# NIMBioS

**National Institute for Mathematical and Biological Synthesis**

**The National Institute for Mathematical and Biological Synthesis**

cordially invites you to an

## Interdisciplinary Seminar

# Dr. Quentin Johnson

on

## *"Utilizing computational methods to predict allosteric networks in protein complexes"*

**Tuesday, October 20, 2015**

3:30-5 p.m.
*Reception & refreshments at 3 p.m.*

Hallam Auditorium, Room 206
1122 Volunteer Boulevard

**Quentin Johnson** (Ph.D., Life Science/Genome Science and Technology, Univ. of Tennessee, Knoxville, 2015) is developing a model to identify allostery and the mechanism by which the allosteric signal is initiated and propagated in the peroxisome proliferator-activated receptor and retinoid X receptor complex, which are proteins involved in preventing growth of cancer cells.

**Abstract:** Allostery is a fundamental control mechanism used to regulate many biological processes that range from ligand binding to transcriptional activation. In the context of proteins and protein complexes, allostery is the ability of one binding site to influence another distant site. This means that proteins can self-regulate or be regulated by other macromolecules without the need for proximity. This type of distal signaling is used as the basis for molecular switches, cellular signaling, and oxygen transport. While the importance of allostery is well appreciated, a clear understanding of the process still eludes modern science. This is chiefly due to the fact that the residual networks involved in this process are vast and complex, also the physical interactions that sustain these networks occur on an atomistic level and a picosecond timescale. Therefore, it can be quite vexing to study allostery using traditional methods. Still, the rewards far outweigh the frustrations, as an understanding of allostery can lead to the physical control of molecular switches and downstream cellular responses. Here, I discuss a novel computational approach for the detection of allostery in protein complexes by way of molecular dynamics simulation and advanced data reduction protocols.

**The seminar will be live streamed. Visit
http://www.nimbios.org/videos/livestream.
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