

**PHYSICS AND ASTRONOMY SEMINAR
SPRING 2009**

**GRAPH THEORY MODELS IN
MOLECULAR BIOLOGY**

DEBRA KNISLEY
Department of Mathematics
ETSU

A number of molecular descriptors of small molecules are derived from graphical representations of the molecule. These descriptors, sometimes called topological indices, are used to identify or relate the structure of a molecule with expected bioactivity and they are an essential tool in the drug design industry. It is generally accepted that these molecular descriptors are not applicable to macromolecules. However, topological indices are equivalent to graphical invariants in graph theory. Graph theory offers a wealth of graphical invariants annotated with structural implications, primarily for large graphs. Thus we consider applying known graphical measures to quantify macromolecules, including secondary RNA structures, amino acids and several families of proteins.

Monday, March 23, 2009, 4:00 pm
Brown Hall 261

Refreshments served at 3:45 pm