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Structural Bioinformatics of Protein-Bound Water. Christopher Bottoms, Tommi White, John J. Tanner, Dept. of Chemistry, Univ. of Missouri-Columbia, MO.

Individual water molecules play specific roles in protein catalysis, in substrate binding, and in the protein structure itself, often bridging amino acid residues within or between secondary structural elements. These roles become especially apparent when water molecules are repeatedly found associated with similar structural motifs in protein families.

We describe a novel computational method of identifying structural solvent motifs within families of protein structures. The method is based on Fourier analysis of the distribution of water molecules in protein families. This method has been validated by successful identification of "known" (i.e. previously described in the literature) as well as "novel" structurally conserved solvent sites in cytochrome C, fatty acid binding proteins, Rossmann-fold dinucleotide-binding proteins, and parvalbumins.

Figure: Structurally conserved solvent sites of cytochrome C, shown with 1YTC1 as the reference protein.

