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RSC Medicinal Chemistry

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ISSN 2632–8682 CODEN RMCSCX 16(4) 1461–1844 (2025)

Cover
See Antonella Ciancetta *et al.*, pp. 1584–1599.
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Inside cover
See Rashmi Sharma *et al.*, pp. 1476–1498.
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PROFILE

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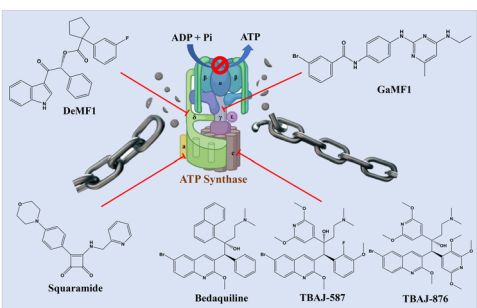
Contributors to our Emerging Investigators collection

REVIEWS

1476

Breaking the energy chain: importance of ATP synthase in *Mycobacterium tuberculosis* and its potential as a drug target

Summaya Perveen, Sunny Pal and Rashmi Sharma*



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PLENARY LECTURES

Dr Ingo HARTUNG
MERCK HEALTHCARE, Darmstadt, Germany

Prof. Paul J. HERGENROTHER
UNIVERSITY OF ILLINOIS, Urbana, IL, United States

Dr Wendy YOUNG
BIOTECH EXECUTIVE & INDEPENDENT BOARD MEMBER, San Francisco, CA, United States

Still possible to register!

SESSIONS AND SESSION COORDINATORS

GPCRS
Dr Tilly BINGHAM *(GIO Therapeutics, Basel, Switzerland)*

A FOCUS ON EARLY CAREER INVESTIGATORS
Prof. Oluseye ONAJOLE *(Roosevelt University, Chicago, IL, United States)*

CHEMICAL BIOLOGY
Prof. Zeynep ATES-ALAGOZ *(Ankara University, Ankara, Turkey)*

AI IN DRUG DISCOVERY
Dr Luc VAN HIJFTE *(Symeres, Nijmegen, The Netherlands)*

INDUCED PROXIMITY
Dr Jennifer ALLEN *(Amgen Inc., South San Francisco, CA, United States)*

PEPTIDE THERAPEUTICS
Prof. Terry MOORE *(University of Illinois, Chicago, IL, United States)*

ANTIVIRAL DRUG DISCOVERY
Prof. Daniel HARKI *(University of Minnesota, Minneapolis, MN, United States)*

CHEMISTRY TOOLS
Dr Hasan A. KHAN *(AbbVie, North Chicago, IL, United States)*

NEW FRONTIERS IN ONCOLOGY AND IMMUNO ONCOLOGY
Dr Darby SCHMIDT *(Violet Therapeutics, Cambridge, MA, United States)*

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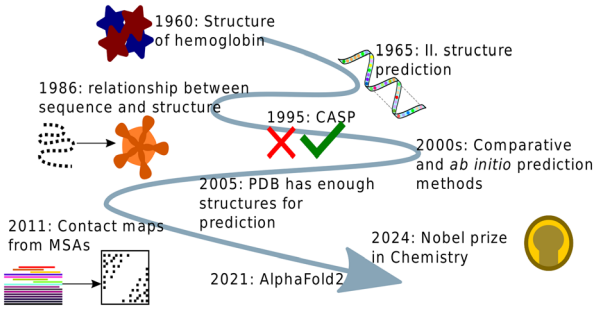
REVIEWS

1499

The physics-AI dialogue in drug design

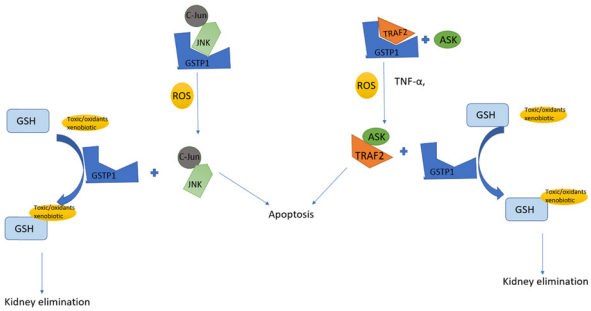
Pablo Andrés Vargas-Rosales and Amedeo Caflisch*



1516

Isozyme-specific inhibition of GSTP1-1: a crucial element in cancer-targeting drugs

