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Specialty training : ~~—Research—~~ ☐ Professional ☐

a few key words to describe the subject of training :

Title of internship:

Comparison of M.D. based techniques for comparing affinities in a congeneric series.

this subject is a first step towards a thesis: ~~—Yes—~~ No

Short texte describing your project

Several techniques related to Molecular Dynamics are being advertised as predictive for ranking the binding thermodynamics or kinetics for new proposals at the lead optimization stage. The objective of the internship is to perform a critical comparison of more or less sophisticated techniques (ABMD, metadynamics, steered Molecular Dynamics, RAMD,...) in congeneric series on at least two targets.