
Titre du stage : Analyse de trajectoires de dynamique moléculaire

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Description du sujet :

We are looking for a motivated student to work on the analysis of Molecular Dynamics data on the regulation of a key enzyme of the neuronal signaling cascade.

We have carried out microsecond-scale molecular dynamics simulations of the Adenyl Cyclase (AC) enzyme alone and in complex with its regulator proteins. The simulations in presence of the activator proteins have shown how the interaction with the activator can promote the enzymatic activity by affecting the flexibility of the catalytic site [1].

Now we want to analyze the MD trajectories of the enzyme in presence of the inhibitor protein, and contrast these results with the enzyme alone and in complex with the activator. Trajectories have already been computed. The goal of the training is to analyze the trajectories.

[1] Frezza E, Martin J, Lavery R: **A molecular dynamics study of adenylyl cyclase: The impact of ATP and G-protein binding.** *PLOS ONE* 2018, **13**:e0196207.