



Identification of Angiotensin 1-7 as potential anti-SARS-CoV-2 therapeutic

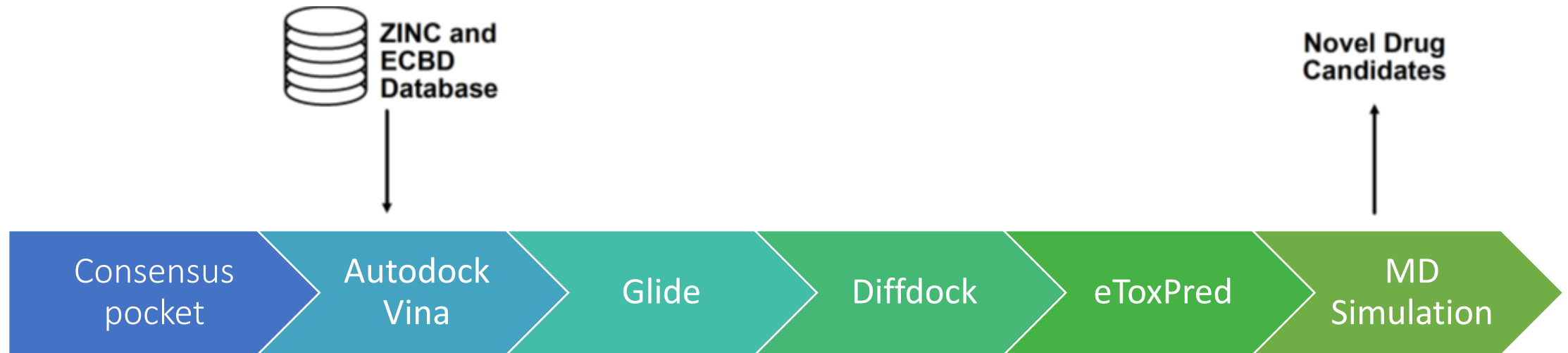
MeetEU Project 2024

Team **Heidelberg**

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Supervisors: Prof. Dr. Carl Herrmann, Dr. Giulia Paiardi

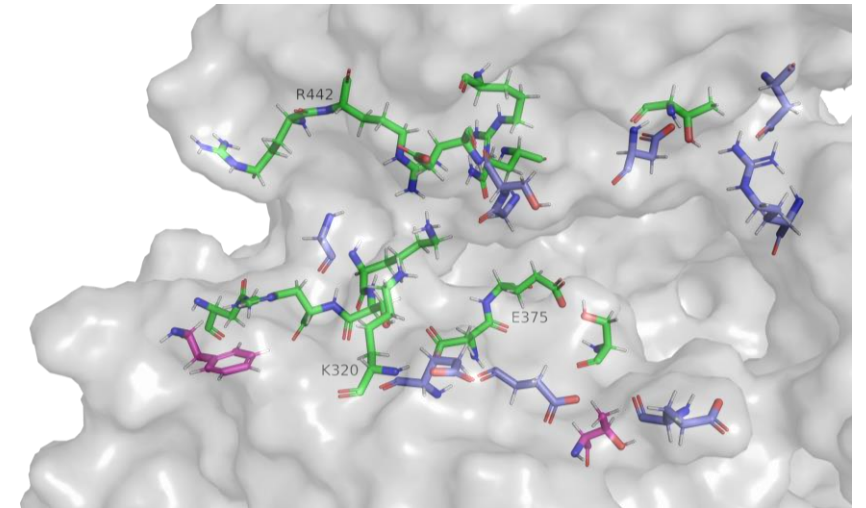
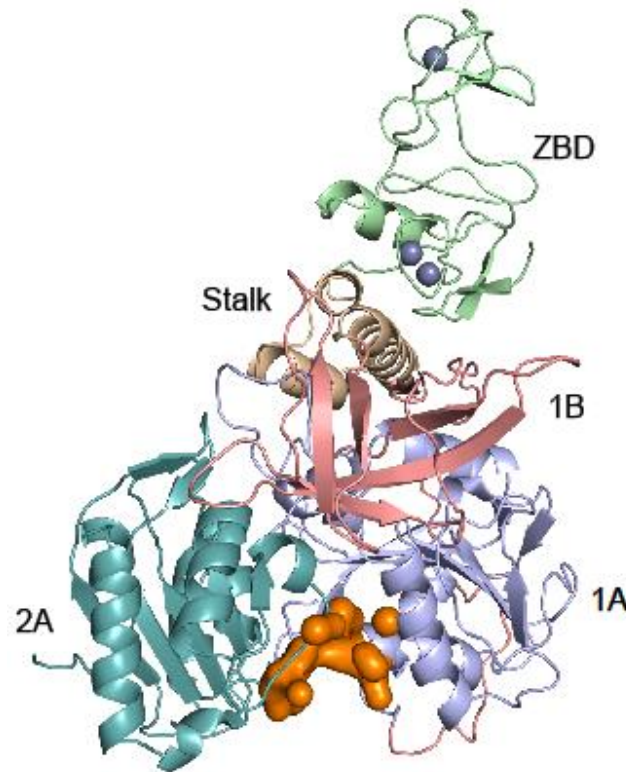
Overview of our pipeline



