# Computer-Aided Design of a New Class of Potent and Selective Inhibitors of Cyclooxygenase 2(COX2), a Key Enzyme in the Inflammatory Pathway

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***Abstract***

Non-steroidal anti-inflammatory drugs (NSAIDs) have been the therapeutic agents of choice for more than a century. However, their adverse gastrointestinal side-effects led to the advent of COX2 selective inhibitors, the coxibs. Recent reports on the harmful cardiovascular and renal side-effects of the conventional NSAIDs as well as the COX2 selective inhibitors valdecoxib and rofecoxib have once again led to the quest for a novel class of inhibitors. Using a structure-based approach, a small, potent and selective peptide inhibitor of COX2 has been identified. The designed peptide is predicted to have a higher activity than the most potent, known inhibitor (celecoxib), and a 800-fold selectivity for COX2 over COX1. It is thus a promising lead compound for the development of a new class of COX2 selective inhibitors.

*Key words*: Structure-based drug design, Cyclooxygenase, Docking, Peptide inhibitor, Anti-Inflammatory drugs.