RSC Medicinal Chemistry

rsc.li/medchem

The Royal Society of Chemistry is the world's leading chemistry community. Through our high impact journals and publications we connect the world with the chemical sciences and invest the profits back into the chemistry community.

IN THIS ISSUE

ISSN 2632-8682 CODEN RMCSCX 14(11) 2117-2428 (2023)



Cover See Jennette A. Sakoff, Christopher J. Scarlett, Adam McCluskey et al., pp. 2246-2267. Image designed by Jennifer R. Baker and reproduced by permission of Adam McCluskey from RSC Med. Chem., 2023, 14, 2246.

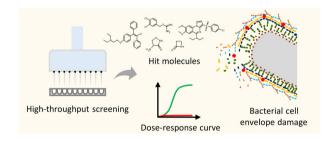


Inside cover See Ranjana Pathania et al., pp. 2125-2154. Image designed by Rinki Gupta and reproduced by permission of Ranjana Pathania from RSC Med. Chem., 2023, 14, 2125.

REVIEWS

Chemical genetic approaches for the discovery of bacterial cell wall inhibitors

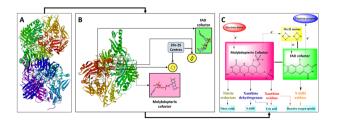
Rinki Gupta, Mangal Singh and Ranjana Pathania*



2155

Past, present and future of xanthine oxidase inhibitors: design strategies, structural and pharmacological insights, patents and clinical trials

Atamjit Singh,* Karanvir Singh, Aman Sharma, Kirandeep Kaur, Renu Chadha and Preet Mohinder Singh Bedi*



Editorial Staff

Executive Editor

Katie Lim

Deputy Editor

Harriet Riley

Editorial Production Manager Sarah Anthony

Saran Anthony

Development Editor Emily Cuffin-Munday

Ellilly Cullill-Muliday

Publishing Editors

Nicola Burton, Tom Cozens, Katie Fernandez, Ryan Kean, Roxane Owen

Editorial Assistant

Amy Cook

Publishing Assistant

Andrea Whiteside

Publisher

Sam Keltie

For queries about submitted papers, please contact Sarah Anthony, Editorial Production Manager, in the first instance. E-mail medchem@rsc.org

For pre-submission queries please contact Katie Lim, Executive Editor. E-mail medchem-rsc@rsc.org

RSC Medicinal Chemistry (electronic: ISSN 2632-8682) is published 12 times a year by the Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, UK CB4 0WF.

All orders, with cheques made payable to the Royal Society of Chemistry, should be sent to the Royal Society of Chemistry Order Department, Royal Society of Chemistry, Thomas Graham House. Science Park, Milton Road.

Cambridge, CB4 0WF, UK Tel +44 (0)1223 432398; E-mail orders@rsc.org

2023 Annual (electronic) subscription price: £1643; US\$2435. Customers in Canada will be subject to a surcharge to cover GST. Customers in the EU subscribing to the electronic version only will be charged VAT.

If you take an institutional subscription to any Royal Society of Chemistry journal you are entitled to free, site-wide web access to that journal. You can arrange access via Internet Protocol (IP) address at www.rsc.org/ip

Customers should make payments by cheque in sterling payable on a UK clearing bank or in US dollars payable on a US clearing bank.

Whilst this material has been produced with all due care, the Royal Society of Chemistry cannot be held responsible or liable for its accuracy and completeness, nor for any consequences arising from any errors or the use of the information contained in this publication. The publication of advertisements does not constitute any endorsement by the Royal Society of Chemistry or Authors of any products advertised. The views and opinions advanced by contributors do not necessarily reflect those of the Royal Society of Chemistry which shall not be liable for any resulting loss or damage arising as a result of reliance upon this material. The Royal Society of Chemistry is a charity, registered in England and Wales, Number 207890, and a company incorporated in England by Royal Charter (Registered No. RC000524), registered office: Burlington House, Piccadilly, London W1J 0BA, UK, Telephone: +44 (0) 207 4378 6556.

Advertisement sales:

Tel +44 (0) 1223 432246; Fax +44 (0) 1223 426017; E-mail advertising@rsc.org

For marketing opportunities relating to this journal, contact marketing@rsc.org

RSC Medicinal Chemistry

rsc.li/medchem

RSC Medicinal Chemistry publishes significant research and review articles in medicinal chemistry and related drug discovery science.

