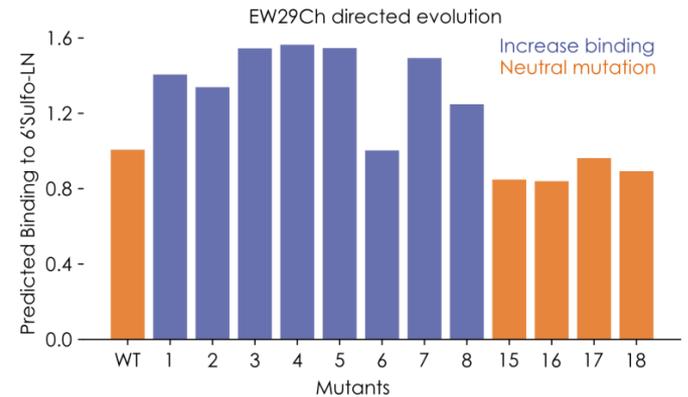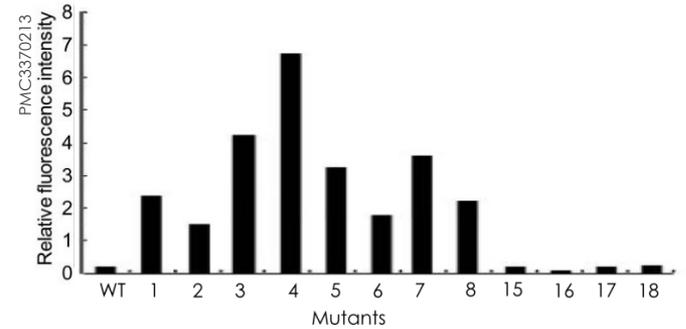
live demo!

Links & Resources

glycowork
- – Publication   doi.org/10.1093/glycob/cwab067
- – Documentation   bojarlab.github.io/glycowork/
- – Code   github.com/BojarLab/glycowork

LectinOracle
- – Publication   doi.org/10.1002/advs.202103807
- – Code   *see glycowork*

Examples
- – Notebook   drive.google.com/drive/folders/1Ro_0VMC-uzEOimJbP9O785aCY3Qk36yS?usp=sharing

      download all, then upload to Google Drive

Contact
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Questions?

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