

Protein-ligand binding kinetics

Franz-Josef Meyer-Almes

University of Applied Sciences Darmstadt, Germany



Abstract

Encyclopedia The importance of binding kinetics in terms of residence time and on-rate in drug discovery has been broadly accepted in the past few years. Furthermore, evidence has accumulated that the optimal binding mechanism of a drug to its target molecule is related to physiological efficacy as well as selectivity and thus drug safety. Homogeneous fluorescence-based binding assays have been shown to enable high throughput kinetics requiring only small amounts of protein. These assays can be used to elucidate even complex mechanisms of molecular recognition. A generalized approach is proposed that combines high quality kinetic and equilibrium data in an Integrated Global Fit analysis yielding the most probable binding mechanism. Arguments will be provided for the thesis that the relationship between quantitative kinetic and mechanistic information and chemical structures of active substances will serve as a valuable tool for drug optimization.

Speaker Publications:

1. Permuted 2,4-thiazolidinedione (TZD) analogs as GLUT inhibitors and their in-vitro evaluation in leukemic cells; European Journal of Pharmaceutical Sciences Volume 154, 1 November 2020, 105512
2. Structure guided design and synthesis of furyl thiazolidinedione derivatives as inhibitors of GLUT 1 and GLUT 4, and evaluation of their anti-leukemic potential; European Journal of Medicinal Chemistry, Volume 202, 15 September 2020, 112603
3. Synthesis and biological evaluation of pyrazoline and pyrrolidine-2,5-dione hybrids as potential antitumor agents; ChemMedChem, 2020 Jul 26. doi: 10.1002/cmdc.202000458
4. Repurposing approved Drugs as potential Inhibitors of 3CL-protease of SARS-CoV-2: Virtual screening and Structure Based Drug Design; Comput Biol Chem, 2020 Jul31;88:107351
5. Switching the Switch: Ligand induced Disulfide Formation in HDAC8; Chemistry, 2020 May 19. doi: 10.1002/chem.202001712

[5th Pharmaceutical Chemistry Conference](#); Webinar, - April27-28, 2020.

Abstract Citation:

Franz-Josef Meyer-Almes, Protein-ligand binding kinetics, Euro Pharma Chemistry 2020, 5th Pharmaceutical Chemistry Conference; Webinar, - April27-28, 2020.

(<https://pharmaceuticalchemistry.annualcongress.com/abstract/2020/protein-ligand-binding-kinetics>)



Biography:

Franz-Josef Meyer-Almes has completed his PhD at the age of 28 years from University of Goettingen. He has 10 years experiences in biotech and pharma companies. He is Professor for Physical Biochemistry and has published more than 40 papers in reputed journals and holds more than 10 patents and patent applications.