Editorial Board

Editor-in-Chief

Mike Waring, Newcastle University, UK

Associate Editors

Cynthia Dowd, George Washington University, USA

Maria Duca, Université Côte d'Azur - CNRS, France Sally-Ann Poulsen, Griffith University, Queensland, Australia Jian Zhang, Shanghai Jiao Tong University School of Medicine, China

Members

Hayley Binch, Hoffmann-La Roche, Switzerland Paola Castaldi, LifeMine Therapeutics, USA Matthew Fuchter, Imperial College London,

Lyn Jones, Dana-Farber Cancer Institute, Boston, USA

Jean-Louis Reymond, University of Bern, Switzerland

Advisory Board

Timor Baasov, Israel Institute of Technology, Israel

Andreas Bender, University of Cambridge, UK Julian Blagg, Institute of Cancer Research, Sutton, UK

Margaret Brimble, University of Auckland, New Zealand Mark Bunnage, Vertex Pharmaceuticals, USA

Christopher Burns, Certa Therapeutics, Australia Andrea Cavalli, University of Bologna, Italy

Andrea Cavain, University of Boogna, Italy Young-Tae Chang, POSTECH, South Korea James Crawford, Genentech, Inc., USA Matthew Duncton, Rigel Pharmaceuticals Inc, San Francisco, USA

Stephen Frye, University of North Carolina at Chapel Hill, USA

Sylvie Garneau-Tsodikova, University of Kentucky, USA

Barry Gold, University of Pittsburgh, USA Jayanta Haldar, Jawaharlal Nehru Centre for Advanced Scientific Research, India Gyoonhee Han, Yonsei University, Korea Mike Hann, GSK Medicine Research Centre,

Christian Heinis, EPFL, Switzerland Laura H. Heitman, Leiden University, Netherlands

Poshinori Ikeura, Axcelead Drug Discovery Partners, Japan Ahmed Kamal, NIPER, Hyderabad, India Bob (Robert) Langer. MIT. USA

Steven V. Ley, University of Cambridge, UK

María Luz López Rodríguez, Complutense University of Madrid, Spain Christa Müller, University of Bonn, Germany Roberto Pellicciari, University of Perugia, Italy David Rees, Astex Therapeutics, Cambridge,

Motonari Uesugi, Kyoto University, Japan John C. Vederas, University of Alberta, Canada Paul Wender, Stanford University, USA Zhen Yang, Peking University, China Ming-Qiang Zhang, Amgen, Shanghai, China

Information for Authors

Full details on how to submit material for publication in RSC Medicinal Chemistry are given in the Instructions for Authors (available from http://www.rsc.org/authors). Submissions should be made via the journal's homepage: rsc.li/medchem

Authors may reproduce/republish portions of their published contribution without seeking permission from the Royal Society of Chemistry, provided that any such republication is accompanied by an acknowledgement in the form: (Original Citation)–Reproduced by permission of the Royal Society of Chemistry.

This journal is © The Royal Society of Chemistry 2023. Apart from fair dealing for the purposes of research or private study for non-commercial purposes, or criticism or review, as permitted under the Copyright, Designs and Patents Act 1988 and the Copyright and Related Rights Regulation 2003, this publication may only be reproduced, stored or transmitted, in any form or by any means, with the prior permission in writing of the Publishers or in the case of reprographic reproduction in accordance with the terms of licences issued by the Copyright Licensing Agency in the UK. US copyright law is applicable to users in the USA.

Registered Charity No. 207890.

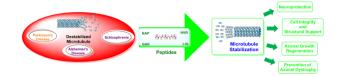


REVIEWS

2192

Microtubule stabilising peptides: new paradigm towards management of neuronal disorders

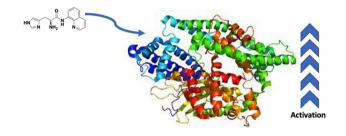
Shubhangi Bhargava, Riya Kulkarni, Bhaskar Dewangan, Neeraj Kulkarni, Chirag Jiaswar, Kunal Kumar, Amit Kumar, Praveen Reddy Bodhe, Hemant Kumar and Bichismita Sahu*



2206

The evolution of small molecule enzyme activators

Louise F. Dow, Alfie M. Case, Megan P. Paustian, Braeden R. Pinkerton, Princess Simeon and Paul C. Trippier*



2231

Recent progress of small-molecule-based theranostic agents in Alzheimer's disease

Furong Gao, Jiefang Chen, Yuancun Zhou, Letong Cheng, Ming Hu and Xiaohui Wang*

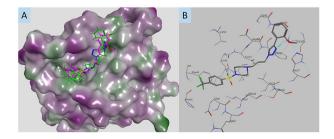


RESEARCH ARTICLES

2246

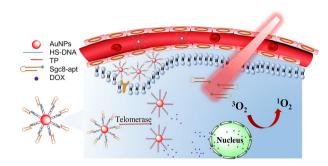
Novel piperazine-1,2,3-triazole leads for the potential treatment of pancreatic cancer

Jufeng Sun, Jennifer R. Baker, Cecilia C. Russell, Hong N. T. Pham, Chloe D. Goldsmith, Peter J. Cossar, Jennette A. Sakoff,* Christopher J. Scarlett* and Adam McCluskey*



RESEARCH ARTICLES

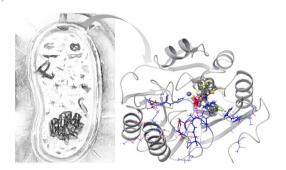
2268



Telomerase-activated Au@DNA nanomachine for targeted chemo-photodynamic synergistic therapy

