

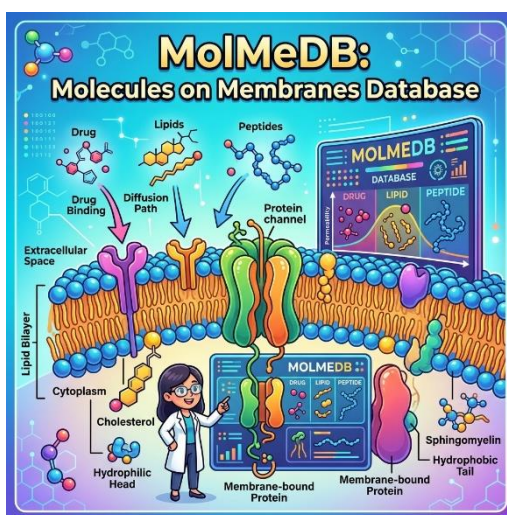
How small molecules interact with lipid membranes, as collected in MolMeDB database

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Interactions of small molecules with lipid membranes play a critical role in determining biological activity, pharmacokinetics, toxicity, and cellular transport. Understanding these processes—such as membrane permeability, partitioning, localization within the lipid bilayer, and energy barriers—is essential for rational drug design and biomaterial research. This lecture introduces MolMeDB (Molecules on Membranes Database) [1], a unique, open-access, and comprehensive repository integrating experimental and computational data on molecule-membrane interactions. Special attention is dedicated to the recent meta-analysis of permeability literature data by Kateřina Storchmannová et al., which comprehensively evaluates the possibilities and limitations of popular measurement and prediction methods for permeabilities.[2] Selected case studies will demonstrate how MolMeDB can be effectively utilized in pharmacology, toxicology, and molecular modeling to gain deeper insights into molecular behavior within biological contexts.

The authors would like to acknowledge support from the Czech Science Foundation (project 24-11986S)



[1] Juračka, J.; Šrejber, M.; Melíková, M.; Bazgier, V.; Berka, K. MolMeDB: Molecules on Membranes Database, Database, 2019, 2019, baz078.

[2] Storchmannová, K.; Balouch, M.; Juračka, J.; Štěpánek, F.; Berka, K. Meta-Analysis of Permeability Literature Data Shows Possibilities and Limitations of Popular Methods. Mol. Pharmaceutics 2025, 22 (3), 1293–1304.