

# ISMB 2005 Tutorial Proposal

**Title:** Computational Geometry of Protein Structure and Function

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## Other relevant qualifications and teaching experience:

- Associate Director of Bioinformatics, NLM Duke-UNC Training Program in Medical Informatics (1999-2000).
  - Director of Computational Resource for Molecular Sciences and Bioinformatics, University of North Carolina at Chapel Hill (1996-2000).
  - Participated in Bioinformatics and Computational Biology curriculum development at the University of North Carolina and George Mason University.
  - Developed and taught graduate courses (high rating by students for all courses taught):
    - [\*Biomolecular Informatics: Sequence to Structure to Function\*](#), BIOC 156, University of North Carolina at Chapel Hill, 1998-present, taught 6 times;
    - [\*Computational Protein Structure Analysis\*](#), BINF 731, George Mason University, 2000-present, taught 4 times;
    - [\*Structural Genomics\*](#), BINF 739, George Mason University, 2002-present, taught twice.
- Developed and taught a Bioinformatics module for the ACS short course in Computational Chemistry and Drug Design (offered 6 times in 2001-2003).  
Developed and taught a Bioinformatics module for the Carolina Workshops in [1995](#) and [1996](#).  
Developed and taught a tutorial at ISMB '95, Cambridge, UK.  
Taught in a number of other [courses and tutorials](#) (more than 500 students total).

**Summary and goals:** The tutorial covers theoretical approaches, techniques and computational tools for computational geometry approach to protein structure analysis, classification, and prediction. Students will acquire knowledge of fundamental principles and methods for protein structure analysis, as well as practical skills necessary to use modern computational tools for such analysis.

**Intended audience:** This tutorial is designed for scientists and graduate students with various backgrounds who have some experience in/exposure to methods and tools for DNA and protein sequence analysis, but no or little experience in protein structure analysis and prediction.

**Length:** Half day

**Presentation outline:**

In the computational geometry methods the nearest neighbor atoms or groups of atoms are identified by statistical analysis of irregular polyhedra obtained as a result of a specific tessellation in three-dimensional space. Voronoi tessellation partitions the space into convex polytopes called Voronoi polyhedra. For a biomolecular system the Voronoi polyhedron is the region of space around an atom, such that each point of this region is closer to the atom than to any other atom of the system. A group of four atoms whose Voronoi polyhedra meet at a common vertex forms another basic topological object called a Delaunay simplex. Delaunay simplices define objectively the nearest neighbor entities in molecular systems. The tutorial will cover applications of computational geometry methods to various problems of protein structure and function, including:

- residue volumes and packing density
- atom-atom and residue-residue contacts
- statistical potentials
- structure classification
- fold recognition
- computational mutagenesis
- functional sites identification