

CHEMISTRY

Fall 2023 SEMINAR SERIES

> 11am-12pm Oct 13th NC 1130

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"Supramolecular behavior of RNA/DNA modified with benzothiophenyl rings. A step towards functional materials"

Chemical modification of oligonucleotides of RNA and DNA enables their use as biomaterials, therapeutics, or in nanotechnology, amongst other applications. This presentation will describe the use of dodecamers of RNA/DNA as platform to generate distinct supramolecular structures, with potential use as nanowires and other 2D-networks. The biopolymers were functionalized with 2-methylbenzothiophene groups at the C2'-O-position. The structural impact varied as a function of salt (monocation) concentration. Circular dichroism (CD) displayed features that were consistent with interstrand interactions amongst the S-containing aromatic rings, as a function of increased [Na+]. Interestingly, thermal denaturation transition measurements displayed a rearrangement that was consistent with the formation of a more stable structure at temperatures above 50° C. To rationalize this observation, the duplexes were modeled using the density functional theory-polarizable continuum model (DFT-PCM). A proposed mechanism involves the hydrophobic surface allowing for an internal nucleobase rearrangement (via H-bonding) into a more thermodynamically stable structure, before undergoing full denaturation, with increased heat. The arrays that are templated, as a function of number and position of the studied chemical modification, self-assemble into distinct motifs with potential as biomaterials, an approach that will be described.

For more information see: https://clas.ucdenver.edu/chemistry/seminars-and-events