



July 2009

Volume 14 · Numbers 13/14
pp. 623–722



Cover Story

The featured review in this issue of *Drug Discovery Today*, by Gerdien de Kloe, David Bailey, Rob Leurs and Iwan de Esch outlines how fragment based drug discovery (FBDD) can draw upon data from diverse inputs, ranging from informatics, structural and physical biology, biochemistry and more mainstream HTS information, amongst others, to aid efficiently the process of lead discovery and optimisation. The authors review a representative set of FBDD studies to highlight various medicinal chemistry strategies employed to develop higher molecular weight drug candidates from these low molecular weight leads.

DRUG DISCOVERY TODAY

REVIEWS

KEYNOTE

630 Transforming fragments into candidates: small becomes big in medicinal chemistry

Gerdien E. de Kloe, David Bailey, Rob Leurs and Iwan J.P. de Esch

647 Proton pump inhibitors: actions and reactions

James M. Mullin, Melissa Gabello, Lisa J. Murray, Christopher P. Farrell, Jillian Bellows, Kevin R. Wolov, Keith R. Kearney, David Rudolph and James J. Thornton

GENE TO SCREEN

661 Proteomics: addressing the challenges of osteoarthritis

Frédéric De Ceuninck and Francis Berenbaum

668 From fragment to clinical candidate—a historical perspective

Gianni Chessari and Andrew J. Woodhead

INFORMATICS

676 Homology modeling in drug discovery: current trends and applications

Claudio N. Cavasotto and Sharangdhar S. Phatak

684 Immunoinformatics: Current trends and future directions

Joo Chuan Tong and Ee Chee Ren

POST SCREEN

690 Neuroplasticity as a target for the pharmacotherapy of anxiety disorders, mood disorders, and schizophrenia

John H. Krystal, David F. Tolin, Gerard Sanacora, Stacy A. Castner, Graham V. Williams, Deane E. Aikins, Ralph E. Hoffman and D. Cyril D'Souza

698 Navigating structure–activity landscapes

Jürgen Bajorath, Lisa Peltason, Mathias Wawer, Rajarshi Guha, Michael S. Lajiness and John H. Van Drie

706 Developments in fluorescent probes for receptor research

Marcello Leopoldo, Enza Lacivita, Francesco Berardi and Roberto Perrone

713 The corticotropin-releasing factor system in inflammatory bowel disease: Prospects for new therapeutic approaches

Konstantinos A. Paschos, George Kolios and Ekaterini Chatzaki