Center of **C**omputational **S**tructural **B**iology (CCSB)

CCSB is focused on the application of computational tools and development of new algorithms to understand the biological mechanism of complex diseases at **molecular level**. The main research topic of our center revolves around the **structure and dynamics of proteins** which play a key role in all human diseases. We believe collaborations between computational groups like ourselves and experimental groups can contribute more to understanding these complex systems and ultimately **creating novel drugs**.

We are especially specialized in structural modeling of membrane receptor-ion channel complexes using enhanced **homology modeling techniques** as well as studying the activation mechanism upon ligand binding. We have strong experience on modeling of pentameric, **nicotinic acetylcholine receptors**, and tetrameric, **glutamate receptors**, ligand gated-ion channel proteins. Theoretical approaches such as normal mode analysis, molecular dynamics simulations, rigid body dynamics, and the analysis of the resulting trajectory by principal component analysis are some of the techniques which are frequently used in our group.

Our research work is based on **interdisciplinary approaches** for which our group members have several years of experience in the fields of computer science, structural biology, bioinformatics, organic chemistry of drug design & action, and statistics.

Our most recent success stories consist of a project funded by the Scientific and Technological Research Council of Turkey (TUBITAK) aiming to identify species-specific binding regions in glycolytic enzymes and their use in **allosteric drug design** studies. Our recently completed projects focused on investigating the mechanism of action in **membrane proteins** and its application in drug design. Other successfully completed projects incorporate the **biological activity of ion channels** such as glutamate receptors and the design of novel azole compounds with potential antifungal and anticonvulsant effects on GABA receptors.

Topics of Interest: We are looking for partners interested in H2020 calls: 1) SC1-BHC-32-2019: Towards a next generation influenza vaccine to protect citizens worldwide – an EU-India collaboration.

Role as an experienced partner: We can contribute to the deeper understanding of physical interactions governing the **function and dynamics of biological systems**, to unravel the **allosteric mechanism** and the **signaling pathways** in proteins. Moreover, we can perform ***in silico*** **screening** of potential drug candidates using a combination of **structure-based docking** and **pharmacophore** modeling approaches. Another value we can add as a group is our ability to develop **machine learning solutions**, including **deep learning architectures** for biological problems. Finally, we can assist in selecting promising vaccine candidates using computational prediction methods based on structural information of target receptors in the early stages of drug design discovery pipeline.

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