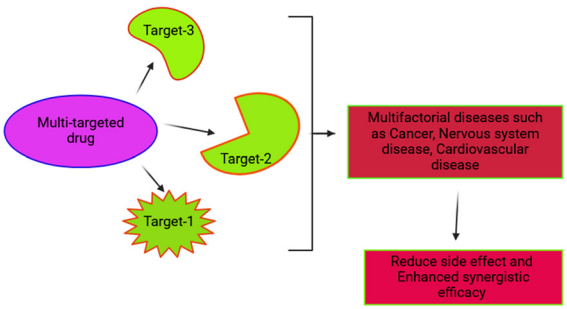
Belal O. Al-Najjar,* M. Helal,* Fadi G. Saqallah and B. Bandy



1532

Synthetic strategies and medicinal chemistry perspectives of dual acting carbonic anhydrase modulators with monoamine oxidase and cholinesterase inhibitors

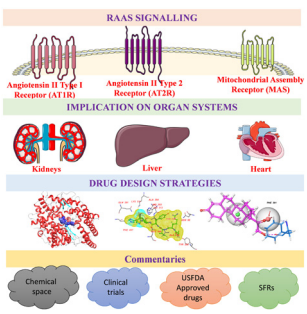
Sandeep Bindra, Ehab M. Mostafa,* Mohamed A. Abdelgawad, Samy Selim, Sunil Kumar and Bijo Mathew*



1550

A perspective on small molecules targeting the renin–angiotensin–aldosterone system and their utility in cardiovascular diseases: exploring the structural insights for rational drug discovery and development

Nisha Bansal, Deepika Kathuria, Arockia M. Babu, Sonia Dhiman, Sorabh Lakhanpal, K. Nagendra Prasad, Roshan Kumar, Yogita Tyagi, Bhupinder Kumar,* Mahendra Pratap Singh and Abhay M. Gaidhane



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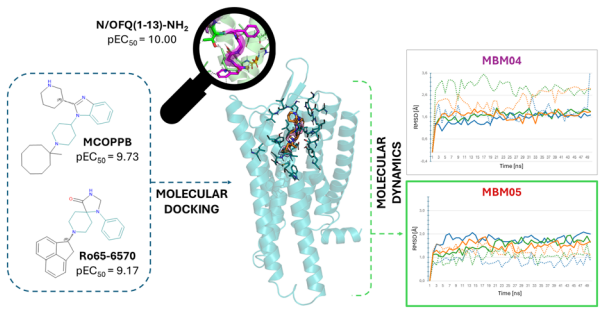
RESEARCH ARTICLES

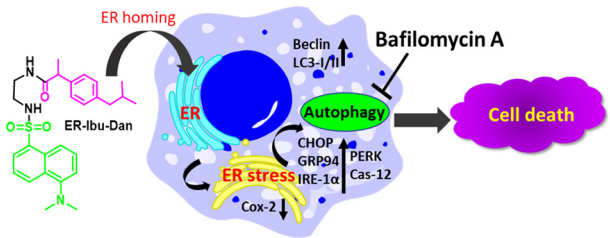
1584



Probing non-peptide agonists binding at the human nociceptin/orphanin FQ receptor: a molecular modelling study

Matteo Gozzi, Davide Malfacini, Valentina Albanese, Salvatore Pacifico, Delia Preti, Remo Guerrini, Girolamo Calò and Antonella Ciancetta*

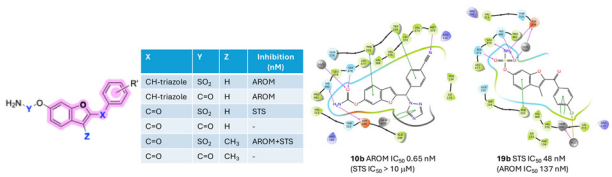
1600



Relocating NSAIDs into the endoplasmic reticulum induces ER stress-mediated apoptosis in cancer cells

