

RSC Medicinal Chemistry

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

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Introduction to the themed collection on 'AI in Medicinal Chemistry'

Jian Zhang,* Ola Engkvist and Gerhard Hessler

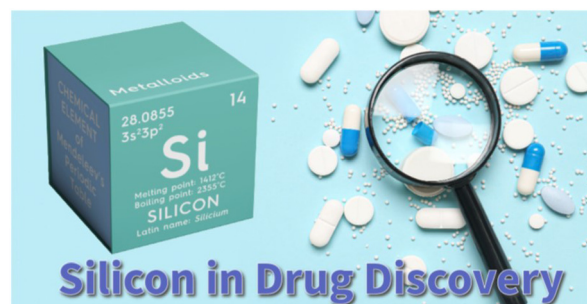


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The role of silicon in drug discovery: a review

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





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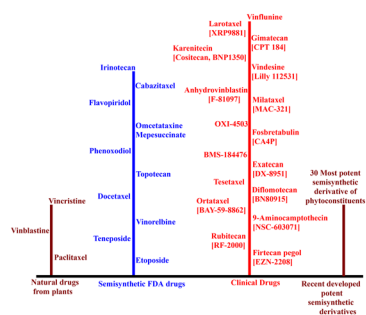


REVIEWS

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Semisynthetic phytochemicals in cancer treatment: a medicinal chemistry perspective

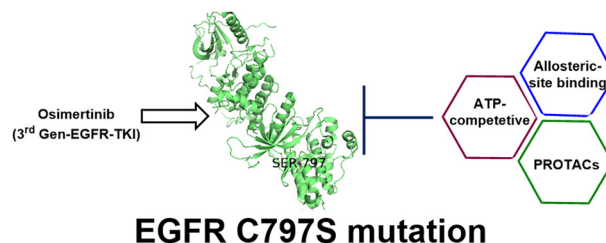
Meghna Arora, Ankit Kumar Singh, Adarsh Kumar, Harshwardhan Singh, Prateek Pathak, Maria Grishina, Jagat Pal Yadav, Amita Verma and Pradeep Kumar*



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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

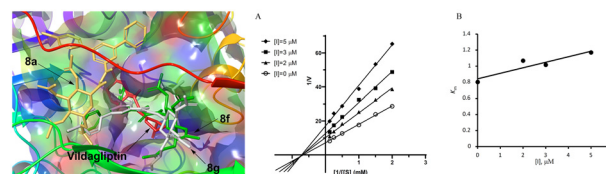


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Design, synthesis, inhibitory activity, and molecular simulations study for D-glucose-conjugated thioureas containing pyrimidine ring as multitarget inhibitors against α -amylase, α -glucosidase, DDP-4, and PTP1B in Type 2 diabetes mellitus

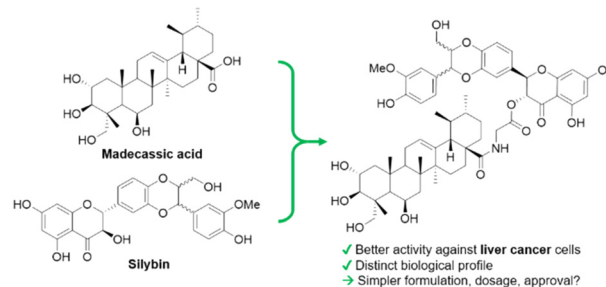
Vu Ngoc Toan, Do Son Hai, Hoang Thi Kim Van, Nguyen Minh Tri, Duong Ngoc Toan, Nguyen Thi Thanh Mai and Nguyen Dinh Thanh*



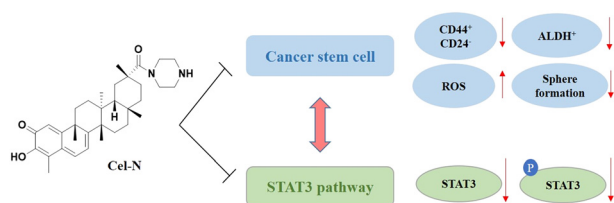
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Synthesis and cytotoxic activity of madecassic acid-silybin conjugate compounds in liver cancer cells

