

TITLE: In silico prediction of pBAE interactions with nucleic acids and in vitro confirmation

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DESCRIPTION: Poly(beta aminoester) (pBAE) polymers have demonstrated outstanding capability to encapsulate a variety of nucleic acids, forming small nanometric polyplexes that can efficiently and selectively deliver nucleic acids inside target cells after in vivo administration, leading to their expression. Although experimental results have shown that depending on the specific nucleic acid type, the use of a certain pBAE variant is preferable, there is not yet a systematic study focused on their rational selection.

Thus, the objective of the present master project is to use biocomputational tools, specifically machine learning algorithms, to predict the best pBAE variant for the encapsulation of a certain nucleic acid. The student will develop a machine learning model that uses experimental data on polymer characteristics and encapsulation efficiency to make accurate predictions. Additionally, molecular docking simulations will be employed to provide insights into the interactions between pBAE polymers and nucleic acids at the molecular level, with docking results integrated into the machine learning model to enhance prediction accuracy.

Through this approach, the student will learn biocomputational skills, complemented by experimental work in the laboratory to confirm the predictions. Wet lab confirmations will include the formulation of the polyplexes, their physico-chemical characterization, and in vitro safety and transfection efficiency evaluation.

SKILLS: nanoformulation, nanocharacterization, cell culture, Machine learning (ML) algorithms, molecular docking simulations, data analysis. (*Ability to work with Python or other computational tools for ML modeling, experience with software for docking simulations would be a plus*)