

Meeting: 1003, Atlanta, Georgia, SS 9A, AMS-MAA-SIAM Special Session on Research in Mathematics by Undergraduates, I

1003-05-171 **Daniel Lamb*** (petetownshend@earthlink.net) and **Bradley Wild**. *Proteins as Simple Graphs*. Preliminary report.

Tertiary protein structures can be modeled as simple graphs in various ways. In this paper, we use two methods. In one method, secondary protein substructures are represented by specified subgraphs and edges are determined by proximity. In the second method, secondary proteins substructures are represented by weighted edges. Edges are incident if the corresponding secondary structures are adjacent on the backbone trace or if they satisfy a distance constraint. Given the simple graph, we then quantify structural parameters by graphical invariants such as eigenvalues, diameter and radius. (Received August 17, 2004)