Yun-Jie Zhou, Jing Zhang, Dong-Xiao Cao, An-Na Tang* and De-Ming Kong*

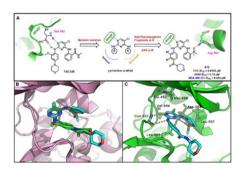
2277



α -Aminophosphonate inhibitors of metallo- β lactamases NDM-1 and VIM-2

Katarzyna Palica, Fritz Deufel, Susann Skagseth, Gabriela Paula Di Santo Metzler, Johannes Thoma, Anna Andersson Rasmussen, Arto Valkonen, Per Sunnerhagen, Hanna-Kirsti S. Leiros, Hanna Andersson* and Mate Erdelyi*

2301



Design, synthesis, and biological evaluation of diaminopyrimidine derivatives as novel focal adhesion kinase inhibitors

Yixiang Sun, Zixuan Gao, Ruifeng Wang, Guoqi Zhang, Tianxiao Wu, Wenbo Yin, Yin Sun, Qiaohua Qin, Dongmei Zhao* and Maosheng Cheng

2315 HYBRID Cinnamic Thiazole **MOLECULES** acids ring Anti-neuroinflammatory and > AChE, BChE AChE, BACE inhibitory activity inhibitory activity antioxidant properties RAGE antagonist Modulation of Aβ Inhibition of Aβaggregation aggregation

Novel styryl-thiazole hybrids as potential anti-Alzheimer's agents

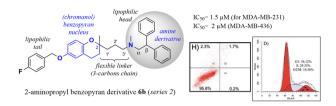
Niki Gouleni, Annalisa Di Rienzo, Ahmet Yılmaz, Harun Selvitopi, Mehmet Enes Arslan, Adil Mardinoglu, Hasan Turkez, Antonio Di Stefano, Stamatia Vassiliou* and Ivana Cacciatore*

RESEARCH ARTICLES

2327

Synthesis of 2-aminopropyl benzopyran derivatives as potential agents against triple-negative breast cancer

Ainhoa García, Sandra Torres-Ruiz, Laura Vila, Carlos Villarroel-Vicente, Álvaro Bernabeu, Pilar Eroles,* Nuria Cabedo* and Diego Cortes



2342

Selective isoxazolopyrimidine PAT1 (SLC26A6) inhibitors for therapy of intestinal disorders

Tifany Chu, Joy Karmakar, Peter M. Haggie, Joseph-Anthony Tan, Riya Master, Keerthana Ramaswamy, Alan S. Verkman, Marc O. Anderson and Onur Cil*



2348

ValCitGlyPro-dexamethasone antibody conjugates selectively suppress the activation of human monocytes

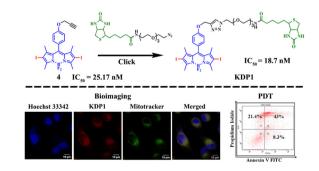
Justin M. Howe, Siteng Fang, Kelsey A. Watts, Fanny Xu, Samantha R. Benjamin and L. Nathan Tumey*



2358

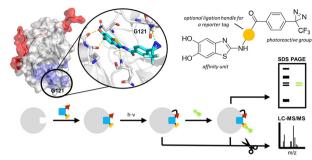
Mitochondria-targeted biotin-conjugated BODIPYs for cancer imaging and therapy

Dhiraj Dutta, Rajshree R. Nair, Kashmiri Neog, S. Asha Nair* and Pranjal Gogoi*



RESEARCH ARTICLES

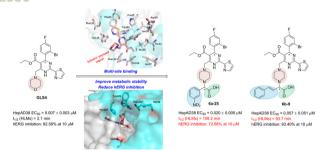
2365



Designing photoaffinity tool compounds for the investigation of the DENV NS2B-NS3 protease allosteric binding pocket

Hannah Maus, Andrea Gellert, Olivia R. Englert, Jia-Xuan Chen, Tanja Schirmeister and Fabian Barthels*

2380



Discovery of carboxyl-containing heteroaryldihydropyrimidine derivatives as novel HBV capsid assembly modulators with significantly improved metabolic stability

Shujie Zhao, Ya Wang, Xujie Zhang, Lijun Qiao, Shuo Wang, Yu Jin, Shuo Wu,* Yuhuan Li,* Peng Zhan* and Xinyong Liu*

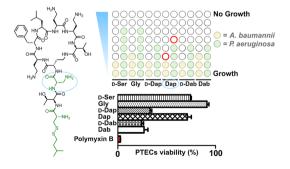
2401



Development of novel thiazolidine-2,4-dione derivatives as PPAR-y agonists through design, synthesis, computational docking, MD simulation, and comprehensive in vitro and in vivo evaluation

Mahendra Gowdru Srinivasa, Revanasiddappa B. C.,* Ashwini Prabhu, Vinitha Rani, Sudeep D. Ghate and Prashantha Kumar B. R.

2417



Semisynthetic polymyxins with potent antibacterial activity and reduced kidney cell toxicity

Cornelis J. Slingerland, Vladyslav Lysenko, Samhita Chaudhuri, Charlotte M. J. Wesseling, Devon Barnes, Rosalinde Masereeuw and Nathaniel I. Martin*