

Seminar 2016

Entropy in molecular recognition by proteins



A. Joshua Wand Professor, Department of Biochemistry & Biophysics University of Pennsylvania Perelman School of Medicine At a fundamental level, biological processes are most often controlled using molecular recognition by proteins. Protein-ligand interactions impact critical events ranging from the catalytic action of enzymes, the assembly of macromolecular structures, complex signaling and allostery, transport phenomena, force generation and so on. The physical origin of high affinity interactions involving proteins continues to be the subject of intense investigation. Conformational entropy represents perhaps the last piece of the thermodynamic puzzle that governs protein structure, stability, dynamics and function. The presence and importance of internal conformational entropy in proteins has been debated for decades but has resisted experimental quantification. Over the past few years we have introduced, developed and validated an NMR-based approach that uses a dynamical proxy to determine changes in conformational entropy. This new approach, which we term the NMR "entropy meter," requires few assumptions, is empirically calibrated and is apparently robust and universal.

Please see Laufer Center website for full abstract.

Friday December 2, 2016

2:30 PM Laufer Center Lecture Hall 101

Host: Ken Dill

Refreshments: Hub 110 after seminar



