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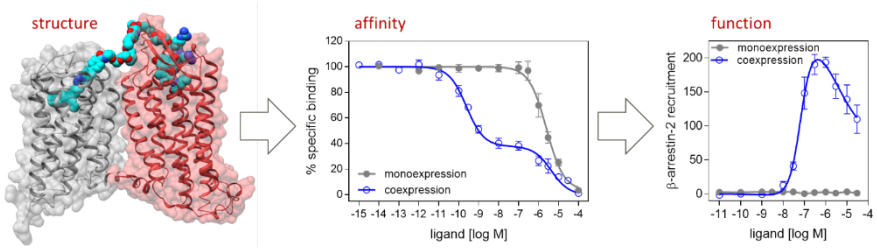
Research

G-Protein coupled receptors (GPCRs) are of particular interest as pharmaceutical target proteins in Medicinal Chemistry since a large number of diseases can be treated by selective GPCR agonists or antagonists. Using tailor-made ligands and probes we investigate the molecular interactions of ligands and GPCRs. A special focus is set on the development of biased ligands, which specifically orient the signaling of a GPCR towards a subset of the available signal transducers. These functionally selective ligands represent promising concepts for the development of novel therapeutics with reduced side effects.

Besides existing as monomers, GPCRs are known to form hetero- and homodimers or -oligomers. Using highly selective (hetero-)bivalent ligands and their monovalent congeners we aim to understand the functional consequences of GPCR dimerization and the specific interactions between bivalent ligands and GPCR dimers. Ultimately, (hetero-)bivalent ligands represent highly selective and unique pharmacological tool compounds which could lead to the development of novel drugs.



Teaching

Seminar on Drug Discovery (Master Molecular Life Sciences)

Publications

5 Structure-guided development of heterodimer-selective GPCR ligands. Harald Hübner, Tamara Schellhorn, Marie Gienger, Carolin Schaab, Jonas Kaindl, Laurin Leeb, Timothy Clark, Dorothee Möller and Peter Gmeiner. *Nat. Commun.* 2016, **7**, 12298.
DOI: 10.1038/ncomms12298.

4 Arrestin-Bound Rhodopsin: A Molecular Structure and its Impact on the Development of Biased GPCR Ligands. Dorothee Möller, Peter Gmeiner. *Angew. Chem. Int. Ed.* 2015, **54**, 13166-13168.
DOI: 10.1002/anie.201507724.
Die Rhodopsin-Arrestin-Kristallstruktur und ihre Bedeutung für die Entwicklung funktionell selektiver GPCR-Wirkstoffe. Dorothee Möller, Peter Gmeiner. *Angew. Chem.* 2015, **127**, 13362-13364.
DOI: 10.1002/ange.201507724.

3 1,4-Disubstituted aromatic piperazines with high 5-HT_{2A}/D_2 selectivity: quantitative structure selectivity investigations, docking, synthesis and biological evaluation. Dorothee Möller, Ismail Salama, Ralf C. Kling, Harald Hübner, Peter Gmeiner, *Bioorg. Med. Chem.* 2015, **23**, 6195-6209.
DOI: 10.1016/j.bmc.2015.07.050.

2 Functionally Selective Dopamine D_2, D_3 Receptor Partial Agonists. Dorothee Möller, Ralf C. Kling, Marika Skultety, Kristina Leuner, Harald Hübner and Peter Gmeiner, *J. Med. Chem.* 2014, **57**, 4861-4875.
DOI: 10.1021/jm5004039.

1 Pharmacological Profile of 2-Bromoterguride at Human Dopamine D_2, Porcine Serotonin 5-HT_{2A} and α_{2C}-Adrenergic Receptors, and its Antipsychotic-Like Effects in Rats. Florian Jantschak, Jan Brosda, Robert T. Franke, Heidrun Fink, Dorothee Möller, Harald Hübner, Peter Gmeiner and Heinz H. Pertz, *JPET* 2013, **347**, 57-68.
DOI: 10.1124/jpet.113.205997.