ACS Local Section
North Jersey

Connecting Chemical Shifts to Structure for Proteins and Nucleic Acids

Speaker: **Prof. David A. Case**
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Date: **May 19th, 2022**

Time: 12:00 pm ET via Microsoft Teams

Abstract

An automated fragmentation quantum mechanics/molecular mechanics approach (AFNMR) has shown promising results in chemical shift calculations for biomolecules. Trends in chemical shift are stable with regards to change in density functional or basis sets, and the use of the small "pcSseg-0" basis, which was optimized for chemical shift prediction, opens the way to more extensive conformational averaging, which can often be necessary, even for fairly well-defined structures. There have also been recent advances in the use of machine learning approaches to develop empirical connections to structure. I will discuss prospects for using both types of calculations to gain insights into biomolecular structure and dynamics.

Connection Information

This will be a virtual meeting hosted via Microsoft Teams. A direct link to the meeting is located HERE. Further information can be found on the NMR Topical Group website (https://www.njacs.org/nmr-spectroscopy-topical-group). Please reach out to Jonathan Williams (jwilliams@njacs.org) or Tom Popp (thomas.osbornpopp@rutgers.edu) with any questions.

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