

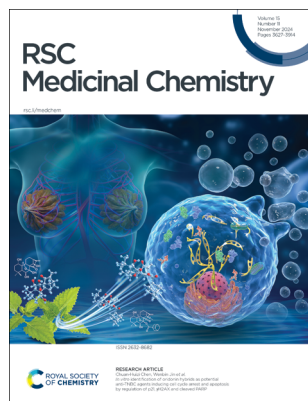
RSC Medicinal Chemistry

rsc.li/medchem

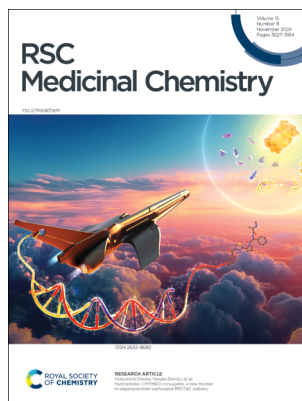
The Royal Society of Chemistry is the world's leading chemistry community. Through our high impact journals and publications we connect the world with the chemical sciences and invest the profits back into the chemistry community.

IN THIS ISSUE

ISSN 2632-8682 CODEN RMCSCX 15(11) 3627-3914 (2024)



Cover
See Chuan-Huizi Chen,
Wenbin Jin *et al.*,
pp. 3674–3694.
Image reproduced by
permission of Wenbin Jin and
Changsha Keyanyihui
Information Technology Co.
Ltd. from *RSC Med. Chem.*,
2024, 15, 3674.



Inside cover
See Nobumichi Ohoka,
Yosuke Demizu *et al.*,
pp. 3695–3703.
Image reproduced by
permission of Yosuke Demizu
from *RSC Med. Chem.*, 2024,
15, 3695.

EDITORIAL

3636

Introduction to the themed collection in honour of Professor Christian Leumann

Marcel Hollenstein* and Eugen Stulz*

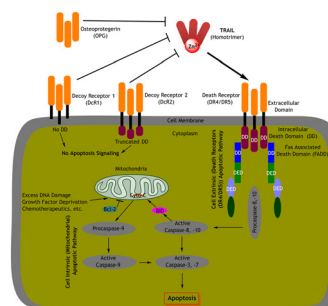


REVIEWS

3639

Chemical synthetic approaches to mimic the TRAIL: promising cancer therapeutics

Abdullah-Al Masum,* Shin Aoki, Md. Mahbubur Rahman
and Yosuke Hisamatsu



ChemComm

Uncover new possibilities
with outstanding
preliminary research

Original discoveries, fuelling
every step of scientific progress

rsc.li/chemcomm

Fundamental questions
Elemental answers

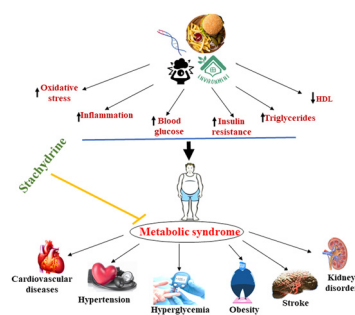


REVIEWS

3652

Stachydrine, a pyrrole alkaloid with promising therapeutic potential against metabolic syndrome and associated organ dysfunction

Semim Akhtar Ahmed, Prasenjit Manna* and Jagat Chandra Borah*

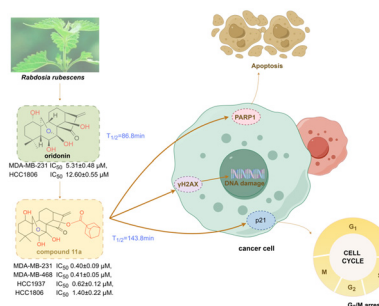


RESEARCH ARTICLES

3674

In vitro identification of oridonin hybrids as potential anti-TNBC agents inducing cell cycle arrest and apoptosis by regulation of p21, γ H2AX and cleaved PARP

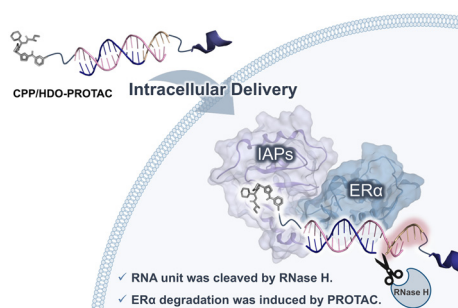
Jinhua Ning, Nini Zhan, Zhanpan Wu, Yuzhe Li, Die Zhang, Yadian Shi, Yingxun Zhou, Chuan-Huizi Chen* and Wenbin Jin*



