Nov 7th, 4:15 PM - 5:30 PM

Computational Investigation of the Interactions Between Bioactive Compounds and Biological Assemblies

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Design of small molecules is an ongoing focus for developing agents against pathogenic viruses and bacteria that are threats to worldwide health. Viruses such as Zika feature assemblies of repeat peptide subunits or capsid proteins which are potential targets for antiviral compounds. Other protein assemblies are implicated in pathology of Alzheimer's Disease (AD) and additional neurodegenerative diseases characterized by large assemblies of misfolded proteins such as amyloid-beta (Aβ) and tau. Recent studies on a class of conjugated polyelectrolytes (CPEs) with phenylene ethynylene moieties and charged functional groups have shown potential both as bioactive antimicrobials and theragnostic sensing agents for tracking Alzheimer's based protein aggregates. A second type of small molecule, curcumin, is used as a therapeutic compound for a number of diseases including AD. Recent evidence shows that this molecule is able to interfere with fibril growth. In addition, curcumin attenuates Aβ-membrane interactions and Aβ toxicity. Our goal is to use computational techniques to better understand the interactions governing small molecule (including OPEs and curcumin) behavior when bound to capsid or fibrillar protein assemblies. We are focused on determining how and where these molecules bind in addition to comparing relative binding strength.