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*



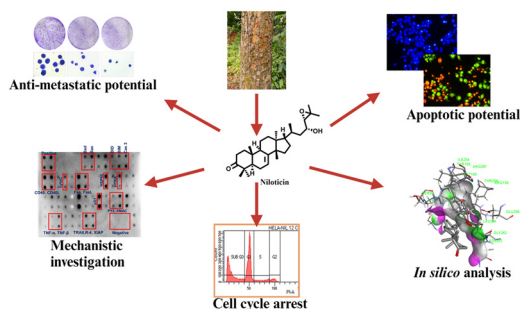
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Synthesis of a celastrol derivative as a cancer stem cell inhibitor through regulation of the STAT3 pathway for treatment of ovarian cancer

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

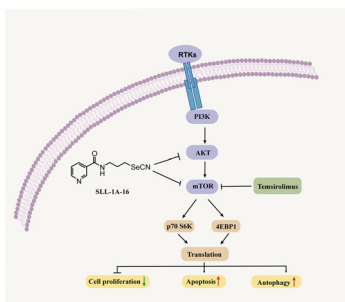
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A comprehensive apoptotic assessment of niloticin in cervical cancer cells: a tirucallane-type triterpenoid from *Aphanamixis polystachya* (Wall.) Parker

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

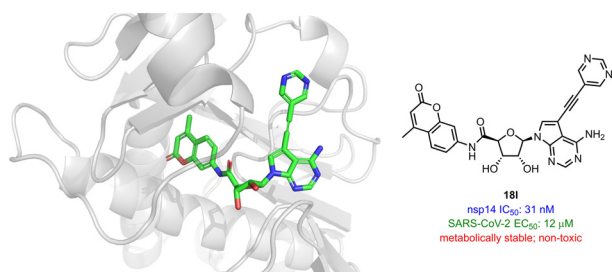
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SLL-1A-16 suppresses proliferation and induces autophagy in non-small-cell lung cancer cells via the AKT/mTOR signaling pathway

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

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

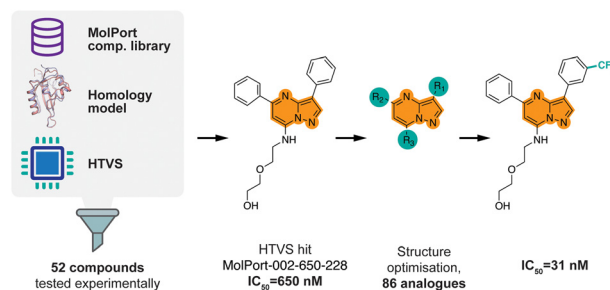
Hugo Kocek, Dominika Chalupská, Milan Dejmeck, Alexandra Dvořáková, Michala Zgarbová, Michal Šála, Karel Chalupský, Petra Krafčíková, Tomáš Otava, Matúš Drexler, Eliška Procházková, Blanka Klepetářová, Milan Štefek, Ján Kozic, Helena Mertlíková-Kaiserová, Evzen Boura, Jan Weber and Radim Nencka*



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

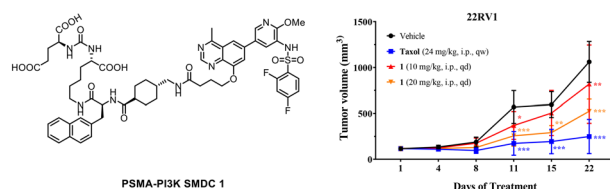
Raitis Bobrovs,* Svetlana Terentjeva, Ninni Elise Olafsen, Zilvinas Dambrauskas, Antanas Gulbinas, Toivo Maimets, Indrek Teino, Aigars Jirgensons, Jason Matthews and Kristaps Jaudzems



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

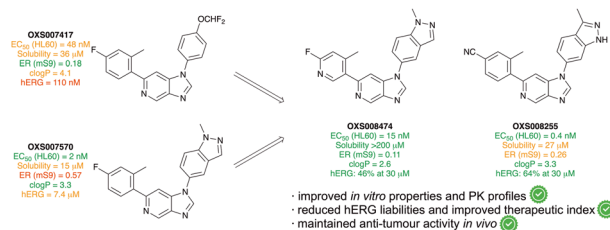
Shouguo Peng, Haixia Li, Weilu Cui, Tianning Xiong, Jiaqi Hu, Haixiang Qi, Songwen Lin, Deyu Wu, Ming Ji* and Heng Xu*



