

## MULTIPLE SEQUENCE ALIGNMENT AND HOMOLOGY MODELING OF SULFOTRANSFERASE ENZYMES

**Keith W. Burdick and Irwin D. Kuntz**  
University of California, San Francisco

burdick@elsinore.compchem.ucsf.edu

Members of the sulfotransferase superfamily of enzymes catalyze the transfer of a sulfuryl group from 3'-phosphoadenosine 5'-phosphosulfate to a wide variety of substrates—ranging from small organic molecules to proteins. The sulfotransferases can be divided into families based on substrate: aryl sulfotransferases, carbohydrate sulfotransferases, and protein sulfotransferases. In addition, there are multiple families of carbohydrate sulfotransferases including nodH, CHST2, and CHST4. Though a few common motifs are shared across the families, the global sequence similarity between the families is low (14–20%), making it difficult to align sequences from disparate families. Aided by the use of secondary structure predictions and analysis of patterns of conserved residues, a global sequence alignment of the sulfotransferases was produced. To translate sequence to structure, the crystal structure of estrogen sulfotransferase was used as a template in modeling the nucleotide binding site of four sulfotransferases. The models propose a similar binding mode across the families and suggest targets for mutations to probe nucleotide binding.