Modeling of Cellular Processes

HEAD:

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GROUP MEMBERS:

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RESEARCH PROFILE:

G protein-coupled receptors (structure prediction, drug design, signal transduction), Solute Carrier Transporters, web applications for computational biology & drug discovery, molecular dynamics simulations of cellular processes

CURRENT RESEARCH ACTIVITIES:

We are focused on transmembrane proteins involved in cell signaling and transportation. Our aim is to characterize them in two major aspects: structure and mechanism of action and as a consequence, we strive for drug discovery.
Main research areas include:

- drug design based on off-target interactions /virtual screening/
- mechanisms of GPCR activation /molecular switches/
- SLC transport cycle /toxins & drug metabolites efflux/
- structure modeling of GPCRs using multiple templates approach and sequence profiles comparison / GPCRM/
- drug design targeting GPCRs from class A and B using flexible-receptor Boost-implementing software /GUT-DOCK/
- NMR methods for biological systems /CABS-NMR, INPHARMA/

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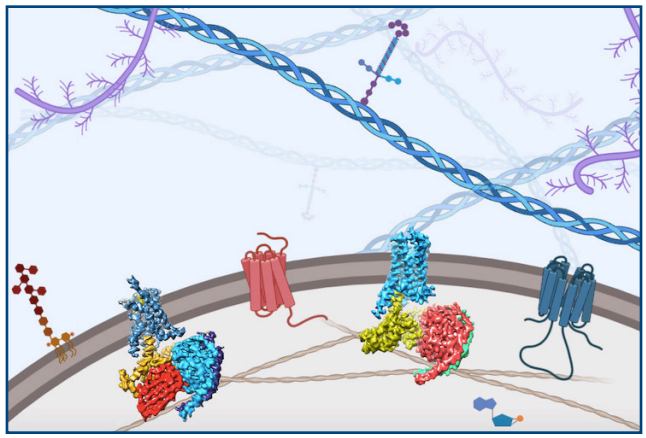

Fig. 1. Extracellular matrix with G protein-coupled receptors located in the cellular membrane. For more information, please visit: http://dlatek.chem.uw.edu.pl/. This figure has been prepared with BioRender (https://biorender.com/).

SELECTED PUBLICATIONS:

1. P. Pasznik, E. Rutkowska, S. Niewieczerzał, J. Cielecka-Piontek, D. Latek, Potential off-target effects of beta-blockers on gut hormone receptors: In silico study including GUT-DOCK—A web service for small-molecule docking, PLOS ONE. 14(1) (2019).
2. D. Latek, E. Rutkowska, S. Niewieczerzal, J. Cielecka-Piontek, Drug-induced diabetes type 2: In silico study involving class B GPCRs, PLOS ONE. 14(1) (2019).
3. D. Latek, I. Langer, K.A. Krzyśko, L. Charzewski, A Molecular Dynamics Study of Vasoactive Intestinal Peptide Receptor 1 and the Basis of Its Therapeutic Antagonism, Int J Mol Sci. 20(18) (2019) 4348.
4. D. Latek, P. Pasznik, T. Carlomagno, S. Filipek, Towards improved quality of GPCR models by usage of multiple templates and profile-profile comparison, PLOS ONE. 8(2) (2013).
5. D. Latek, M. Bajda, S. Filipek, A hybrid approach to structure and function modeling of G protein-coupled receptors, J Chem Inf Model. 56(4) (2016) 630-641.
6. P. Miszta, P. Pasznik, J. Jakowiecki, A. Sztyler, D. Latek, S. Filipek, GPCRM: a homology modeling web service with triple membrane-fitted quality assessment of GPCR models, NAR. 46(W1) (2018) W387–W395.
7. D. Latek, Rosetta Broker for membrane protein structure prediction: concentrative nucleoside transporter 3 and corticotropin-releasing factor receptor 1 test cases, BMC Struct Biol. 17(1) (2017) 8.
8. B. Trzaskowski, D. Latek, S. Yuan, U. Ghoshdastider, A. Dębiński, S. Filipek, Action of molecular switches in GPCRs-theoretical and experimental studies, Curr Med Chem. 19(8) (2012) 1090-1109.
9. S. Yuan, R. Wu, D. Latek, B. Trzaskowski, S. Filipek, Lipid receptor S1P1 activation scheme concluded from microsecond all-atom molecular dynamics simulations, PLOS Comp Biol. 9(10) (2013).
10. L. Skjærven, L. Codutti, A. Angelini, M. Grimaldi, D. Latek, P. Monecke, M.K. Dreyer, T. Carlomagno, Accounting for conformational variability in protein–ligand docking with NMR-guided rescoring, JACS. 135(15) (2013) 5819-5827.