

JANUARY 2008

VOLUME 41

NUMBER 9

ACCOUNTS

of chemical research

SPECIAL ISSUE ON
**Modern Molecular
Approaches to Drug
Design & Discovery**

0

1

4

ation
merican
Society

pubs.acs.org/acr

ACCOUNTS

of chemical research

January 2008 • Volume 41 • Number 9

Registered in U.S. Patent and Trademark Office

© 2008 American Chemical Society

ACHRE4 41(1) 1-156 (2008)

ISSN 0001-4842

Special Issue on Modern Molecular Approaches to Drug Design and Discovery

GUEST EDITOR: IWAO OJIMA

TABLE OF CONTENTS

- 1 **Editorial**
JOAN SELVERSTONE VALENTINE, KENDALL N. HOUK, PAUL F. BARBARA
- 2 **Guest Editorial: Modern Molecular Approaches to Drug Design and Discovery**
IWAO OJIMA
- 4 **The Chemical Versatility of Natural-Product Assembly Lines**
CHRISTOPHER T. WALSH
- 11 **Inhibitors of FabI, an Enzyme Drug Target in the Bacterial Fatty Acid Biosynthesis Pathway**
HAO LU AND PETER J. TONGE*
- 21 **Epothilones as Lead Structures for the Synthesis-Based Discovery of New Chemotypes for Microtubule Stabilization**
FABIAN FEYEN, FRÉDÉRIC CACHOUX, JÜRG GERTSCH, MARKUS WARTMANN, AND KARL-HEINZ ALTMANN*
- 32 **Discovery and Combinatorial Synthesis of Fungal Metabolites Beauveriolides, Novel Antiatherosclerotic Agents**
HIROSHI TOMODA* AND TAKAYUKI DOI
- 40 **Function-Oriented Synthesis, Step Economy, and Drug Design**
PAUL A. WENDER,* VISHAL A. VERMA, THOMAS J. PAXTON, AND THOMAS H. PILLOW
- 50 **Challenges in Modern Drug Discovery: A Case Study of Boceprevir, an HCV Protease Inhibitor for the Treatment of Hepatitis C Virus Infection**
F. GEORGE NJORGE,* KEVIN X. CHEN, NENG-YANG SHIH, AND JOHN J. PIWINSKI
- 60 **Functionalized Carbon Nanotubes in Drug Design and Discovery**
MAURIZIO PRATO,* KOSTAS KOSTARELOS,* AND ALBERTO BIANCO*
- 69 **Hybrid Molecules with a Dual Mode of Action: Dream or Reality?**
BERNARD MEUNIER