***In silico* approaches for exploring the functional mechanism of transmembrane proteins**

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The transmembrane proteins play a significant role in a broad range of biological processes, initiating cellular responses and signaling pathways. With significant progress in membrane protein structural biology over the past few years, cutting-edge biophysical and computational tools have been combined with vast amounts of experimental structural data to provide new insights. In this talk, our recent studies on transmembrane proteins will be presented. Focusing on three target proteins, i.e., adenosine receptor as a GPCR family, TRPV1 as an ion channel, and TM4SF5 as a tetraspanin family, it will be described how simulations have been successfully applied to elucidate structural, functional, and molecular interactions of protein families and their modulators.