Consensus pocket was detected in ATP binding site

6ZSL, 5RME, 5RM2

Fpocket,
PrankWeb 3,
FTMap



Consensus pocket

Autodock Vina

Glide

Diffdock

eToxPred

MD Simulation

Top scorers were identified with molecular docking



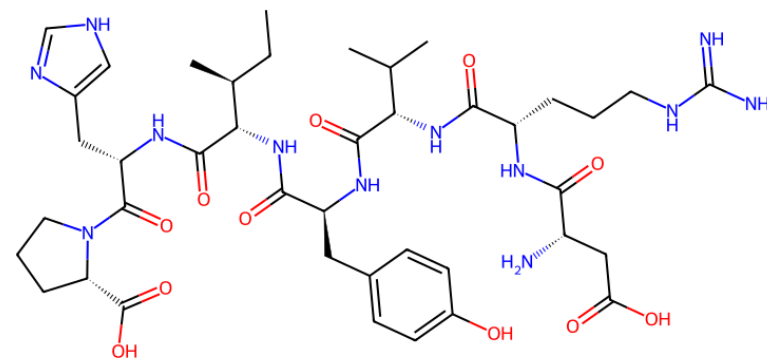
ZINC and
ECBD
Database

Autodock
Vina

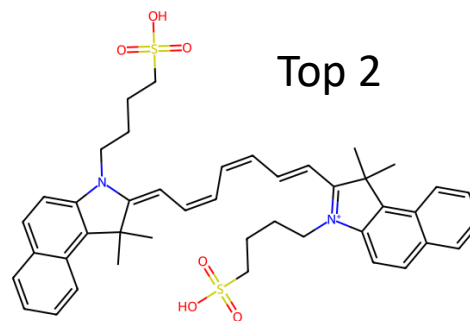
Top100

Glide

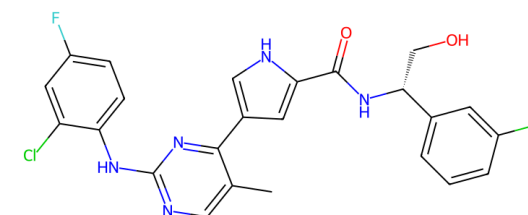
Top 1 Angiotensin 1-7



Top 2



Top 3



Consensus pocket

Autodock Vina

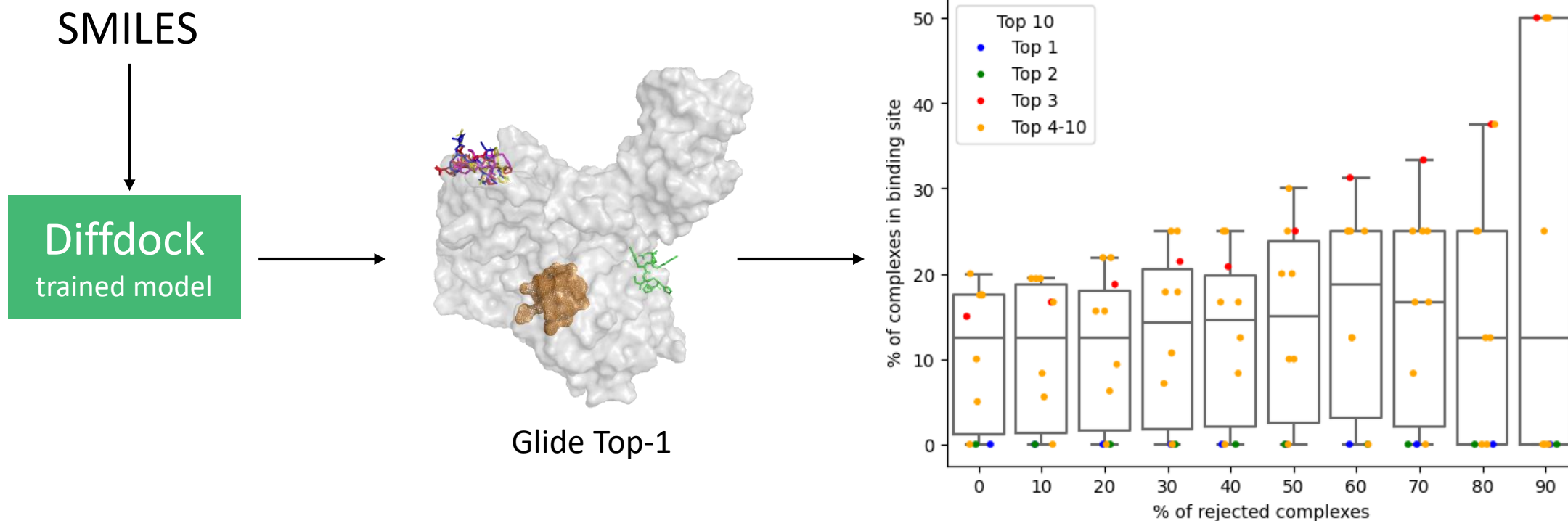
Glide

Diffdock

eToxPred

MD Simulation

Diffdock could not find binding site for Top 1



Consensus pocket

Autodock Vina

