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Protein crystallography has become an integral part of modern pharmaceutical research. Recent technological advances have led to a rapid expansion of its role in low molecular weight drug discovery, from the traditional structure-based drug design approaches to fragment-based screening and the triaging, validation and characterization of high-throughput screening hits. Moreover, protein crystallography supports the design, optimization and characterization of novel therapeutic antibodies, a very fast-growing class of biological drugs. Our interest is in applying X-ray analysis, combined with other biophysical approaches (SPR, DSF, DSC, ITC, NMR, etc), to better understand molecular recognition processes such as ligand binding and protein-protein interactions, with the objective of supporting current drug discovery projects. In addition, a more fundamental research endeavor of our laboratory is to augment our structural understanding of cytokine-receptor signaling by determining crystal structures of selected, disease-relevant cytokine-receptor complexes.

Selected Publications

Discovery of cyclic sulfoxide hydroxyethylamines as potent and selective γ -site APP-cleaving enzyme 1 (BACE1) inhibitors: structure based design and in vivo reduction of amyloid γ -peptides.

[2]
Rueeger H, Lueoend R, Machauer R, Veenstra SJ, Jacobson LH, Staufenbiel M, Desrayaud S, Rondeau JM, Moebitz H, Neumann, U.
Bioorg Med Chem Lett. 2013 Oct 1;23(19):5300-6.

Discovery of cyclic sulfone hydroxyethylamines as potent and selective γ -site APP-cleaving enzyme 1 (BACE1) inhibitors: structure-based design and in vivo reduction of amyloid γ -peptides. [3]

Rueeger H, Lueoend R, Rogel O, Rondeau JM, Moebitz H, Machauer R, Jacobson L, Staufenbiel M, Desrayaud S, Neumann U.
J Med Chem. 2012 Apr 12;55(7):3364-86.

Ligand Binding: The Crystallographic Approach.

Rondeau JM, Klebe G, Podjarny A.

In "Biophysical Approaches Determining Ligand Binding to Biomolecular Targets. Detection, Measurement and Modelling" Podjarny A, Dejaegere A and Kieffer B, Eds. RSC Biomolecular Sciences No.22, RSC Publishing" 2011, Cambridge, UK.

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[3] <https://www.ncbi.nlm.nih.gov/pubmed/22380629>

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