Maciej Bagiński, Assoc. Prof.

The possible offered Ph.D. thesis may cover different areas of computer-aided drug design. It includes molecular properties of drug targets, drug-target interactions as well as studies of new potential target inhibitors/modulators. All these studies will be performed using molecular modeling methods. In particular, proposed subjects may include studies on polyene macrolide antifungal antibiotics (amphotericin B and its derivatives), drug-DNA interactions, telomeric proteins and their interaction with telomeric DNA as well as membrane interacting systems (protein transporters) responsible for multi-drug resistance transporters.

List of papers:

1. A. Neumann, M. Baginski, J. Czub, How do sterols determine the antifungal activity of Amphotericin B? Free energy binding between the drug and its membrane targets. *J. Am. Chem. Soc.* 132, 18266-18272 (2010)
2. A. Neumann, M. Baginski, S. Winczewski, J. Czub, The effect of sterols on amphotericin B self-aggregation in a lipid bilayer as revealed by free energy simulations. *Biophys. J.* 104, 1485-1494 (2013)
3. J. Bidzinska, M. Baginski, A. Skladanowski, Novel anticancer strategy aimed at targeting shelterin complexes by the induction of structural changes in telomeric DNA: hitting two birds with one stone. *Curr. Cancer Drug Targets* 14, 201-216 (2014)
4. U. Kalathiya, M. Padariya, M. Baginski, Molecular modeling and evaluation of novel dibenzopyrrole derivatives as telomerase inhibitors and potential drug for cancer therapy. *IEEE-ACM Trans. Comput. Biol. Bioinform.* – 11, 1196-1207 (2014)
5. L. Nierzwicki, M. Wieczór, V. Censi, M. Baginski, L. Calucci, S. Samaritani, J. Czub, C. Forte, Interaction of cisplatin and two potential antitumoral platinum(II) complexes with model lipid membranes: a combined NMR and MD study. *Phys. Chem. Chem. Phys.* 17, 1458-1468 (2015)