

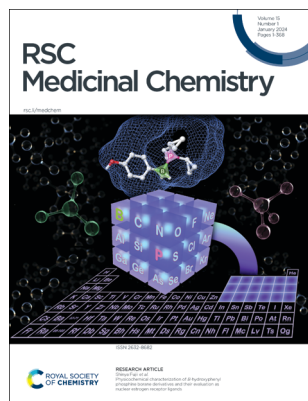
# RSC Medicinal Chemistry

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 RMCSX 15(1) 1-368 (2024)



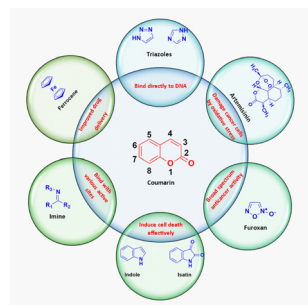
**Cover**  
See Shinya Fujii *et al.*,  
pp. 119–126.  
Image reproduced by  
permission of Shinya Fujii  
from *RSC Med. Chem.*,  
2024, 15, 119.

## REVIEWS

10

### Latest developments in coumarin-based anticancer agents: mechanism of action and structure–activity relationship studies

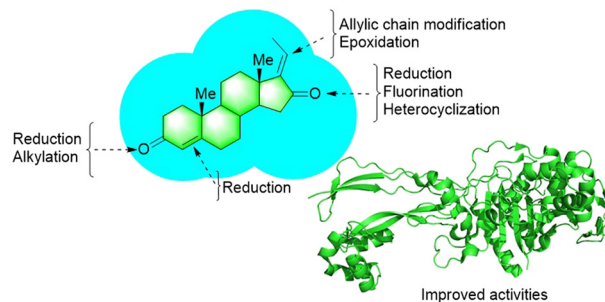
Manankar Koley, Jianlin Han, Vadim A. Soloshonok, Subhajit Mojumder, Ramin Javahershenas and Ata Makarem\*



55

### Guggulsterone – a potent bioactive phytosteroid: synthesis, structural modification, and its improved bioactivities

T. P. Adarsh Krishna,\* T. P. Ajeesh Krishna, Baldev Edachery and S. Antony Ceasar



# Fuelling your energy research



## Energy & Environmental Science

Agenda-setting research in energy science and technology

### Chair of the Editorial Board

Jenny Nelson, Imperial College London, UK

Impact factor 2021: 39.714, median time to first decision (peer reviewed articles only): 46 days\*.

[rsc.li/ees](https://rsc.li/ees)



## EES Catalysis

Exceptional research on energy and environmental catalysis

### Editor-in-Chief

Shizhang Qiao, University of Adelaide, Australia

Median time to first decision (peer reviewed articles only): 24 days\*.

[rsc.li/ees-catalysis](https://rsc.li/ees-catalysis)



## Sustainable Energy & Fuels

Driving the development of sustainable energy technologies through cutting edge research

### Editor-in-Chief

Garry Rumbles, National Renewable Energy Laboratory and University of Colorado Boulder, USA

Impact factor 2021: 6.813, median time to first decision (peer reviewed articles only): 28 days\*.

[rsc.li/sustainable-energy](https://rsc.li/sustainable-energy)



## Energy Advances

Embracing research at the nexus of energy science and sustainability

### Editor-in-Chief

Volker Presser, Leibniz Institute for New Materials, Germany

Median time to first decision (peer reviewed articles only): 32 days\*.

[rsc.li/energy-advances](https://rsc.li/energy-advances)

Submit your work today

[rsc.li/energy](https://rsc.li/energy)

\*Visit [rsc.li/metrics-explainer](https://rsc.li/metrics-explainer) for more information

