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Methods Differentiating Agonists and Non-Agonists Binding to GPCRs (G-Protein-Coupled Receptors)

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G-protein-coupled receptors (GPCRs) represent the largest family of surface receptors, with approximately 800 members in human genome. The participation of GPCRs in numerous physiological and pathological processes entails a potential role for their modulation by ligands of various functions: agonists (increase receptor activity), antagonists (block the receptor not changing the activity), and inverse agonists (decrease activity). GPCRs are extremely important as molecular targets for drugs in medicine since their ligands are used in the treatment of many diseases including cardiovascular, mental disorders, cancer and viral infections. There is also well documented direct and indirect involvement of GPCRs on neurological disorders like Parkinson's and Alzheimer's diseases. Currently, approximately 30%-50% of drugs in clinical use exert their effects by acting on GPCR-mediated signaling pathways. It is estimated that global market for GPCRs reached over $100 billion therefore, the pharmaceutical industry is greatly interested in reliable methods to assess the function of GPCR ligands with their multi-dimensional spectrum of actions. The approaches used for GPCR agonist/non-agonist differentiation involve: the molecular fingerprints; ligand docking to active and inactive receptor structures; molecular dynamics and meta dynamics simulations, network correlation analysis, methods using specific parameters of the ligand binding site.

Biography:

Prof. Sławomir Filipek is a leader of Biomodeling Laboratory. His research interests are molecular dynamics simulations of biological systems mainly the membranous proteins and their complexes with small ligands and with other proteins. His research group investigates how the activation processes are going on in proteins, especially in G-protein-coupled receptors (GPCRs), and how the allosteric factors (lipids, ions) are influencing their functions. His group also performs ligand docking to proteins and employ a range of methods for drug design. In the material science area his group investigates how graphene, carbon nanotubes as well as lipid cubic phases interact with proteins.