

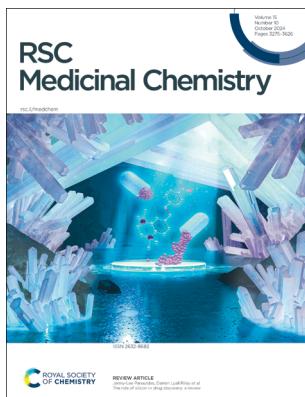
RSC Medicinal Chemistry

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IN THIS ISSUE

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Cover

See Jenny-Lee Panayides,
Darren Lyall Riley et al.,
pp. 3286–3344.
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3286.

EDITORIAL

3284

Introduction to the themed collection on ‘AI in Medicinal Chemistry’

Jian Zhang,* Ola Engkvist and Gerhard Hessler



REVIEWS

3286

The role of silicon in drug discovery: a review

Jenny-Lee Panayides,* Darren Lyall Riley,*
Felix Hasenmaile and Willem A. L. van Otterlo





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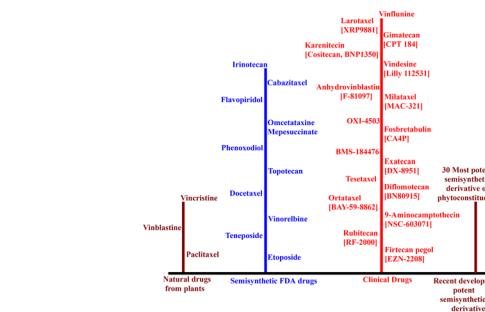
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REVIEWS

3345

Semisynthetic phytochemicals in cancer treatment: a medicinal chemistry perspective

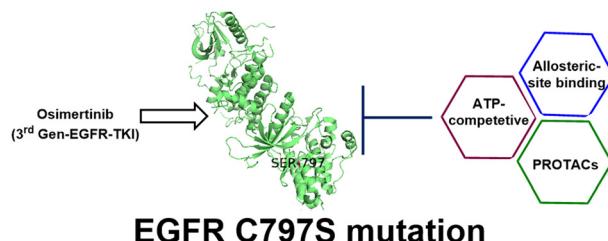
Meghna Arora, Ankit Kumar Singh, Adarsh Kumar, Harshwardhan Singh, Prateek Pathak, Maria Grishina, Jagat Pal Yadav, Amita Verma and Pradeep Kumar*



3371

Next-generation EGFR tyrosine kinase inhibitors to overcome C797S mutation in non-small cell lung cancer (2019–2024)

Debasis Das,* Lingzhi Xie and Jian Hong

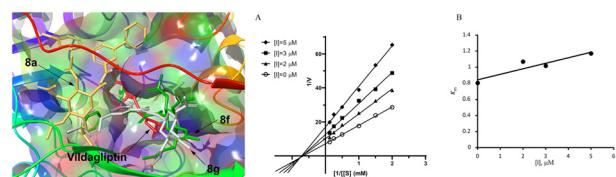


RESEARCH ARTICLES

3395

Design, synthesis, inhibitory activity, and molecular simulations study for D-glucose-conjugated thioureas containing pyrimidine ring as multitarget inhibitors against α -amylase, α -glucosidase, DDP-4, and PTP1B in Type 2 diabetes mellitus

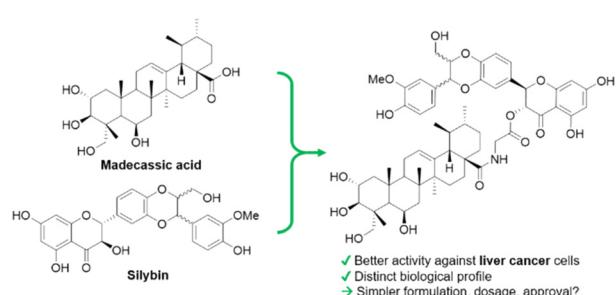
Vu Ngoc Toan, Do Son Hai, Hoang Thi Kim Van, Nguyen Minh Tri, Duong Ngoc Toan, Nguyen Thi Thanh Mai and Nguyen Dinh Thanh*



