

# Physical Chemistry Seminar

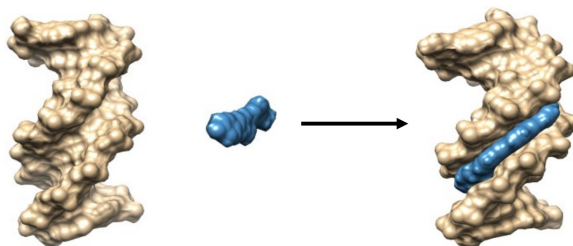
## Elucidating Small Molecule- DNA Binding Mechanisms with Molecular Dynamics Simulations

**Steve Corcelli**

Professor and Chair of the  
Department of Chemistry and Biochemistry  
University of Notre Dame



Biomolecular binding is ubiquitous and central to biological function. However, the detailed molecular mechanisms by which small molecules bind to DNA are not well understood. The tremendous computational power of graphics processor units (GPUs) combined with advanced sampling algorithms such as weighted ensemble (WE) offers the opportunity to use molecular dynamics (MD) to simulate such binding processes directly. Moreover, harvesting and analyzing a statistically meaningful ensemble of binding events allows for unprecedented mechanistic understanding. Here, we have applied WE to simulate the binding of a minor groove ligand (Hoechst 33258) and an anti-cancer intercalator (daunomycin) to double-stranded DNA. The simulations reveal new insights about specific biomolecular and hydration dynamics involved in the binding processes.



Wednesday, February 19, 2025



10:30am



BRWN 4102



**PURDUE**  
UNIVERSITY®

James Tarpo Jr. and Margaret Tarpo  
Department of Chemistry

## Corcelli Bio

Dr. Corcelli is a theoretical chemist whose research focuses on the structure, dynamics, and spectroscopy of molecular and biomolecular solutes in solution. He graduated from Brown University in 1997 (Sc.B. in Chemistry). In 2002, he was awarded a Ph.D. from Yale University, where he trained with Dr. John Tully. From 2002 – 2005, he was a postdoctoral scholar with Dr. Jim Skinner at the University of Wisconsin-Madison. Dr. Corcelli began his independent academic career in 2005 at the University of Notre Dame, where he has been the grateful recipient of several awards, including the Camille and Henry Dreyfus New Faculty Award, an NSF CAREER Award, and a Sloan Research Fellowship. Dr. Corcelli was promoted to Associate Professor in 2011 and to Professor in 2017. He has published over 90 research papers and given over 100 invited presentations. He has twice won the Rev. Edmund P. Joyce, C.S.C. Award for Excellence in Undergraduate Teaching (2012 and 2019), as well as the Thomas P. Madden Award for Excellence in Teaching First-Year Undergraduates (2020). Dr. Corcelli served as the Associate Dean of Interdisciplinary Programs and Faculty Development in the College of Science (2019-2022) and is now Chair of the Department of Chemistry and Biochemistry (2022-present).