Tripti Mishra, Preeti, Jaypalsing Ingle, Aditi Saha and Sudipta Basu*

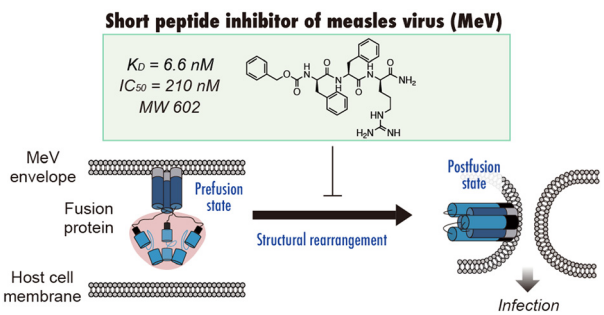
1606



Development of benzofuran-derived sulfamates as dual aromatase-steroid sulfatase inhibitors (DASIs): design, synthesis and biological evaluation

Ahmed G. Eissa, Francesca Gozzi, Oqab Aloqab, Charlotte E. Parrish, Nadira Mohamed, Irene Shiali, Harith Al-Baldawi, Paul A. Foster and Claire Simons*

1619



Discovery of potent measles virus fusion inhibitor peptides *via* structure-guided derivatization

Ziwei Gao, Jiei Sasaki, Tateki Suzuki, Tomoaki Suzuki, Yuki Miwa, Shinsuke Sando,* Takao Hashiguchi* and Jumpei Morimoto*

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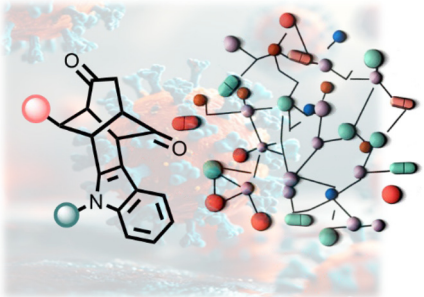
RESEARCH ARTICLES

1626

Expanding the chemical space for antiviral discovery: the potential of twistenediones

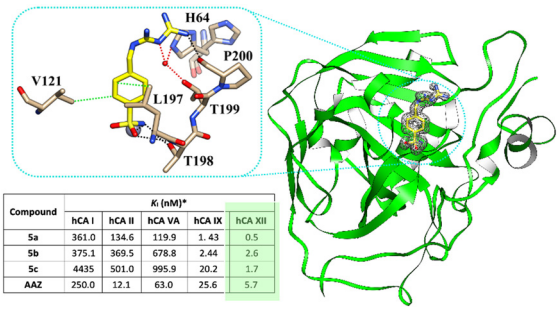
Aida Jaafar, Daniel Guerra-González, Ana Pascual, Ana M. Ortuño, Carlos M. Cruz, Juan M. Cuerva, Paula Bueno, Victoria Castro, Urtzi Garaigorta, Pablo Gastaminza,* Javier Adrio* and María Ribagorda*



1633

X-ray crystallographic and kinetic studies of biguanide containing aryl sulfonamides as carbonic anhydrase inhibitors

Chiara Baroni, Murat Bozdag, Gioele Renzi, Viviana De Luca, Clemente Capasso, Carla Bazzicalupi, Silvia Selleri, Marta Ferraroni,* Fabrizio Carta* and Claudiu T. Supuran

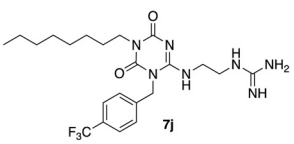


Compound	K_i (nM)*				
	hCA I	hCA II	hCA VA	hCA IX	hCA XII
5a	361.0	134.6	119.9	1. 43	0.5
5b	375.1	369.5	678.8	2.44	2.6
5c	4435	501.0	995.9	20.2	1.7
AAZ	250.0	12.1	63.0	25.6	5.7

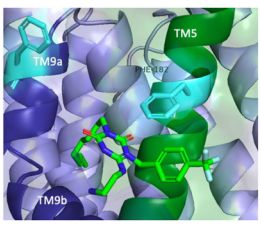
1641

Antimicrobial triazinedione inhibitors of the translocase MraY–protein E interaction site: synergistic effects with bacitracin imply a new mechanism of action

Julia A. Fairbairn, Rachel V. Kerr, Nika-Kare A. Pierre-White, Anthony Jacovides, Becca W. A. Baileeves, Phillip J. Stansfeld, Gerhard Bringmann, Andrew T. Merritt and Timothy D. H. Bugg*



