You are cordially invited to a talk in the Edmond J. Safra Center for Bioinformatics Distinguished Speaker Series.
The speaker is Prof. Tom Kurtzman, Department of Chemistry, Lehman College, City University of New York

Title: "Exploiting active site solvation structure and thermodynamics for drug discovery and design"

Time: Sunday, March 11 2018, at 11:15 sharp (refreshments from 11:00)

Place: Sherman 631, Life Sciences Faculty

Host: Prof. Nir Ben-Tal, bental@tauex.tau.ac.il, Life Sciences Faculty, TAU

Abstract: Understanding the underlying physics of the binding of small-molecule drugs to protein active sites is a key objective of computational chemistry and biology. The displacement and reorganization of water molecules from the active site upon the binding of a ligand is a principal, and often dominant, source of binding free energy. We will discuss how statistical mechanics and molecular dynamics simulations help characterize the solvation of protein active sites and how this information may be incorporated into computational tools aimed at aiding early stage drug discovery and design efforts.