BioData

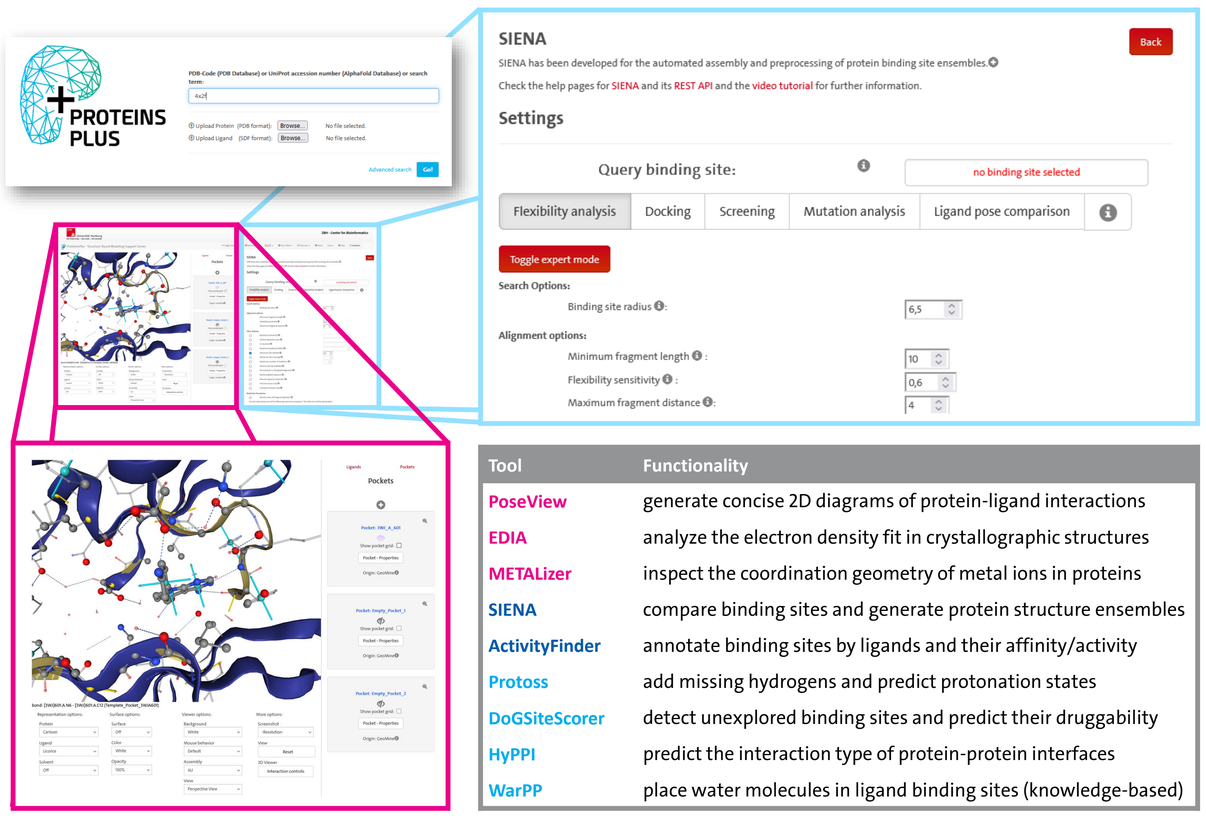
Proteins*Plus* – Services for Computational Analyses of Protein-Ligand Complexes

Joel Graef, Christiane Ehrt, Matthias Rarey
Computational Molecular Design, ZBH - Center for Bioinformatics, University of Hamburg

