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*

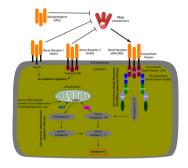


REVIEWS

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

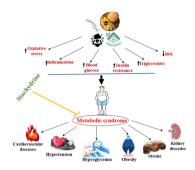
Registered charity number: 207890

REVIEWS

3652

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

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

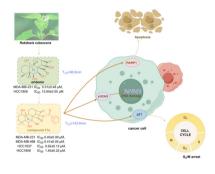


RESEARCH ARTICLES

3674

In vitro identification of oridonin hybrids as potential anti-TNBC agents inducing cell cycle arrest and apoptosis by regulation of p21, yH2AX and cleaved PARP

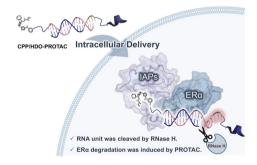
Jinhua Ning, Nini Zhan, Zhanpan Wu, Yuzhe Li, Die Zhang, Yadian Shi, Yingxun Zhou, Chuan-Huizi Chen* and Wenbin Jin*



3695

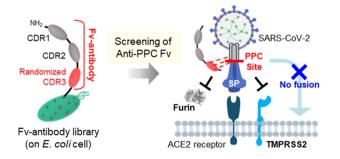
Hydrophobic CPP/HDO conjugates: a new frontier in oligonucleotide-warheaded PROTAC delivery

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



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

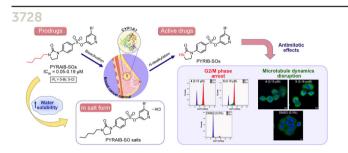
Jaeyong Jung, Jeong Soo Sung, Soonil Kwon, Hyung Eun Bae, Min-Jung Kang, Joachim Jose, Misu Lee* and Jae-Chul Pyun*



3711

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

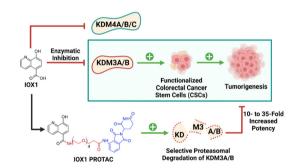
Sara C. Silva-Reis, Vera M. Costa, Daniela Correia da Silva, David M. Pereira, Xavier Cruz Correia, Xerardo García-Mera, José E. Rodríguez-Borges and Ivo E. Sampaio-Dias*



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

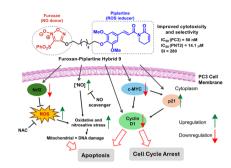
New ATP-competitive inhibitors of E. coli GyrB obtained from the mapping of the hydrophobic floor at the binding site: synthesis and biological evaluation

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

3778

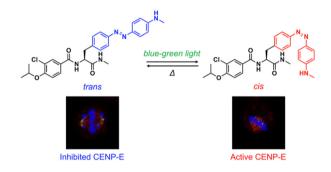
Furoxan-piplartine hybrids as effective NO donors and ROS inducers in PC3 cancer cells: design, synthesis, and biological evaluation

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



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

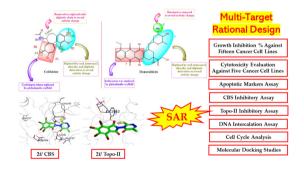
Kazuya Matsuo,* Takashi Kikukawa, Tomonori Waku, Akio Kobori and Nobuyuki Tamaoki*



3800

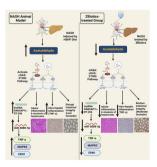
Design and synthesis of novel multi-target tetrabromophthalimides as CBS and Topo-II inhibitors and DNA intercalators

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*



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

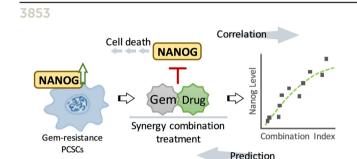
Maha Saad, Walaa Ibrahim, Amany Helmy Hasanin, Aya Magdy Elyamany and Marwa Matboli*



3837

Fexinidazole optimization: enhancing antileishmanial profile, metabolic stability and hERG safety

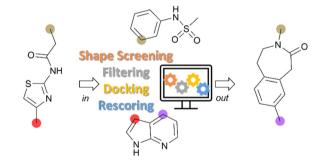
Abdrrahman Shemsu Surur,* Chin Fung Chan, Frieda-Marie Bartz, Iris L. K. Wong, Van T. D. Nguyen, Lukas Schulig, Andreas Link, Tak Hang Chan, Larry M. C. Chow and Patrick J. Bednarski



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

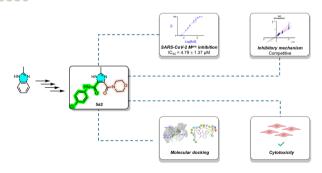
Jiongjia Cheng,* Ting Zhu, Shaoxian Liu, Jiayu Zhou, Xiaofeng Wang and Guangxiang Liu*

3862



Design and synthesis of novel 8-(azaindolyl)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*



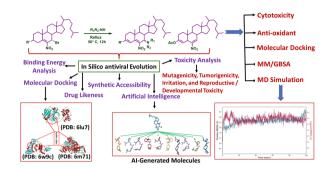
Asymmetric imidazole-4,5-dicarboxamide derivatives as SARS-CoV-2 main protease inhibitors: design, synthesis and biological evaluation

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 Choowongkomon* and Cam-Van T. Vo*

3889

Exploring 7β-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 3β-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