Contributors to this Issue

Cover Photograph, *Bioorganic & Medicinal Chemistry Letters*

2002: Representation of the inhibitor celecoxib in the active site of the COX-2 enzyme. The model has been derived from the 1cx2 crystal structure via docking and force-field calculations [Price, M. L. P.; Jorgensen, W. L. *J. Am. Chem. Soc.* **2000**, *122*, 9455–9466]. Monte Carlo simulations have then been used to develop a computational model to reproduce the observed activities of 45 celecoxib analogues [Wesolowski, S. S.; Jorgensen, W. L. *Bioorg. Med. Chem. Lett.* **2002**, *12*, 267]. In the illustration, the shading reflects the distance between atoms of the inhibitor and the protein: the more red, the shorter the distance. The deep red region near the sulfonamide group includes residues H/R 513 and I/V 523, which provide the primary differences between the COX-1 and COX-2 binding sites. The figure was prepared using the Sybyl program by Dr. Erin M. Duffy.