**MolMeDB - Molecules on Membranes Database**

Jakub Juračka1,2, Kateřina Storchmannová1, Dominik Martinát1, Václav Bazgier1, Karel Berka1

1 Department of Physical Chemistry, Faculty of Science, Palacký University Olomouc, Czech Republic
2 Department of Computer Sciences, Faculty of Science, Palacký University Olomouc, Czech Republic

Biological membranes are natural barriers to cells. They play a key role in cell life and the pharmacokinetics of drug-like small molecules. A small molecule can pass through the membranes in two ways: via passive diffusion or actively via membrane transport proteins. There is a huge amount of data available about interactions of the small molecules with membranes and about interactions among the small molecules and the transporters.

MolMeDB (molmedb.upol.cz) is a comprehensive and interactive database of interactions of small molecules with membranes.1 From the start, we have collected data about partitioning and penetration of the small molecules crossing the membranes. Recently, we have expanded our area of interest to include interactions of small molecules with transporters and ion channels. Nowadays, more than 930,000 interactions for almost 500,000 molecules are available in MolMeDB.

The data within the MolMeDB is collected from scientific papers, our in-house calculations (COSMOmic/COSMOperm2), and obtained by data mining from several databases (e.g. ChEMBL, PubChem, The IUPHAR/BPS Guide to PHARMACOLOGY3). Data in the MolMeDB are fully searchable and browsable by name, SMILES, membrane, method, transporter, or dataset, and we offer collected data openly for further reuse. Also, the content of the database is available via REST API and the RDF model of MolMeDB (docs.molmedb.upol.cz).

**References**

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