

ASRC - City College of New York

Seminar in Biochemistry, Biophysics & Biodesign

SEMINAR LOCATION:

ASRC Main Auditorium
85 St. Nicholas Terrace

For non-CUNY attendees,
advance registration is required;
please contact Hyacinth
Camillieri at
hcamillieri@gc.cuny.edu

THE SEMINAR WILL ALSO BE AVAILABLE VIA ZOOM:

[Click here for Zoom link](#)

Meeting ID: 916 3796 4386

Passcode: asrc+ccny

HOST:

Kevin Gardner

kgardner@gc.cuny.edu

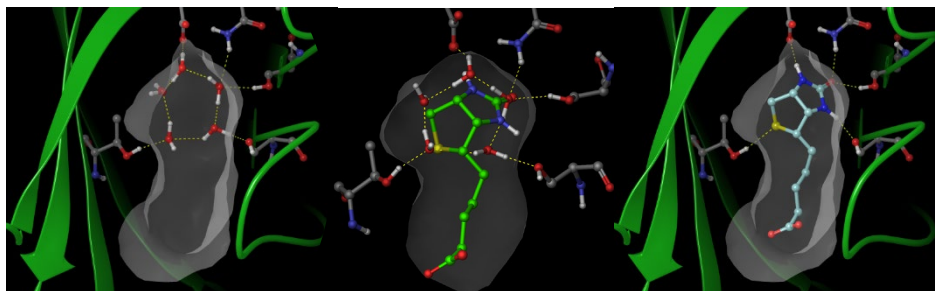
FOR MORE INFORMATION, CONTACT:

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Wednesday, February 21, 2024

Coffee & tea 11:30 AM

Seminar 12:00-1:00 PM

Thomas Kurtzman

Professor, Department of Chemistry
Lehman College, New York, NY

How can water structure and thermodynamics inform lead drug discovery and design?

ABSTRACT Water plays an instrumental role in the recognition between small molecule drugs and their biomolecular targets. When a drug is unbound, the structure and thermodynamics of water in the binding site reveal information that can be used to inform the discovery of lead drug compounds and their subsequent rational optimization. We will discuss how computer simulations and statistical mechanical liquid state theory can be used to map out the properties of water on the surface of proteins and how these ‘maps’ may be used to improve modern drug discovery and optimization efforts.

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