Molecular dynamics simulations of poly(2-oxazolines) for drug delivery applications.

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Poly(2-oxazolines) or POx are emerging as promising alternatives to polyethylene glycol (PEG) in drug delivery due to their biocompatibility, tunable properties, and high functionalization potential [1, 2]. To investigate how stereochemistry and solvent polarity influence their structural behavior, we conducted molecular dynamics (MD) simulations on chiral poly(2-oxazoline) polymers with varying side-chain compositions in different solvents. This study aims to provide molecular-level insights into how these molecular features influence the structural dynamics and stability of these polymers in drug formulation and drug delivery.

Simulations of enantiopure and racemic conformers of poly(2-propyl-4-methyl-2-oxazoline) (pPrMeOx), poly(2-ethyl-4-ethyl-2-oxazoline) (pEtEtOx), and poly(2-butyl-4-ethyl-2-oxazoline) (pBuEtOx) were conducted in methanol, ethanol, and butanol using GROMACS software with the OPLS-AA force field. The results show that solvent polarity and side-chain structure strongly affect polymer dynamics and stability.

Our findings offer valuable insights into the design of poly(2-oxazoline)-based drug delivery systems. Solubility and structural behavior are strongly influenced by chain length, side-chain composition, and enantiomeric ratio, indicating that optimizing these parameters can enhance drug formulation process. The agreement between our simulations and experimental data further supports these observations [3], highlighting the role of poly(2-oxazolines) for enhanced drug delivery applications.

References:

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