



BIOINFORMATICS 2016 FALL SEMINAR SERIES

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<http://bioinformatics.udel.edu/Seminars/Current>

MONDAY, February 8, 2016
3:30pm
DBI Room 102

**Accurate Scoring of Drug Conformations
at the Extreme Scale**

Michela Taufer

***David and Beverly J.C. Mills Career Development Chair
Computer and Information Sciences***

Acting Director, Center for Bioinformatics and Computational Biology

Acting Director, Master's Programs in Bioinformatics & Computational Biology

Acting Director, PhD Program in Bioinformatics & Systems Biology

ABSTRACT: In this talk we present a scalable method to extensively search for drug candidates in large distributed datasets of drug conformations. For each conformation in the dataset, our method first extracts relevant geometrical properties and transforms the properties into a single metadata point. Then, the method performs an octree-based clustering on the metadata to search for predominant clusters. We scale the analysis of our datasets a factor of 400X higher in performance and 500X larger in size than ever before. We also show that our method achieves higher accuracy compared with that of traditional methods.