3695

Hydrophobic CPP/HDO conjugates: a new frontier in oligonucleotide-warhead PROTAC delivery

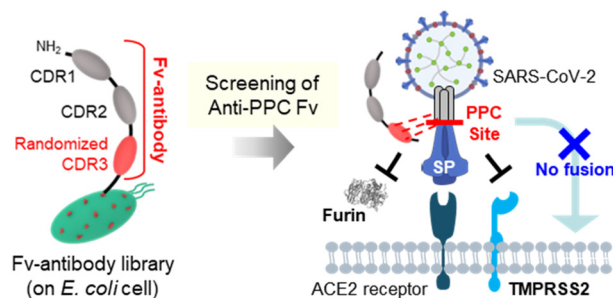
Miyako Naganuma, Nobumichi Ohoka,* Motoharu Hirano, Daishi Watanabe, Genichiro Tsuji, Takao Inoue and Yosuke Demizu*



3704

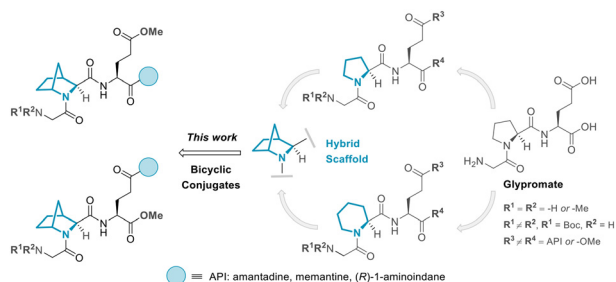
Preventing SARS-CoV-2 infection using Fv-antibodies targeting the proprotein convertase (PPC) cleavage site

Jaeyong Jung, Jeong Soo Sung, Soonil Kwon, Hyung Eun Bae, Min-Jung Kang, Joachim Jose, Misu Lee* and Jae-Chul Pyun*



RESEARCH ARTICLES

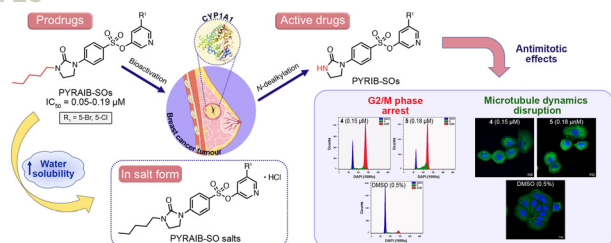
3711



Discovery of hybrid Glypromate conjugates with neuroprotective activity against paraquat-induced toxicity

Sara C. Silva-Reis, Vera M. Costa, Daniela Correia da Silva, David M. Pereira, Xavier Cruz Correia, Xerardo Garcia-Mera, José E. Rodríguez-Borges and Ivo E. Sampaio-Dias*

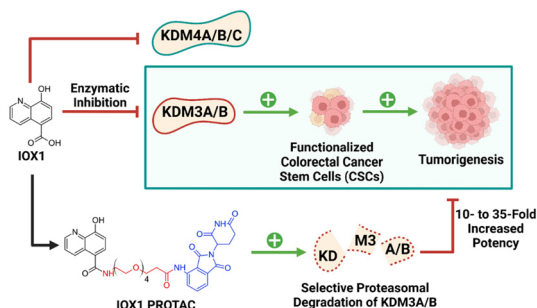
3728



Pyridinyl 4-(2-oxoalkylimidazolidin-1-yl) benzenesulfonates and their hydrochloride salts as novel water soluble antimitotic prodrugs bioactivated by cytochrome P450 1A1 in breast cancer cells

Vincent Ouellette, Chahrazed Bouzriba, Atziri Corin Chavez Alvarez, Quentin Bruxelles, Geneviève Hamel-Côté and Sébastien Fortin*

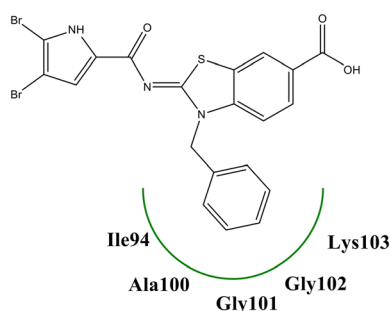
3746



Novel PROTAC probes targeting KDM3 degradation to eliminate colorectal cancer stem cells through inhibition of Wnt/ β -catenin signaling

Shadid U. Zaman, Piyusha P. Pagare, Hongguang Ma, Rosalie G. Hoyle, Yan Zhang* and Jiong Li*

3759



New ATP-competitive inhibitors of *E. coli* GyrB obtained from the mapping of the hydrophobic floor at the binding site: synthesis and biological evaluation

