Numerical simulations of proteins

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Propositions thesis

Numerical simulations of proteins: molecular dynamics, docking, and deep learning

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1. Computational modelling can be a powerful tool in enzyme design campaigns
2. A combination of computational methods can yield fast yet accurate workflows to model enzymatic activity
3. To verify that simulations represent reality, it is important to contrast predictions with experimental observations
4. The Rosetta score can be used as the objective function to guide the design of improved ω-transaminase variants
5. Enzymatic selectivity can be modelled via analysis of binding poses of the protein-ligand complex
6. Martini 3 allows the observation of protein-ligand binding events in unbiased molecular dynamics simulations
7. A neural network can learn to score unseen enzyme variants at millisecond-scale evaluation times
8. Deep learning is currently underused in molecular modelling workflows
9. Overspecialization kills creativity