Registered charity number: 207890

## REVIEWS

70

## Recent advances of phenotypic screening strategies in the application of anti-influenza virus drug discovery

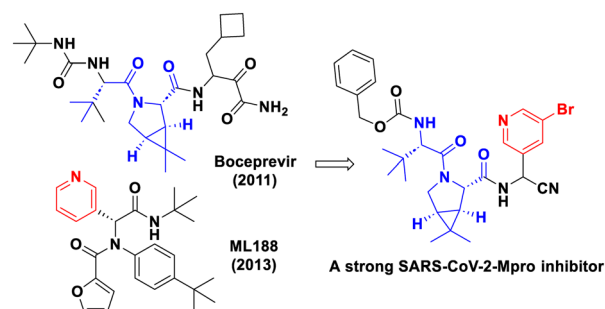
Huinan Jia, Lide Hu, Jiwei Zhang, Xing Huang, Yuanmin Jiang, Guanyu Dong, Chuanfeng Liu,\* Xinyong Liu,\* Meehyein Kim\* and Peng Zhan\*



81

## On the origins of SARS-CoV-2 main protease inhibitors

Yves L. Janin



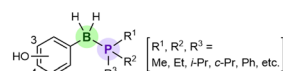
## RESEARCH ARTICLES

119

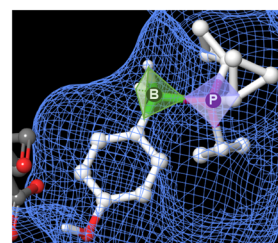
## Physicochemical characterization of *B*-hydroxyphenyl phosphine borane derivatives and their evaluation as nuclear estrogen receptor ligands

Yu Miyajima, Tomomi Noguchi-Yachide, Kotaro Ochiai and Shinya Fujii\*

### Phosphine borane Novel chemical entry for drug discovery



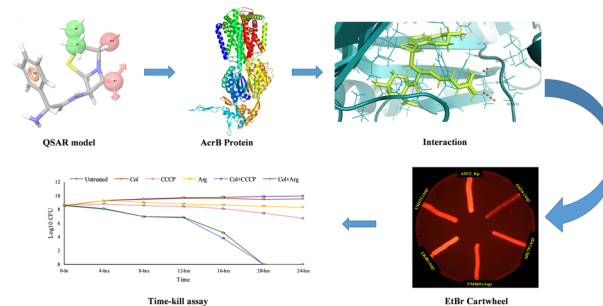
- ✓ Stable in aqueous media
- ✓ Less hydrophobic than hydrocarbons
- ✓ Desirable membrane affinity
- ✓ Estrogen receptor agonistic activity with favorable lipophilicity



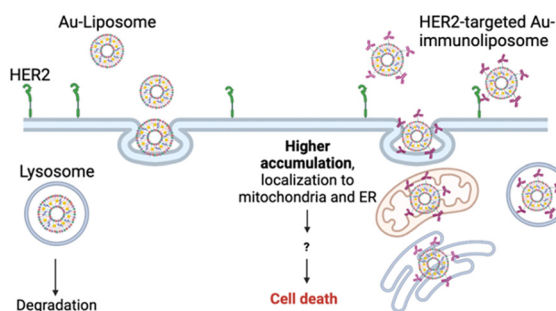
127

## Development of pharmacophore models for AcrB protein and the identification of potential adjuvant candidates for overcoming efflux-mediated colistin resistance

Dibyajyoti Uttameswar Behera, Mahendra Gaur, Maheswata Sahoo, Enketeswara Subudhi\* and Bharat Bhusan Subudhi\*



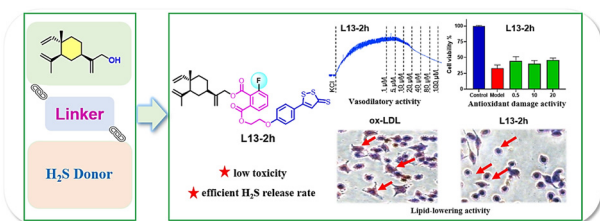
139



### Development of immunoliposomes containing cytotoxic gold payloads against HER2-positive breast cancers

Afruja Ahad, Fatima Aftab, Alexa Michel, Jason S. Lewis\* and Maria Contel\*

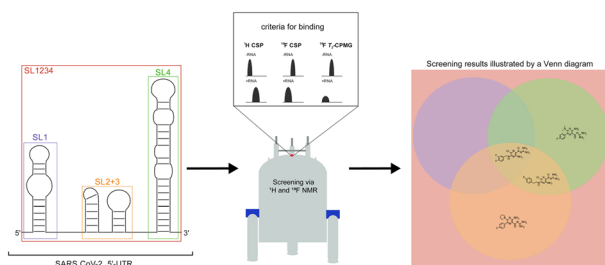
151



### Discovery of novel $\beta$ -elemene hybrids with hydrogen sulfide-releasing moiety possessing cardiovascular protective activity for the treatment of atherosclerosis

