Joint Math Colloquium

Millersville University and Franklin & Marshall College

Speaker: **Dr. Jason Labonte**
Department of Chemistry
Franklin & Marshall College

Topic: **RosettaCarbohydrate: Using Geometry & Statistics to Predict the Structures of the "Forgotten" Biopolymer**

Date: **November 1, 2018 (Thursday)**

Time: **4 – 5 p. m.**

Place: **Stager 219, Franklin & Marshall College**

Contact: **Baoling Ma (717) 871-4263 Baoling.Ma@millersville.edu**
Kevin S. Robinson (717) 871-7313 krobinson@millersville.edu

Abstract: In 1969, Professor Levinthal presented a mathematical paradox: Even if huge approximations were made, and even if we could sample a conformation every picosecond, it would take longer than the age of the universe to enumerate all the conformations of a protein to find the most stable one. Nevertheless, Nature can find the most stable conformation in only milliseconds!
Rosetta is a computational modeling tool that tries to solve this problem, not by sampling every conformation but by sampling random conformations in a Monte-Carlo–minimization method and relying on statistical "scoring" to recognize "good" protein structures. Unfortunately, proteins are not the only biopolymer out there. Carbohydrates have largely been ignored by modelers, because they are supposedly even more "floppy" and hard to model than proteins. My research seeks to expand on Rosetta's modeling algorithms with sugar-specific statistical and geometrical insights, teaching Rosetta to recognize favorable carbohydrate interactions.

All are Welcome