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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

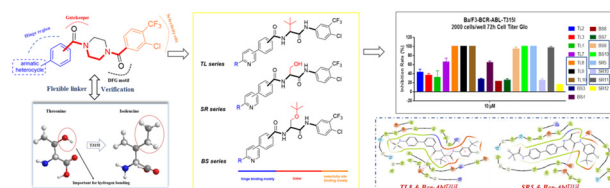
Thomas J. Cogswell, Laia Josa-Culleré, David Zimmer, Sébastien R. G. Galan, Morgan Jay-Smith, Kate S. Harris, Carole J. R. Bataille, Thomas R. Jackson, Douzi Zhang, Stephen G. Davies, Pares Vyas, Thomas A. Milne, Graham M. Wynne and Angela J. Russell*



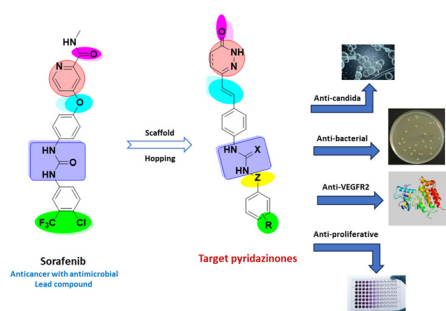
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Integrating amino acids into Bcr-Abl inhibitors: design, synthesis, biological evaluation, and *in silico* studies

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



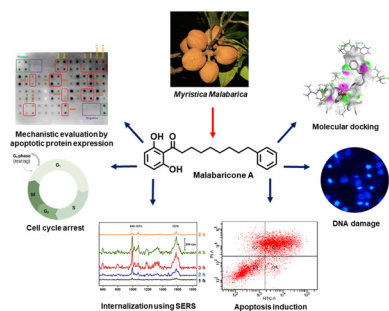
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Pyridazinone-based derivatives as anticancer agents endowed with anti-microbial activity: molecular design, synthesis, and biological investigation

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

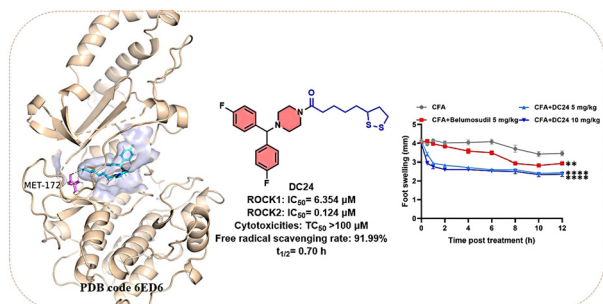
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Exploring apoptotic induction of malabaricone A in triple-negative breast cancer cells: an acylphenol phyto-entity isolated from the fruit rind of *Myristica malabarica* Lam.

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

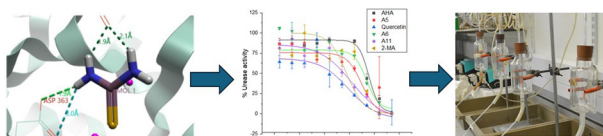
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The synthesis and bioactivities of ROCK2 inhibitors with 1,2-dithiolan-3-yl motif

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

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

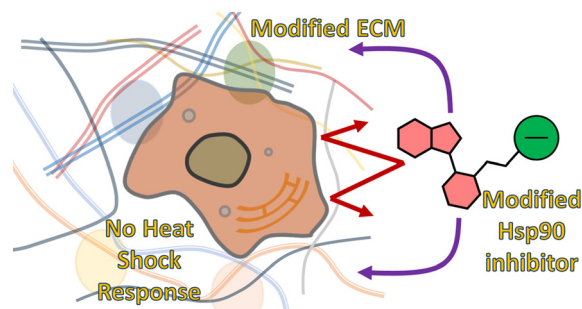
Rachel A. Heylen, Nicola Cusick, Tom White, Emily J. Owen, Bethany L. Patenall, Martin Alm, Peter Thomsen, Maisem Laabei and A. Toby A. Jenkins*



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

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



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Sidechain structure–activity relationships of cyclobutane-based small molecule $\alpha\text{v}\beta\text{3}$ 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*

