

Biomodellab in Biological and Chemical Research Centre



HEAD:

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RESEARCH PROFILE:

- Investigations of drugs and proteins especially in biological membrane environments
- molecular dynamics simulations of biological systems
- study of activation processes in G-protein-coupled receptors (GPCRs)
- ligand docking to proteins and use of other methods for drug design
- interactions of proteins with graphene, carbon nanotubes and lipid cubic phases

CURRENT RESEARCH ACTIVITIES:

- Research on rhodopsin and other proteins involved in vision processes. Oligomerization of rhodopsin as a universal feature for other G-protein-coupled receptors (GPCRs). Large biological complexes of oligomeric rhodopsin with G protein and arrestin (publications 1-3)
- Study of activation processes of GPCRs (opioid receptors, adenosine receptors, serotonin receptors, and others) (publications 4-6)
- Homology modeling of GPCRs – construction of web service GPCRM (publications 7-8)
- Interactions of proteins with graphene and lipid cubic phases (publications 9-10)

SELECTED PUBLICATIONS:

1. S. Gulati, B. Jastrzębska, S. Banerjee, A. Placeres, P. Miszta, S. Gao, K. Gunderson, G. Tochtrop, S. Filipek, K. Katayama, P.D. Kiser, M. Mogi, P.L. Stewart, K. Palczewski, Photocyclic behavior of rhodopsin induced by a novel isomerization mechanism, *Proc. Natl. Acad. Sci. USA*. 114 (2017) E2608-E2615.
2. S. Filipek, K.A. Krzyśko, D. Fotiadis, Y. Liang, D.A. Saperstein, A. Engel, K. Palczewski, A concept for G protein activation by G protein-coupled receptor dimers: the transducin/ rhodopsin interface, *Photochem. Photobiol. Sci.* 3 (2004) 628-638.
3. D. Fotiadis, Y. Liang, S. Filipek, D.A. Saperstein, A. Engel, K. Palczewski, Atomic force microscopy: Rhodopsin dimers in native disc membranes, *Nature*. 421 (2003) 127-128.
4. S. Yuan, Q. Peng, K. Palczewski, H. Vogel, S. Filipek, Mechanistic studies on the stereoselectivity of the serotonin 5-HT1A receptor, *Angew. Chem. Int. Ed.* 55 (2016) 8661-8665.
5. S. Yuan, H.C.S. Chan, H. Vogel, S. Filipek, R.C. Stevens, K. Palczewski, The molecular mechanism of P2Y1 receptor activation, *Angew. Chem. Int. Ed.* 55 (2016) 10331-10335.
6. S. Yuan, K. Palczewski, Q. Peng, M. Koliński, H. Vogel, S. Filipek, The mechanism of ligand-induced activation or inhibition of mu- and kappa-opioid receptors, *Angew. Chem. Int. Ed.* 54 (2015) 7560-7563.
7. P. Miszta, P. Pasznik, J. Jakowiecki, A. Szttyler, D. Latek, S. Filipek, GPCRM: a homology modeling web service with triple membrane-fitted quality assessment of GPCR models, *Nucleic Acids Research*. 46 (2018) W387-W395.
8. D. Latek, M. Bajda, S. Filipek, A hybrid approach to structure and function modeling of G protein-coupled receptors, *J. Chem. Inf. Model.* 56 (2016) 630-641.
9. U. Ghoshdastider, R. Wu, B. Trzaskowski, K. Młynarczyk, P. Miszta, M. Gurusaran, S. Viswanathan, V. Renugopalakrishnan, S. Filipek, Molecular Effects of Encapsulation of Glucose Oxidase Dimer by Graphene, *RSC Advances*. 5 (2015) 13570-13578.
10. S. Viswanathan, T.N. Narayanan, K. Aran, K.D. Fink, J. Paredes, P.M. Ajayan, S. Filipek, P. Miszta, H.C. Tekin, F. Inci, U. Demirci, P. Li, K.I. Bolotin, D. Liepmann, V. Renugopalakrishnan, Graphene-protein field effect biosensors: glucose sensing, *Mater. Today*. 18 (2015) 513-522.