3418

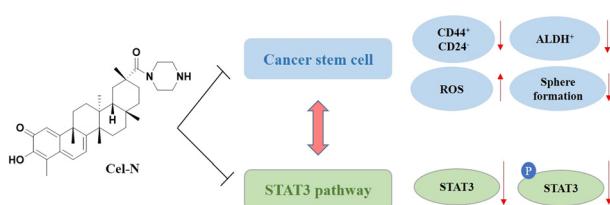
Synthesis and cytotoxic activity of madecassic acid–silybin conjugate compounds in liver cancer cells

Chien Van Tran, Thao Thi Phuong Tran, Anh The Nguyen, Loc Van Tran, Ninh Thi Pham, Luu Thi Nguyen, Dung Thi Nguyen, Michelle D. Garrett, Nga Thi Nguyen, Thao Thi Do, Christopher J. Serpell* and Sung Van Tran*



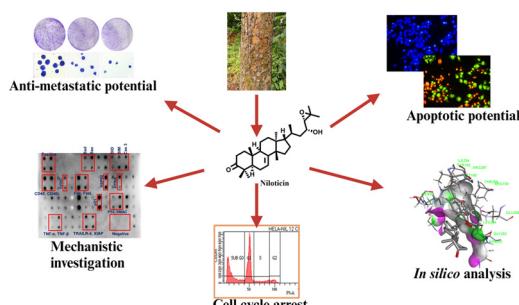
RESEARCH ARTICLES

3433

**Synthesis of a celastrol derivative as a cancer stem cell inhibitor through regulation of the STAT3 pathway for treatment of ovarian cancer**

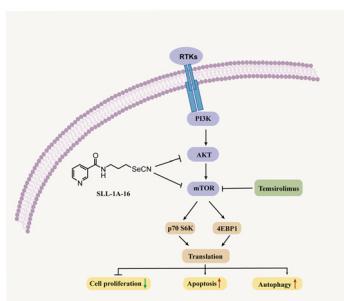
Meijuan Liu, Na Li, Zhaoxue Wang, Shuo Wang, Shaoda Ren* and Xiaojing Li*

3444

**A comprehensive apoptotic assessment of nilotinib in cervical cancer cells: a tirucallane-type triterpenoid from *Aphanamixis polystachya* (Wall.) Parker**

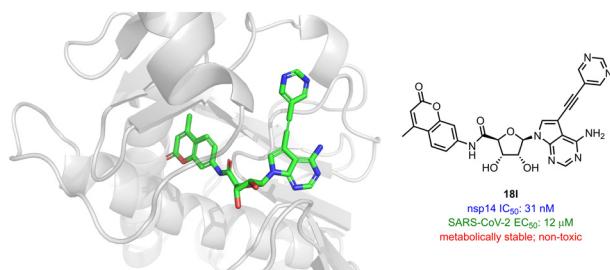
Anuja Gracy Joseph, Mohanan Biji, Vishnu Priya Murali, Daisy R. Sherin, Alisha Valsan, Vimalkumar P. Sukumaran, Kokkuvalayil Vasu Radhakrishnan* and Kaustabh Kumar Maiti*

3460

**SLL-1A-16 suppresses proliferation and induces autophagy in non-small-cell lung cancer cells via the AKT/mTOR signaling pathway**

Xiaoqin Luo, Jin Wang, Ruichang Wang, Jiabing Lian, Mengnan Guo, Hongrui Zhou, Mengxue Zhang, Zhe Yang, Xiaolong Li, Xianran He and Xiuli Bi*

3469

**Discovery of highly potent SARS-CoV-2 nsp14 methyltransferase inhibitors based on adenosine 5'-carboxamides**

Hugo Kocek, Dominika Chalupská, Milan Dejmek, Alexandra Dvořáková, Michala Zgarbová, Michal Šála, Karel Chalupský, Petra Krafčíková, Tomáš Otava, Matúš Drexler, Eliška Procházková, Blanka Klepetářová, Milan Štefek, Ján Kozic, Helena Mertlíková-Kaiserová, Evzen Boura, Jan Weber and Radim Nencka*

