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“Probing the dynamics of macromolecules and energetics of molecular interactions with high-performance, fast and accessible computational methods”

In this talk I will discuss recent methods developed within our group for ultra-massive virtual screening, protein engineering and understanding macromolecular dynamics all based on basic simple biophysical principles leading to fast, accessible and high-performing computational methods with examples of their application in the study of GPCRs, SARS-CoV-2 and Ebola.