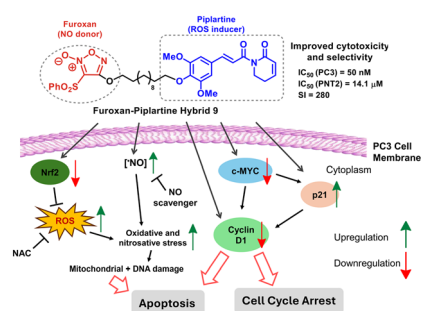
Lucas Gutierrez, Peter Peršolja, Rodrigo Tosso, Nace Zidar, Danijel Kikelj and Ricardo D. Enriz



3778

Furoxan–piplartine hybrids as effective NO donors and ROS inducers in PC3 cancer cells: design, synthesis, and biological evaluation

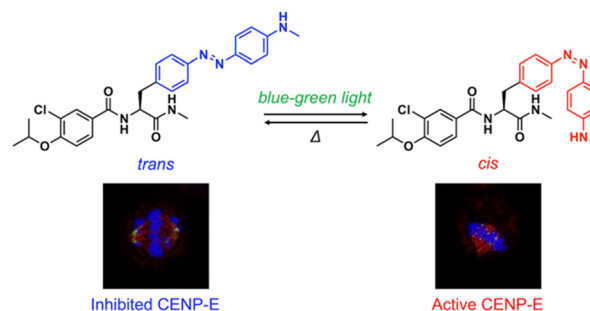
Carolyne Brustolin Braga, Julio Cesar Milan, Matheus Andrade Meirelles, Bruno Zavan, Guilherme Álvaro Ferreira-Silva, Ester Siqueira Caixeta, Marisa Ionta and Ronaldo A. Pilli*



3795

A photoswitchable CENP-E inhibitor with single blue-green light to control chromosome positioning in mitotic cells

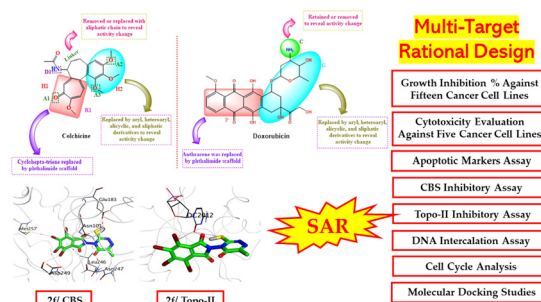
Kazuya Matsuo,* Takashi Kikukawa, Tomonori Waku, Akio Kobori and Nobuyuki Tamaoki*



3800

Design and synthesis of novel multi-target tetrabromophthalimides as CBS and Topo-II inhibitors and DNA intercalators

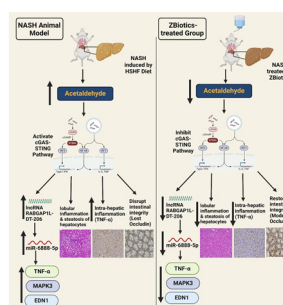
Marwa Abdel-Motaal, Dalal Ali Aldakhili,* Ayman B. Farag, Ayman Abo Elmaaty, Marwa Sharaky, Nadia A. Mohamed, Saad Shaaban, Abdullah Yahya Abdullah Alzahrani and Ahmed A. Al-Karmalawy*



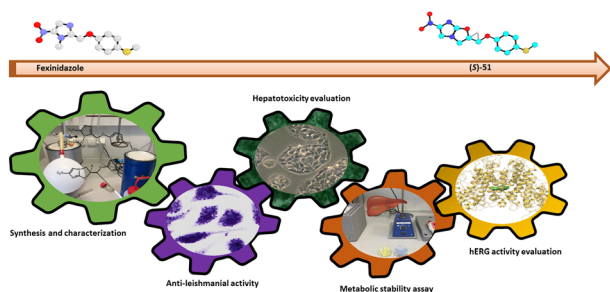
3817

Evaluating the therapeutic potential of genetically engineered probiotic ZbioTics (ZB183) for non-alcoholic steatohepatitis (NASH) management via modulation of the cGAS-STING pathway

Maha Saad, Walaa Ibrahim, Amany Helmy Hasanin, Aya Magdy Elyamany and Marwa Matboli*



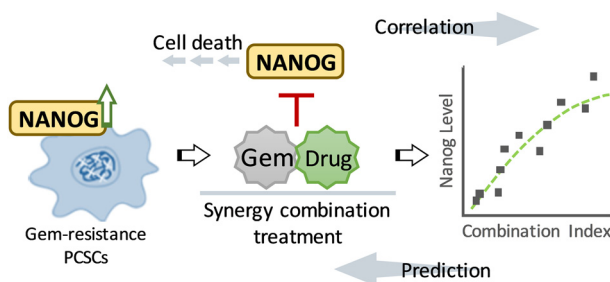
3837



Fexinidazole optimization: enhancing anti-leishmanial profile, metabolic stability and hERG safety

