Analyzing Conformational Ensembles using Machine Learning

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Aim: Molecular dynamics simulations enable to follow the time evolution of complex systems made of tens to hundreds of thousand of atoms with an atomistic resolution. Such an approach produces such an amount of data that it is difficult to analyze it by visual inspection. In this project we analyze large datasets using data analysis tools such as clustering, regression and classification algorithms. This will lead to the identification of the degrees of freedom (collective variables) that can help interpret the simulations and build mechanistic models of their function.

What will you do in practice? You will be given a set of simulations and will analyze them using python scripts. Basic scripts will be provided in the form of google Colab notebooks and one of your roles will be to modify them to fit the needs of the projects. You will interpret the results using molecular visualization tools.