Molecular Dynamics simulations of Supramolecular Nanotubes containing Cancer Therapeutic

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Supramolecular structures have diverse applications, including drug delivery.[i] A well-known drug molecule camptothecin (CPT) is a proven cancer therapeutic that has been combined with other molecules to increase its biological activity and solubility properties in physiological conditions.[ii] TT1(a type of tubustecan) is one of such structures and has been shown to be more effective at treating certain types of cancer in biological studies when compared to CPT alone, owing to its increased efficacy due to the self assembling nanotubes it forms.[iii] Studies involving TT1 using Molecular dynamics (MD) simulations have focused on the initial stages of nanotube formation.[iv] Expanding on these results by simulating a Pre-formed nanotube using MD has allowed us to hone in on quantifiable predictors of these types of structures while also reducing computational cost.[v]

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[i] Bellavita et al., "An Overview of Supramolecular Platforms Boosting Drug Delivery."
[ii] Venditto and Simanek, "Cancer Therapies Utilizing the Camptothecins: A Review of in Vivo Literature."
[iii] Su et al., "Macrocyclization of a Class of Camptothecin Analogues into Tubular Supramolecular Polymers."
[iv] Tang et al., "Exploration of the Nucleation Pathway for Supramolecular Fibers."