### CHEMICAL BIOLOGY & DRUG DESIGN

### **TABLE OF CONTENTS**

#### Inaugural Issue of Chemical Biology & Drug Design – January 2006

#### Editorial

**Chemical Biology & Drug Design: Inaugural issue!** (by Tomi Sawyer, ARIAD Pharmaceuticals and University of Massachusetts, USA)

#### Perspective

**Overcoming roadblocks in lead optimization: A thermodynamic perspective** (by Adam Ruben, Yoshiaki Kiso and Ernesto Friere, John Hopkins University, USA, and Kyoto Pharmaceutical University, Japan)

#### Perspective

Structural interaction fingerprints: A new approach to organizing, mining, analyzing and designing protein-small molecule inhibitors complexes (by Juswinder Singh, Zhan Deng, Gaurav Narale and Claudio Chuaqui, Biogen-IDEC, USA)

#### Review

Peptide, peptidomimetic and small-molecule drug discovery targeting HIV-1 host-cell attachment and entry through gp120, gp41, CCR5 and CXCR4

(by Wieslaw Kazmierkski, Terry Kenakin, and Kristjan Gudmundsson, GlaxoSmithKline, USA)

#### Review

## Inhibition of amyloid fibril formation by polyphenols: Structural similarity and aromatic interactions as a common inhibition mechanism

(by Yair Porat, Adel Abramowitz, and Ehud Gazit, Tel Aviv University, Israel)

#### Research Article

## The role of water in computational and experimental derivation of binding thermodynamics in SH2 domains

(by Sebastien Geroult, Satpal Virdee, and Gabriel Waksman, University College London/Birbeck College, UK)

#### Research Article

### Structural basis of Src tyrosine kinase inhibition with a new class of potent and selective trisubstituted purine-based compounds

(by David Dalgarno, Thilo Stehle, et al. and Tomi Sawyer, ARIAD Pharmaceuticals and Massachusetts General Hospital, USA)

#### Research Article

#### Structure-based optimization of MurF inhibitors

(by Geoffrey Stamper, Kenton Longenecker, et al. and Vincent Stoll, Abbott, USA)

#### Research Article

## Cellular analysis of disorazole C1 and structure-activity relationship of analogs of the natural product

(by Peter Wipf, Thomas Graham, et al. and John Lazo, University of Pittsburgh, USA)

#### Research Article

# The discovery of small molecule inhibitors of neutral endopeptidase: Structure-activity studies on functionalized glutaramides

(by Graham N. Maw, Alan Stobie, et al. and Kevin Beaumont, Pfizer, UK)

#### Research Article

**Stability of gold nanoparticle-bound DNA toward biological, physical and chemical agents** (by Gang Han, Craig Martin, and Vincent Rotello, University of Massachusetts, USA)

#### Technology Forum

**Use of an induced fit receptor structure in virtual screening** (by Woody Sherman, Hege Beard, and Ramy Farid, Schrodinger Inc, USA

#### Technology Forum

A chemogenomic approach to discovering of target-selective drugs (William Janzen and C. Nicholas Hodge, Amphora Discovery Corp., USA)

#### *Technology Forum* **Biochemical microarrays for studying chemical biology interactions: DiscoveryDot**<sup>TM</sup> **Technology**

(Kurumi Horiuchi, Yuan Wang and Haiching Ma, Reaction Biology Corp., USA )

## *Who's Who in Chemical Biology and Drug Design* **CB&DD Senior Editor Team**

Calendar of Events