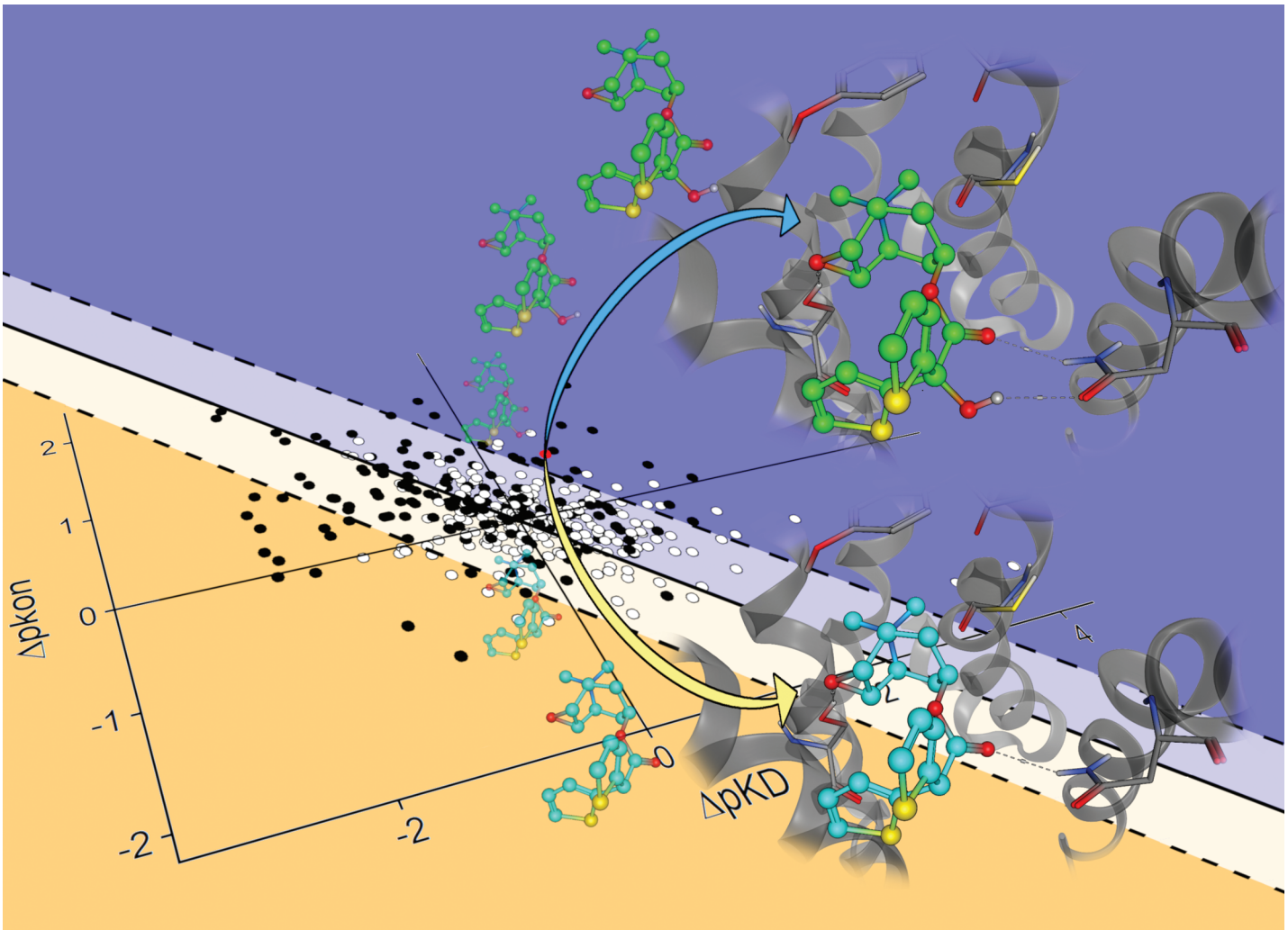

Showcasing research from Professor Ecker's Pharmacoinformatics research group, Department of Pharmaceutical Chemistry, University of Vienna, Austria.

A structure–kinetic relationship study using matched molecular pair analysis

In order to gain a better understanding of drug-target binding kinetics, the hitherto largest kinetic data collection called KIND (KINetic Dataset) has been assembled and released. Matched Molecular Pair analysis allowed to identify the fundamental contribution of a small molecule's polarity to the lifetime of a drug-target complex. The study showcases how molecular properties of small molecules trigger kinetic on- and off-rates.

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As featured in:

See Gerhard F. Ecker *et al.*, *RSC Med. Chem.*, 2020, **11**, 1285.

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