Wenjian Zhu, Hongyu Wu, Chen He, Huajian Zhu, Hong Yao, Yun Cao, Yueman Shi, Xiaotong Chen, Xue Feng, Shengtao Xu,\* Zheyong Zhu and Jinyi Xu\*

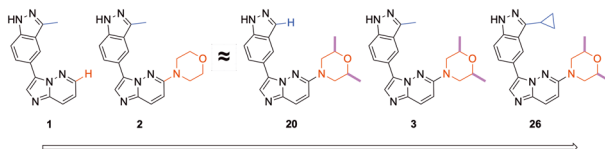
165



### NMR $^1\text{H}$ , $^{19}\text{F}$ -based screening of the four stem-looped structure 5\_SL1-SL4 located in the 5'-untranslated region of SARS-CoV 2 RNA

Daniel Hymon, Jason Martins, Christian Richter, Sridhar Sreeramulu, Anna Wacker, Jan Ferner, Neeraj N. Patwardhan, Amanda E. Hargrove and Harald Schwalbe\*

178



### Discovery of imidazo[1,2-*b*]pyridazine-containing TAK1 kinase inhibitors with excellent activities against multiple myeloma

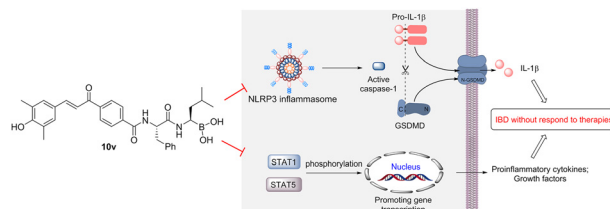
Desmond Akwata, Allison L. Kempen, Jones Lamptey, Neetu Dayal, Nickolas R. Brauer and Herman O. Sintim\*



193

## Discovery of a dual-acting inhibitor of interleukin-1 $\beta$ and STATs for the treatment of inflammatory bowel disease

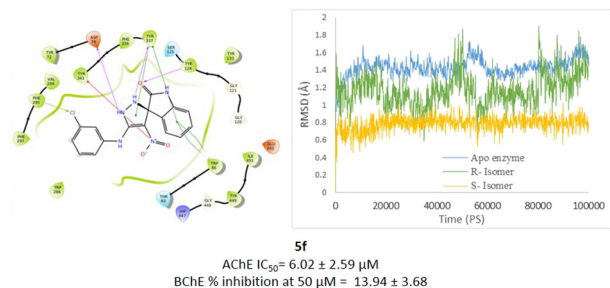
Haowei Cai, Zhuorong Liu, Ping Sun, Yinghua Zhou, Yuyun Yan, Yiming Luo, Xiuxiu Zhang, Ruiwen Wu, Xiangting Liang, Dan Wu, Wenhui Hu\* and Zhongjin Yang\*



207

## Highly efficient, catalyst-free, one-pot sequential four-component synthesis of novel spiroindolinone-pyrazole scaffolds as anti-Alzheimer agents: *in silico* study and biological screening

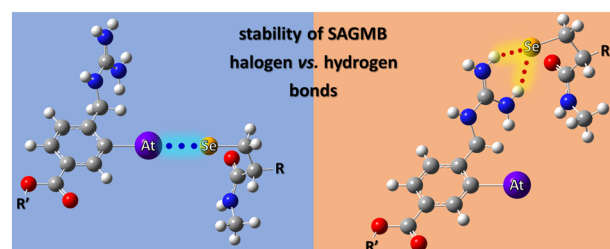
Hormoz Pourtaher, Yasaman Mohammadi, Alireza Hasaninejad\* and Aida Irajji\*