Abdrrahman Shemsu Surur,* Chin Fung Chan, Frieda-Marie Bartz, Iris L. K. Wong, Van T. D. Nguyen, Lukas Schulig, Andreas Link, Tak Hang Chan, Larry M. C. Chow and Patrick J. Bednarski

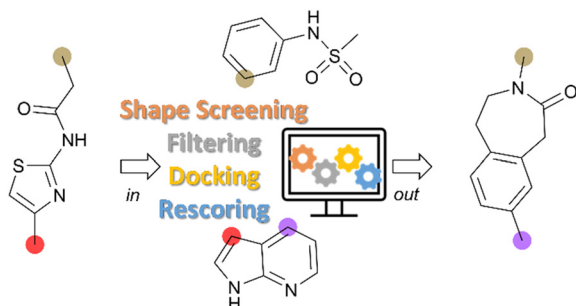
3853



Prediction of synergistic gemcitabine-based combination treatment through a novel tumor stemness biomarker NANOG in pancreatic cancer

Jiongjia Cheng,* Ting Zhu, Shaoxian Liu, Jiayu Zhou, Xiaofeng Wang and Guangxiang Liu*

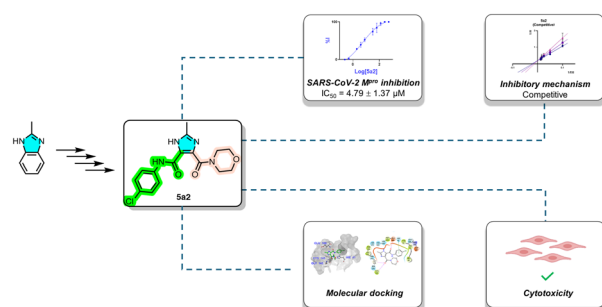
3862



Design and synthesis of novel 8-(azaindoly)-benzoazepinones as potent and selective ROCK inhibitors

Daniele Pala,* David Clark, Christine Edwards, Elisa Pasqua, Laura Tigli, Barbara Pioselli, Piotr Malysa, Fabrizio Facchinetti, Fabio Rancati and Alessandro Accetta*

3880



Asymmetric imidazole-4,5-dicarboxamide derivatives as SARS-CoV-2 main protease inhibitors: design, synthesis and biological evaluation

Phuong Nguyen Hoai Huynh, Phatcharin Khamplong, Minh-Hoang Phan, Thanh-Phuc Nguyen, Phuong Ngoc Lan Vu, Quang-Vinh Tang, Phumin Chamsodsai, Supaphorn Seetaha, Truong Lam Tuong, Thien Y. Vu, Duc-Duy Vo, Kiattawee Choowongkamon* and Cam-Van T. Vo*

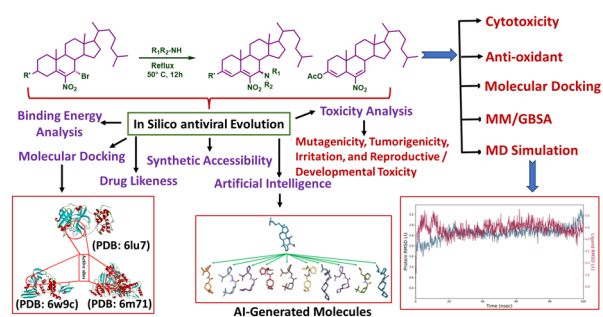


RESEARCH ARTICLES

3889

Exploring 7 β -amino-6-nitrocholestens as COVID-19 antivirals: *in silico*, synthesis, evaluation, and integration of artificial intelligence (AI) in drug design: assessing the cytotoxicity and antioxidant activity of 3 β -acetoxynitrocholestane

Shahabuddin, Uzma, Mohammad Azam, Mehtab Parveen,* Nurul Huda Abd Kadir, Kim Min and Mahboob Alam*



CORRECTION

3912

Correction: computational design, synthesis, and assessment of 3-(4-(4-(1,3,4-oxadiazol-2-yl)-1H-imidazol-2-yl)phenyl)-1,2,4-oxadiazole derivatives as effective epidermal growth factor receptor inhibitors: a prospective strategy for anticancer therapy

Nilesh Raghunath Khedkar, Milind Sindkhedkar* and Alex Joseph