Contract Nr. W-de.NBI-012

Short Description of the Project

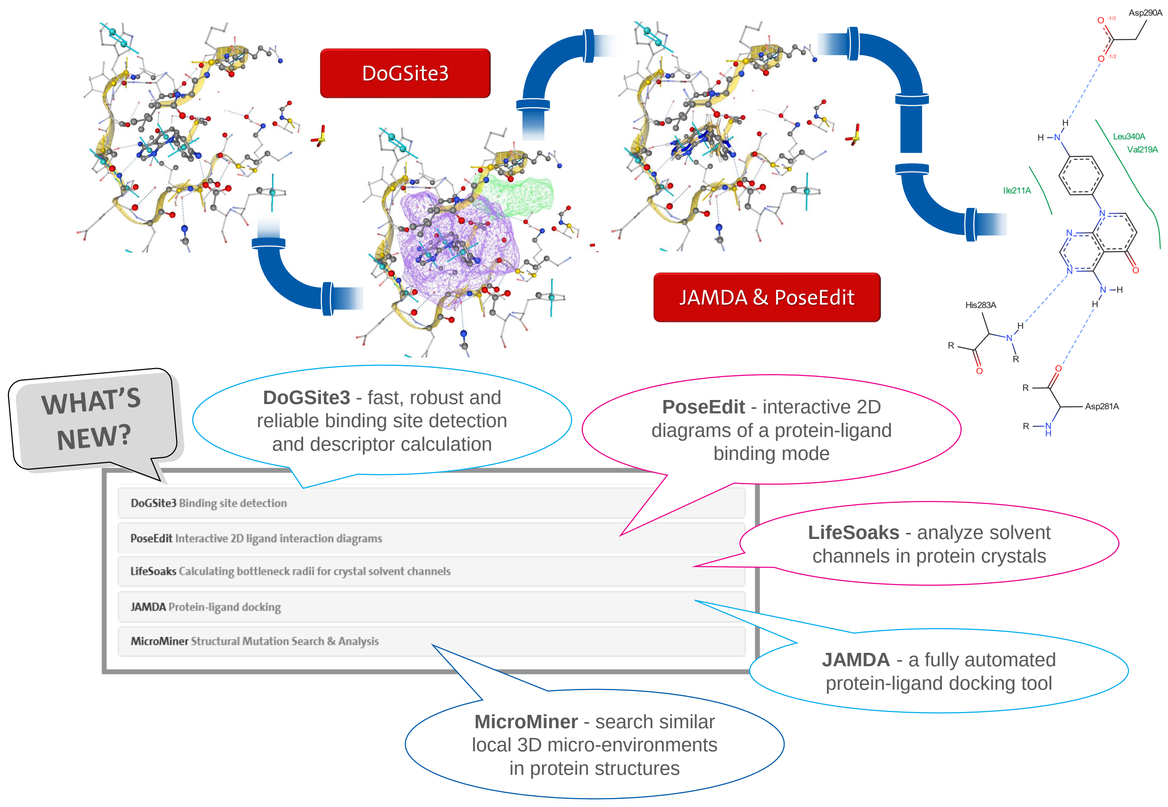
The Proteins*Plus* Web Server enables users to ***analyze***, ***mine***, and ***predict*** protein-ligand complexes on the web. Its availability is ensured by regularly updating hardware and software. Furthermore, new state-of-the-art methods through independent research activities are constantly added.



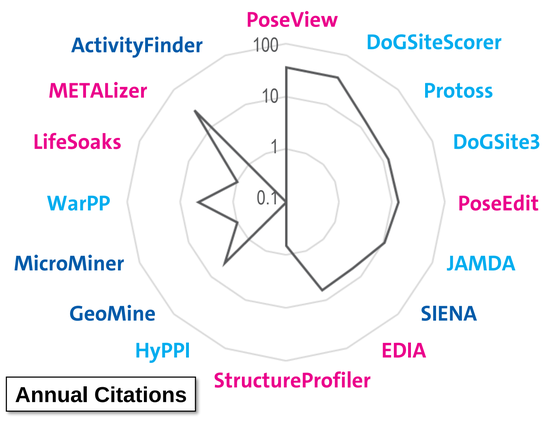
Tool	Functionality
PoseView	generate concise 2D diagrams of protein-ligand interactions
EDIA	analyze the electron density fit in crystallographic structures
METALizer	inspect the coordination geometry of metal ions in proteins
SIENA	compare binding sites and generate protein structure ensembles
ActivityFinder	annotate binding sites by ligands and their affinity/activity
Protoss	add missing hydrogens and predict protonation states
DoGSiteScorer	detect unexplored binding sites and predict their druggability
HyPPI	predict the interaction type of protein-protein interfaces
WarPP	place water molecules in ligand binding sites (knowledge-based)