223

## *In vivo* stability of $^{211}\text{At}$ -radiopharmaceuticals: on the impact of halogen bond formation

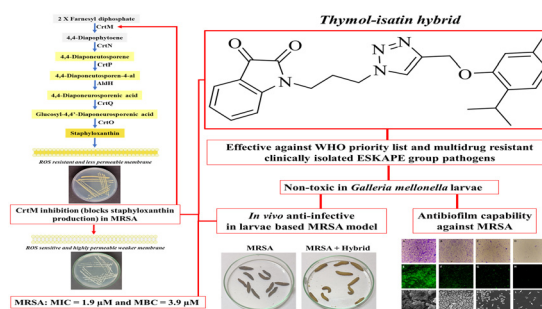
Thibault Yssartier, Lu Liu, Sylvain Pardoue, Jean-Yves Le Questel, François Guérard, Gilles Montavon\* and Nicolas Galland\*



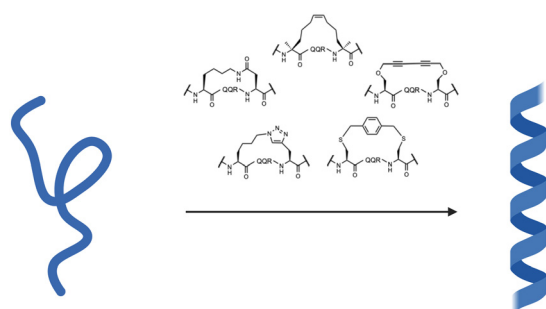
234

## The development of thymol-isatin hybrids as broad-spectrum antibacterial agents with potent anti-MRSA activity

Atamjit Singh,\* Kirandeep Kaur, Pallvi Mohana, Karanvir Singh, Aman Sharma, Jignesh Prajapati, Dweipayan Goswami, Neha Khosla, Uttam Kaur, Rajanbir Kaur, Rajinder Kaur, Abhineet Rana, Sandeep Kour, Puja Ohri, Saroj Arora, Renu Chadha and Preet Mohinder Singh Bedi\*



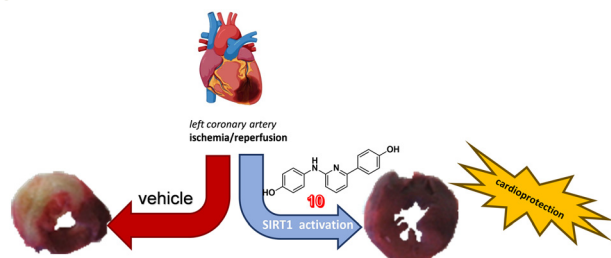
254



### A survey of stapling methods to increase affinity, activity, and stability of ghrelin analogues

Juan J. Esteban, Julia R. Mason, Jakob Kaminski, Rithwik Ramachandran and Leonard G. Luyt\*

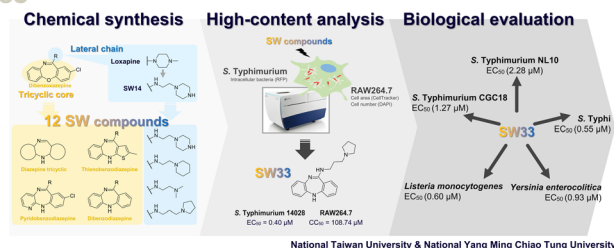
267



### Sirtuin 1-activating derivatives belonging to the anilino-pyridine class displaying *in vivo* cardioprotective activities

Giulia Bononi, Valentina Citi, Alma Martelli, Giulio Poli, Tiziano Tuccinardi, Carlotta Granchi,\* Lara Testai,\* Vincenzo Calderone and Filippo Minutolo

