Katedry informatiky a aplikovanej informatiky FMFI
Katedry genetiky a biochémie PriF UK
a občianske združenie *NATURA*

Vás pozývajú na 122. prednášku v rámci Kuželových seminárov:

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USING CHEMISTRY TO UNDERSTAND GENOMIC DATA

ktorá sa uskutoční **24. novembra 2021** (streda) o **14:00**

hybridnou formou:
Prezenčne (pre plne zaočkovaných): FMFI UK, poslucháreň C
online: https://bit.ly/3ogObXo

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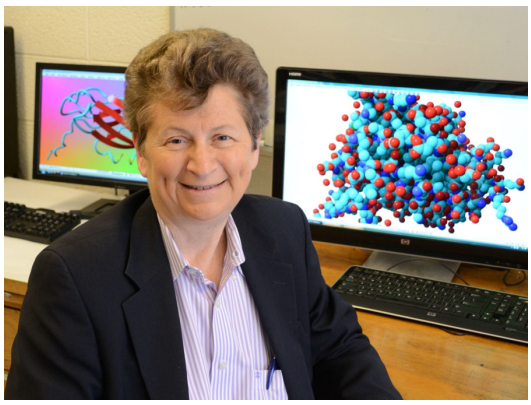

1974: B.A., Chemistry, Reed College, Portland, OR, USA
1978: Ph.D., Physical Chemistry, Northwestern University, Evanston, IL, USA
1978-1980: Postdoctoral Researcher, University of Chicago, IL, USA
1980: NATO Postdoctoral Fellow, Tel-Aviv University, Israel
1980-present: Faculty member, Northeastern University, Boston, MA, USA

Prof. Ondrechen's research group develops novel computational methods, and also deploys established computational and informatics methods, for structure-based drug design, for understanding enzyme function, for understanding key interactions within protein structures, for enzyme design, for genomics studies, and for prediction of protein function.

Over 15,000 Structural Genomics (SG) protein structures have been deposited in the Protein Data Bank (PDB) and most of these are of unknown or uncertain biochemical function. Typically, functions are assigned using informatics approaches based on similarities in sequence and/or 3D structure. However similar sequence or similar structure does not always imply similar function.The annotation of protein function by automated means has led to high rates of misannotations in some databases. A complementary and powerful approach is presented, based on computed chemical properties of the individual amino acids in a protein structure. Partial Order Optimum Likelihood (POOL) is a machine learning method that predicts the amino acids in the query protein structure that are important for catalysis. Local arrays of POOL-predicted residues of the query (SG) protein are aligned with those of proteins of known function. These alignments, each SG protein against each known functional family, are scored to predict the most likely function of the SG proteins. Results are reported for the SG members of the Ribulose Phosphate Binding Barrel (RPBB), Clp-Crotonase, and Haloacid Dehalogenase superfamilies. Of particular interest are cases of predicted misannotation, where our prediction differs from that of the assigned function. Experimental testing of our predictions is performed by direct biochemical assays. Supported by the U.S. National Science Foundation under grant number CHE-1905214.

Selected publications:

"Amino acid interactions that facilitate enzyme catalysis," Timothy A. Coulther, Jaeju Ko, and Mary Jo Ondrechen, J. Chem. Phys. 154, 195101 doi.org/10.1063/5.0041156 (2021).
"Reintegrating Biology Through the Nexus of Energy, Information, and Matter," Kim L. Hoke, Sara L. Zimmer, Adam B. Roddy, Mary Jo Ondrechen, Craig E. Williamson, Nicole R. Buan, Integrative and Comparative Biology, https://doi.org/10.1093/icb/icab174 (2021).
"Analysis of electrostatic coupling throughout the laboratory evolution of a designed retroaldolase," Timothy A. Coulther, Moritz Pott, Cathleen Zeymer, Donald Hilvert, Mary Jo Ondrechen, Protein Science, 30(8), 1617-1627 (2021).
"Functional classification of protein structures by local structure matching in graph representation," Caitlyn L. Mills, Rohan Garg, Joslynn S. Lee, Liang Tian, Alexandru Suciu, Gene Cooperman, Penny J. Beuning, Mary Jo Ondrechen, Protein Science 27, 1125-1135 (2018).
"Prediction of distal residue participation in enzyme catalysis," Heather R. Brodkin, Nicholas A. DeLateur, Srinivas Somarowthu, Caitlyn L. Mills, Walter R. Novak, Penny J. Beuning, Dagmar Ringe, Mary Jo Ondrechen, Protein Science 24 (5), 762-778 (2015).
"Protein Function Annotation with Structurally Aligned Local Sites of Activity (SALSAs), Zhouxi Wang, Pengcheng Yin, Joslynn S. Lee, Ramya Parasuram, Srinivas Somarowthu," and Mary Jo Ondrechen, BMC Bioinformatics, 14(Suppl 3):S13 (2013).