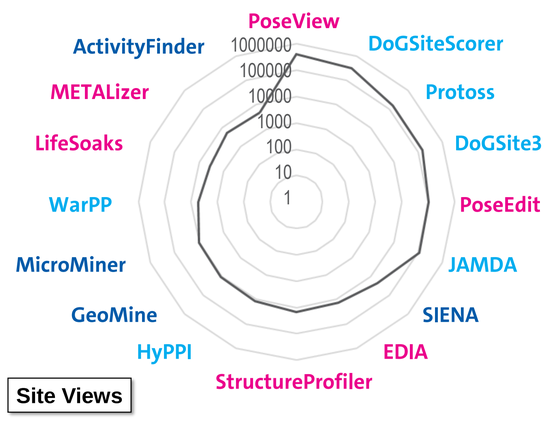
Progress Report

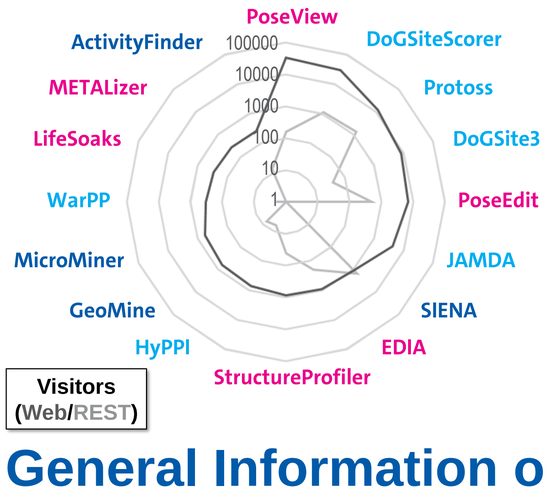
- New tools added to the Proteins*Plus* server
- Currently developing an easier maintainable successor of Proteins*Plus* where tools can be used in the style of a pipeline, e.g., calculate binding sites using DoGSite3, dock a ligand of interest using JAMDA, and visualize the interactions with PoseEdit

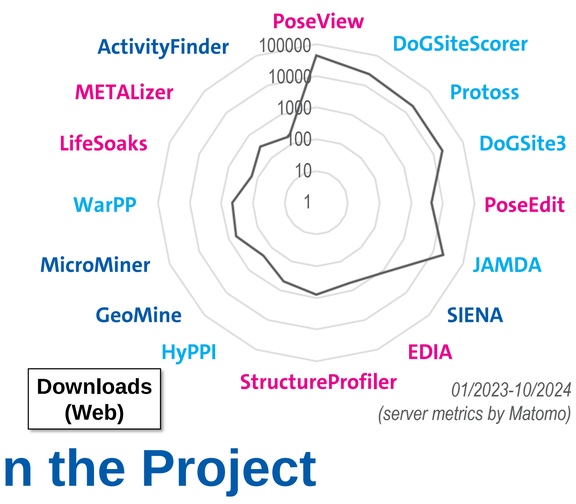


de.NBI services









01/2023-10/2024
(server metrics by Matomo)

de.NBI Training and Education

- Workshops
  "Proteins*Plus* – Supporting Structure-Based Design on the Web"
  - 4th CIC Summer School on Cheminformatics 2023 in Halle, Germany (August 21st-25th, 2023)
  - 36th Molecular Modeling Workshop in Erlangen, Germany (March 3rd-6th, 2024)
  - Spring School Structure-based Computer-aided Drug Design in Lausanne, Switzerland (June 10th-14th, 2024)
- Presentation of activities at the Science City Day in Hamburg

General Information on the Project

Staff paid from de.NBI grant (1.6 FTE)
- *Joel Graef (Services)*
- *Christiane Ehrt (Training)*
- *Gerd Embruch (Web Server)*

Other staff involved
- *Thorben Schulze*
- *Konrad Diedrich*
- *Martin Poppinga*
- *Emanuel Ehmki*
- *Florian Flachsenberg*
- *Jonathan Pletzer-Zelgert*
- *Jochen Sieg*

Modelling Support Server:
http://proteins.plus

SMARTS Pattern Server:
http://smarts.plus

NAOMI ChemBio Suite:
http://uhh.de/naomi

Publications

- Graef, J.; Ehrt, C.; Rarey, M. ***Binding Site Detection Remastered: Enabling Fast, Robust, and Reliable Binding Site Detection and Descriptor Calculation with DoGSite3***. *J Chem Inf Model* 63 (10), 3128-3137 (2023). doi: 10.1021/acs.jcim.3c00336
- Diedrich, K.; Krause, B.; Berg, O.; Rarey, M. ***PoseEdit: enhanced ligand binding mode communication by interactive 2D diagrams***. *J Comput Aided Mol Des* 37, 491–503 (2023). doi: 10.1007/s10822-023-00522-4
- Diedrich, K.; Ehrt, C.; Graef, J.; Poppinga, M.; Ritter, N.; Rarey, M. ***User-Centric Design of a 3D Search Interface for Protein-Ligand Complexes***. *J Comput Aided Mol Des* 38(1), 23 (2024). doi: 10.1007/s10822-024-00563-3
- Flachsenberg, F.; Ehrt, C.; Gutermuth, T.; Rarey, M. ***Redocking the PDB***. *J Chem Inf Model* 64 (1), 219-237 (2024). doi: 10.1021/acs.jcim.3c01573

GEFÖRDERT VOM
Bundesministerium für Bildung und Forschung