Using Neural Networks to Classify Three Dimensional Hint Maps

[1]Nathan Smith and [2]Glenn Kellogg

[1]Dept. of Computer Science, Grinnell College
[2]Dept. of Medicinal Chemistry, Virginia Commonwealth University

Hint is a program/paradigm that derives a non-covalent force field from partitioning coefficient between 1-octanol and water. The Hint program is capable of producing three-dimensional maps of both polar and hydrophobic interactions. While these maps are currently used for visualization there is a great deal of mathematical data encoded within them. It is hypothesized that HINT maps of the interactions between residues and the proteins in which they reside can be used to classify environments for individual amino acids. If a set of typical environments could be derived from this information it would then be possible to apply this information to low-resolution crystallographic maps to evaluate the most likely placement of a particular residue. Artificial neural networks a form of artificial intelligence are currently being used to extract useful features from maps