Interactions between molecules constitute fundamental events in the processing of a biological information. The process of a ligand recognition in one of the most critical steps in signaling. Also ligand's residence time in a receptor is of crucial importance in regulatory processes of living organisms. Therefore, the association and dissociation mechanisms of the ligand-receptor complexes are extensively studied by theoretical and experimental techniques. To pass a signal, the ligand usually binds to a specific receptor docking site. Usually, before the ligand reaches the docking site, it may experience a complex migration through the channels or cavities accessible in a receptor. Uncovering distributions of ligand transport routes and egress pathways is important not only in understanding mechanisms of signal transductions, but also in molecular diseases (i.e. diabetes) and optogenetics. Structural biology is currently focused on biological molecules conformations in the ground electronic state. However, processes involving excited electronic energy play a crucial role in many biophysical phenomena, i.e. molecular recognition and ligand binding as well. The excitation to the excited state may be induced by light, which usually leads to the allosteric modification of its conformation. Therefore, the excited ligand entry/egress pathways in excited state may be fundamentally different than that in the ground state. The main objective of this project is to proceed with molecular dynamics simulations involving electronic excited states. We plan to study two model protein systems, channelrhodopsin (ChR) and EPAC2, both important in optogenetics. ChRs are light-gated cation channels derived from algae that have shown empirical utility in optogenetics (neurons expressing ChRs can be controlled via light even in such complex systems like moving mammals). Despite applying ChRs to neuroscience research, knowledge about molecular mechanism exploited by this proteins is very limited. In terms of structure, ChRs have seven-transmembrane part and contain the light-isomerizable chromophore all-*trans-retinal*. Thus, ChRs are perfect model for our novel methods of light induced ligand-receptor association and dissociation problem. The second protein - EPAC2 is promising player in a therapy of diabetes, a disease affecting 1:12 people worldwide. Recently, a possibility of optical control of insulin release from pancreatic beta cells has been opened. Based on existing drugs other authors have synthesized a compound JB235 that undergoes cis-trans photo-isomerization under blue light. This drug binds to the EPAC2 protein. When the light is switched on the cis-isomer of JB235 is being produced from the normal trans-form. That photon-induced transition modifies a structure of the EPAC protein receptor and that, in turn, exerts a positive effect of expulsion of insulin from the beta cell. Insulin may be therefore delivered to the body by simple shining photons on the activated cell, i.e. fully controlled, an optical release of insulin is possible. This opens new exciting possibilities in the research and the treatment. The aim of our project is to study the dissociation of JB235-EPAC2 complex in order to understand the molecular processes important in conformation changes accompanying JB235 transport in EPAC2. This novel methodology promises future advances that would shift the paradigm in the studies of excited ligand recognition process, which is a crucial aspect of developing selective drugs in brain-related diseases. Better understanding of the dissociation pathways of a ligand from the docking site will provide a knowledge necessary to build light-sensitive molecular “semaphores”, crucial in modern medicine.