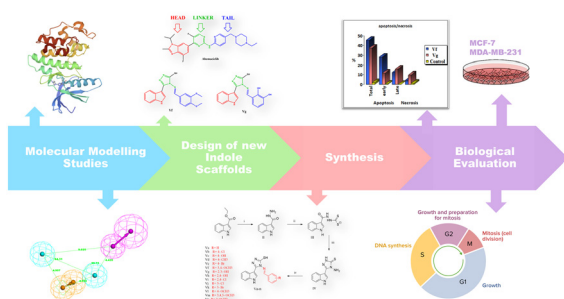
283



### Discovery of new dibenzodiazepine derivatives as antibacterials against intracellular bacteria

Ling-Han Chen, Man-Yi Lin, Hsueh-Chun Lin, Fan-Wei Yang, Hsiao-Wei Liao, Chung-Wai Shiau, Hao-Chieh Chiu\* and Jung-Chen Su\*

293



### Novel indolyl 1,2,4-triazole derivatives as potential anti-proliferative agents: *in silico* studies, synthesis, and biological evaluation

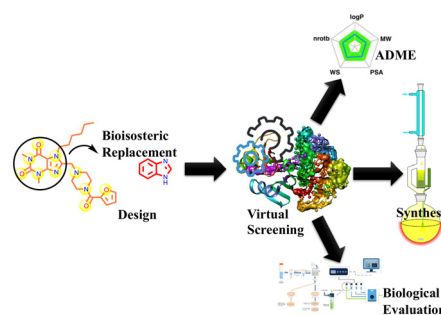
Sarah A. Ghobish, Khaled O. Mohamed, Nahla Farag\* and Doaa B. Farag\*



309

### Scaffold hopping based designing of selective ALDH1A1 inhibitors to overcome cyclophosphamide resistance: synthesis and biological evaluation

Gera Narendra, Baddipadige Raju, Himanshu Verma, Manoj Kumar, Subheet Kumar Jain, Gurleen Kaur Tung, Shubham Thakur, Rasdeep Kaur, Satwinderjeet Kaur, Bharti Sapra and Om Silakari\*

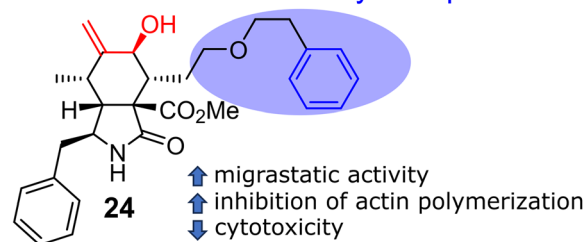


322

### Synthesis and migrastatic activity of cytochalasin analogues lacking a macrocyclic moiety

Bedřich Formánek, Dorian Dupommier, Tereza Volfová, Silvie Rimpelová, Aneta Škarková, Jana Herciková, Daniel Rösel, Jan Brábek and Pavla Perlíková\*

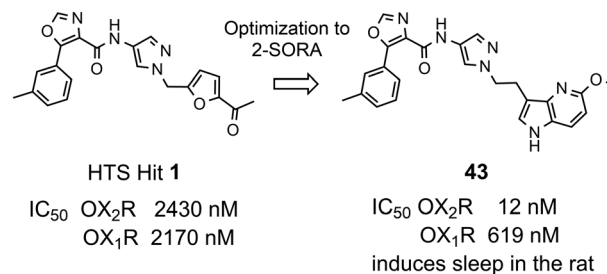
core modifications macrocycle replacement



344

### Pyrazole derivatives as selective orexin-2 receptor antagonists (2-SORA): synthesis, structure–activity–relationship, and sleep-promoting properties in rats

Christine Brotschi,\* Martin H. Bolli,\* John Gatfield, Catherine Roch, Thierry Sifferlen, Alexander Treiber, Jodi T. Williams and Christoph Boss



355

### Impact of dipeptide on ADC physicochemical properties and efficacy identifies Ala–Ala as the optimal dipeptide

Lu Wang,\* Adrian D. Hobson, Julia Fitzgibbons, Axel Hernandez Jr., Ying Jia, Zhou Xu, Zhongyuan Wang, Yajie Yu and Xiang Li