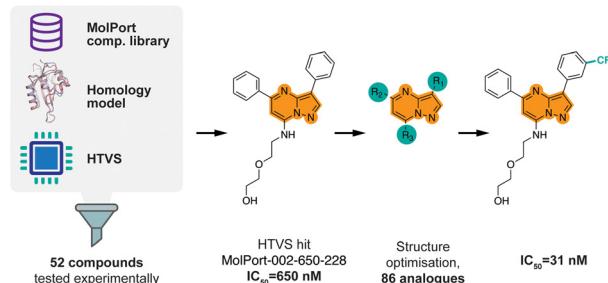


RESEARCH ARTICLES

3477

Discovery and optimisation of pyrazolo[1,5-a]pyrimidines as aryl hydrocarbon receptor antagonists

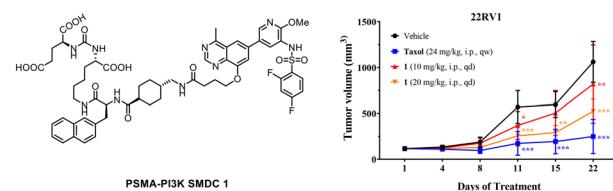
Raitis Bobrovs,* Svetlana Terentjeva, Ninni Elise Olafsen, Zilvinas Dambrauskas, Antanas Gulbinas, Toivo Maimets, Indrek Teino, Aigars Jurgensons, Jason Matthews and Kristaps Jaudzems



3485

Design, synthesis and biological evaluation of a novel PSMA-PI3K small molecule drug conjugate

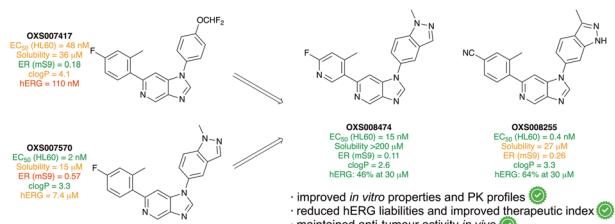
Shouguo Peng, Haixia Li, Weiliu Cui, Tianning Xiong, Jiaqi Hu, Haixiang Qi, Songwen Lin, Deyu Wu, Ming Ji* and Heng Xu*



3495

Lead optimisation of OXS007417: *in vivo* PK profile and hERG liability modulation to optimise a small molecule differentiation agent for the potential treatment of acute myeloid leukaemia

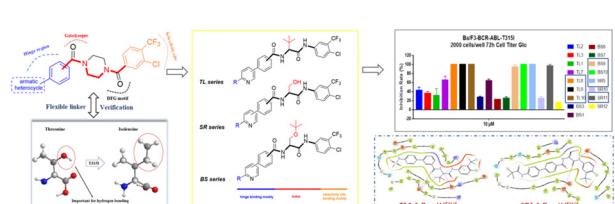
Thomas J. Cogswell, Laia Josa-Culleré, David Zimmer, Sébastien R. G. Galan, Morgan Jay-Smith, Kate S. Harris, Carole J. R. Bataille, Thomas R. Jackson, Douzi Zhang, Stephen G. Davies, Paresh Vyas, Thomas A. Milne, Graham M. Wynne and Angela J. Russell*



3507

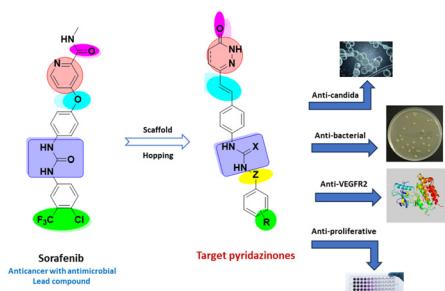
Integrating amino acids into Bcr-Abl inhibitors: design, synthesis, biological evaluation, and *in silico* studies

Yuying Liu, Zeyu Yang, Jie Zhang, Na Guo, Nanxin Liu, Qingqing Zhang, Xintao Dang, Yanchen Li, Jie Zhang and Xiaoyan Pan*



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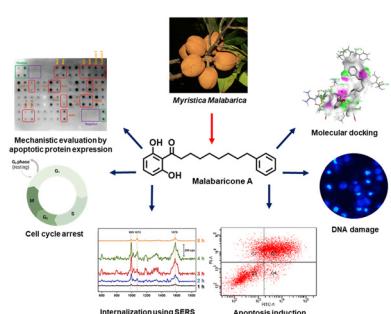
3529