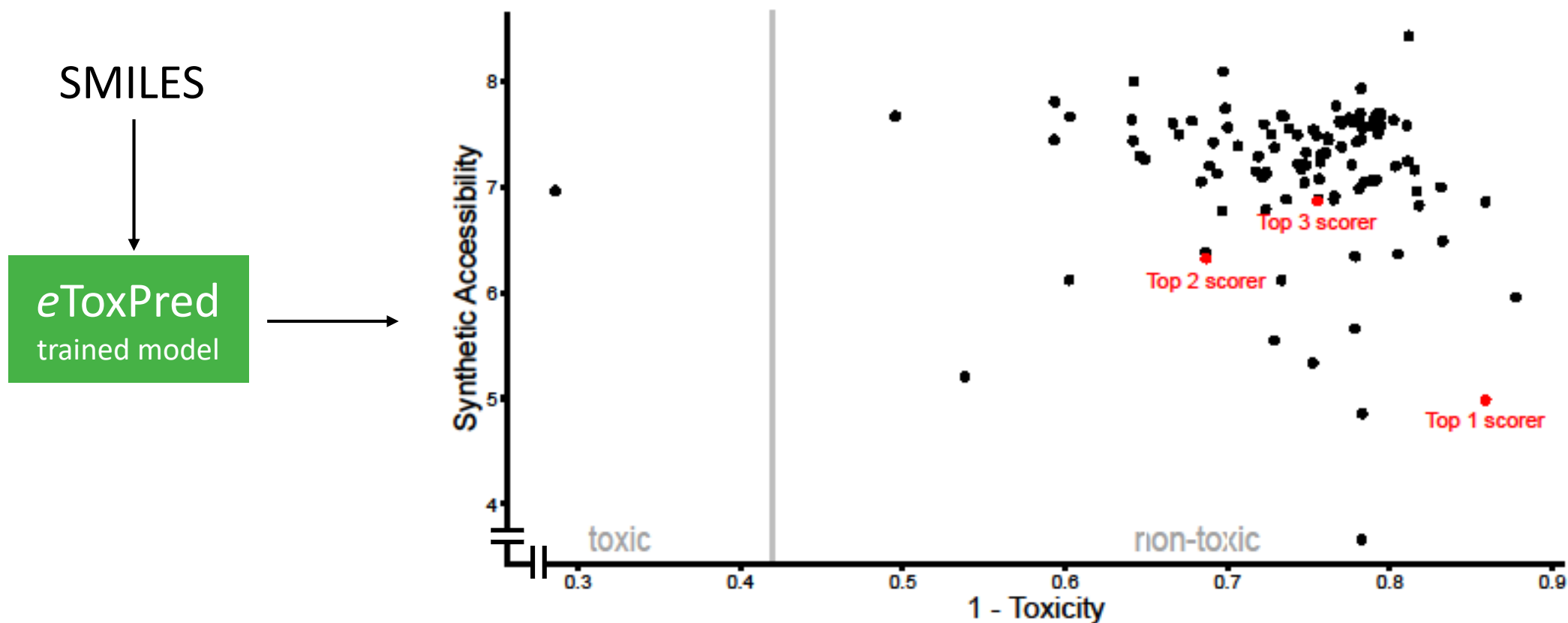
Glide

Diffdock

eToxPred

MD Simulation

Majority of compounds predicted non-toxic



Consensus pocket

Autodock Vina

Glide

Diffdock

eToxPred

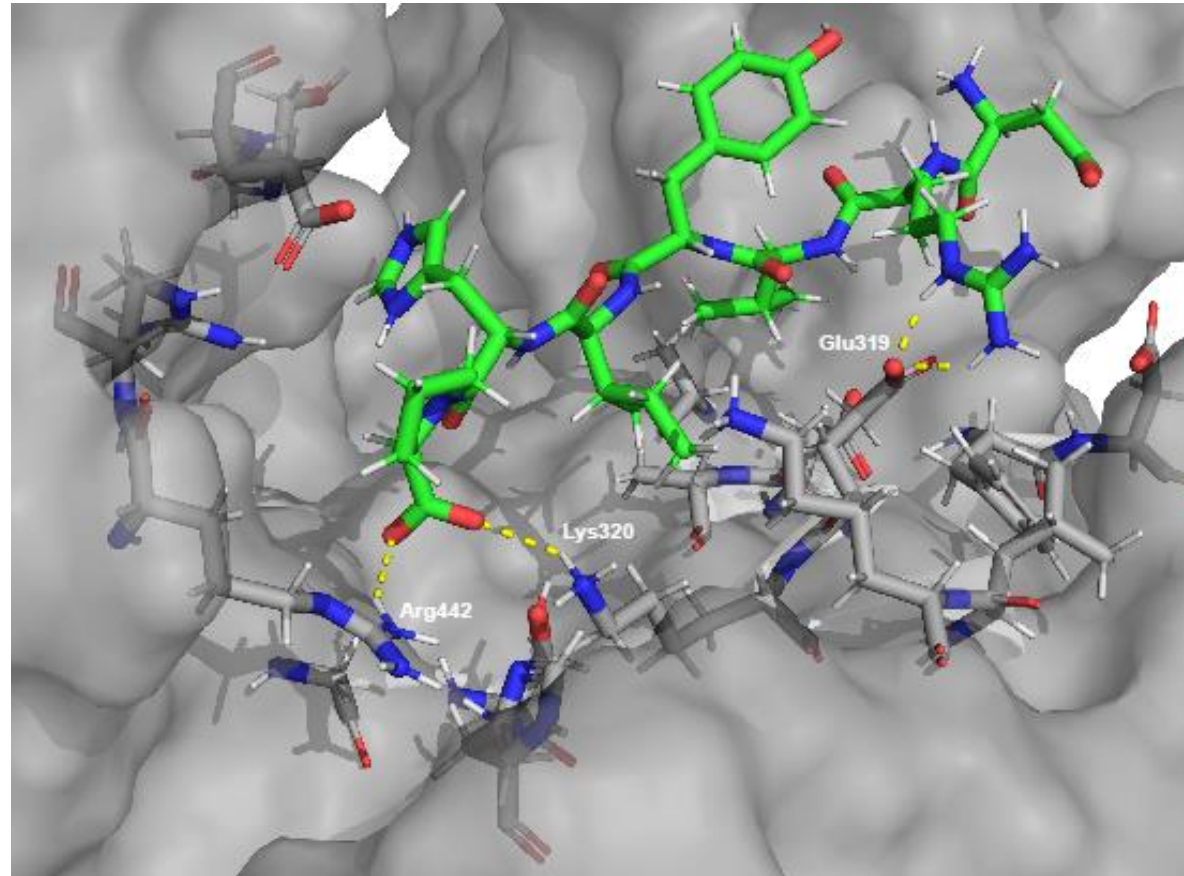
MD Simulation

MD-Simulation validates binding of Top ligand

Glide Top 1



GROMACS



