PL | Medicinal chemistry site

Institute of Biochemistry and Biophysics (IBB PAS)

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Prof. Dr. Piotr Zielenkiewicz (Head of Unit)

„I hope our involvement in EU-OPENSCREEN will not only increase the participation of Polish researchers in screening tests, but will also show the added value of in silico studies in search for the new drugs."

At a glance

- Bioinformatics platform for optimization of lead compounds structure
- A wide range of bioinformatics services provided by experienced scientists
- Methodology for the construction of protein-protein interaction peptide inhibitors
- Design of small molecule-, peptide- as well as peptidomimetic- inhibitors, and miRNAs as modulators of metabolism
- Physicochemical and ADME profiling (State of the art equipment and highly qualified staff performing experimental measurements)

Infrastructure and technical focus

- NEST computing cluster based on Intel and AMD processors, professional graphic computing cards and programmable coprocessor cards
- Large-scale in silico screening system, based on our molecular fitting solutions and machine learning based assessments
- Tools for the analysis and visualization of the results of large scale screening experiments, both experimental and in silico
- Systems biology tools, including reactome analysis and FBA/FVA
- Cheminformatics and Target Modelling Course

Projects past and present

2021 | Speeding up discovery for mutation diagnostic therapies in cystic fibrosis: an approach based on Artificial Intelligence and Systems Biology (VERTEX Innovation Award) Link

2019 | Integrated laboratory for large-scale gene and protein analyses

2018 | POL-OPENSCREEN (Polish Platform of Screening Infrastructure for Biological Chemistry) Link

Our science in selected publications

Development and evaluation of a deep learning model for protein-ligand binding affinity prediction
Bioinformatics, 2018, 34(21), 3666-3674

Open Drug Discovery Toolkit (ODDT): A new open-source player in the drug discovery field.
Journal of Cheminformatics, 2015, 7, 26

DeCAF-Discrimination, Comparison, Alignment Tool for 2D PHarmacophores
Molecules, 2017, 22 (7), 1128

DiSCuS: An Open Platform for (Not Only) Virtual Screening Results Management
Journal of Chemical Information and Modeling, 2014, 54(1), 347-354

Performance of machine-learning scoring functions in structure-based virtual screening.
Scientific Reports, 2017, 7, 46710

Further info and site-contact

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