Pyridazinone-based derivatives as anticancer agents endowed with anti-microbial activity: molecular design, synthesis, and biological investigation

Mohamed K. S. El-Nagar, Mai I. Shahin, Mohammed F. El-Behairy, Ehab S. Taher, Mohamed F. El-Badawy, Marwa Sharaky, Dalal A. Abou El Ella,* Khaled A. M. Abouzid* and Mai Adel

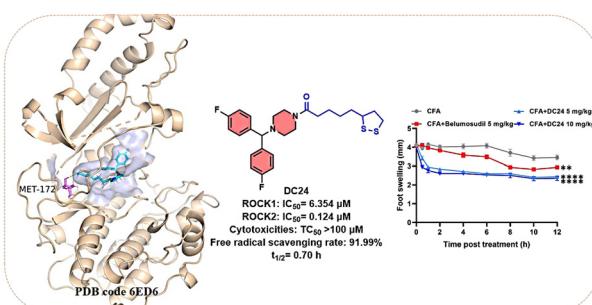
3558



Exploring apoptotic induction of malabaricone A in triple-negative breast cancer cells: an acylphenol phyto-entity isolated from the fruit rind of *Myristica malabarica* Lam.

Pothiyil S. Vimalkumar, Neethu Sivadas, Vishnu Priya Murali, Daisy R. Sherin, Madhu Krishnan Murali, Anuja Gracy Joseph, Kokkuvalayil Vasu Radhakrishnan,* and Kaustabh Kumar Maiti*

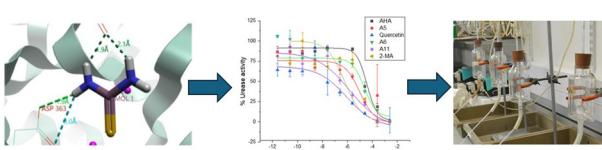
3576



The synthesis and bioactivities of ROCK2 inhibitors with 1,2-dithiolan-3-yl motif

Ruolin Cao, Fangyu Du, Zhiqiang Liu, Pengcheng Cai, Minggang Qi, Wei Xiao,* Xuefei Bao* and Guoliang Chen*

3597



Rational design and *in vitro* testing of new urease inhibitors to prevent urinary catheter blockage

Rachel A. Heylen, Nicola Cusick, Tom White, Emily J. Owen, Bethany L. Patenall, Martin Alm, Peter Thomsen, Maisem Laabei and A. Toby A. Jenkins*

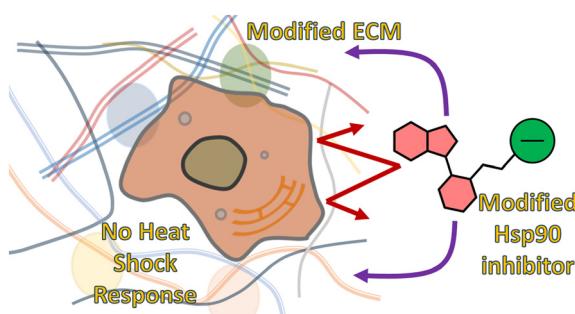


RESEARCH ARTICLES

3609

Rationally modified SNX-class Hsp90 inhibitors disrupt extracellular fibronectin assembly without intracellular Hsp90 activity

Gciniwe S. Mathenjiwa, Abir Chakraborty,
Abantika Chakraborty, Ronel Muller, Mathew P. Akerman,
Moira L. Bode, Adrienne L. Edkins*
and Clinton G. L. Veale*



3616

Sidechain structure–activity relationships of cyclobutane-based small molecule $\alpha v\beta 3$ antagonists

Adam Throup, Manar Saleh Zraikat, Andrew Gordon,
Shohreh Jafarinejad Soumehsaraei, Kathrin D. Haase,
Laurence H. Patterson, Patricia A. Cooper,
Katherine Hanlon, Paul M. Loadman, Mark Sutherland,
Steven D. Shnyder and Helen M. Sheldrake*