Consensus pocket

Autodock Vina

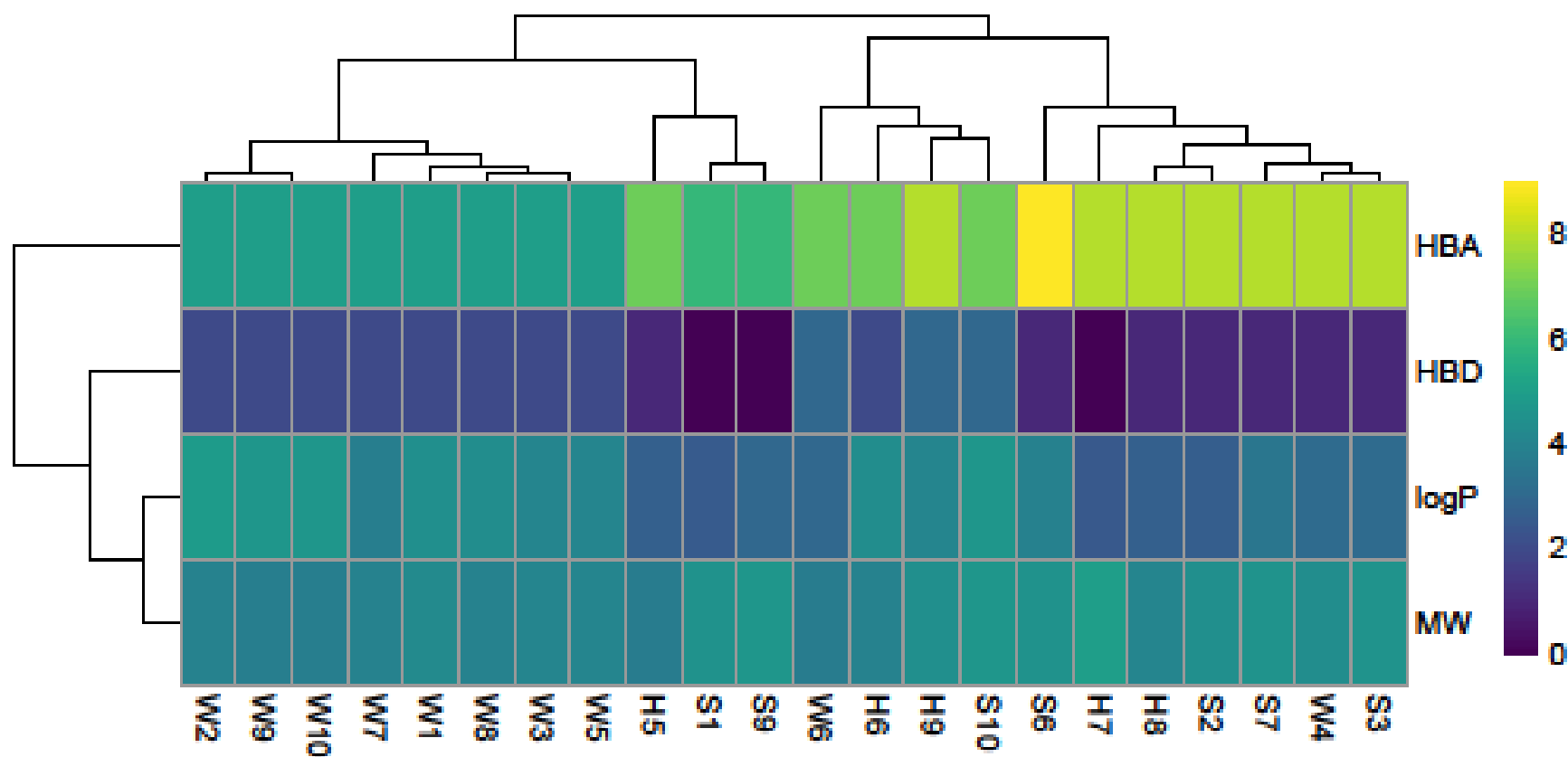
Glide

Diffdock

eToxPred

MD Simulation

22/30 compounds from all paired teams are drug-like



Our take a way

Results are highly dependent on tools and selected data

Communication is key to teamwork and collaboration

Set realistic goals and plan ahead