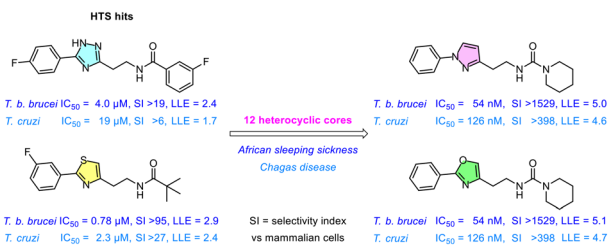
Acinetobacter baumannii MIC 16 μg/mL,
Staphyloccoccus aureus MRSA MIC 2-4 μg/mL



1654

Heterocyclic core modifications in trypanosomacidal 2-[(phenylheteroaryl)ethyl]ureas

Arthur Toynton, Lori Ferrins, Harriet L. Newson, Melissa L. Sykes, Swapna Varghese, Nghi Nguyen, Stephanie Russell, Raphaël Rahmani, Jeremy Cheang, Gavin R. Flematti, Brian W. Skelton, Bilal Zulfiqar, Vicky M. Avery,* Jonathan B. Baell* and Matthew J. Piggott*



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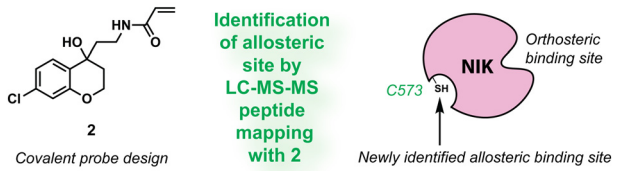
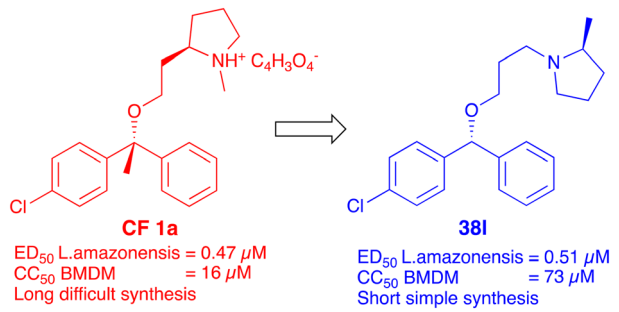
1681



Identification of a novel allosteric binding site on the catalytic domain of NF-κB inducing kinase (NIK)

Jared J. Anderson and Daniel A. Harki*

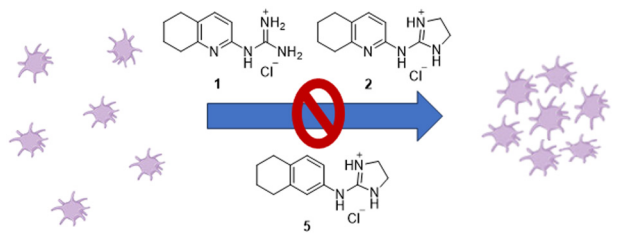
1686



Simple accessible clemastine fumarate analogues as effective antileishmanials

Rebecca L. Charlton, Douglas O. Escrivani, Christopher Brown, Niranjan Thota, Victor S. Agostino, Exequiel O. J. Porta, Timur Avkiran, Andrew T. Merritt, Paul W. Denny, Bartira Rossi-Bergmann and Patrick G. Steel*

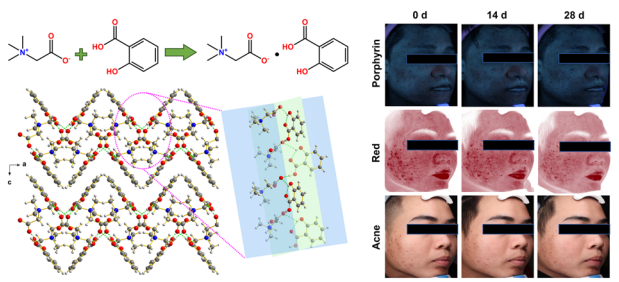
1695



Effect of mono-guanidine-like derivatives on platelet aggregation and tumour cell induced platelet aggregation

Nadhim Kamil Hante, Aaron P. Keogh, Yanni Huang, Tanya Kapoor, Harriet Bennett-Lenane, Eleanor Walsh, Isabel Rozas,* Carlos Medina* and Maria Jose Santos-Martinez*

1705



Betaine–salicylic acid cocrystal for enhanced skincare and acne treatment

Zhenyuan Wang, Mi Wang,* Qingsheng Tao, Yufei Li, Hao Wang, Mei Zhang, Xueli Liu and Jiaheng Zhang*

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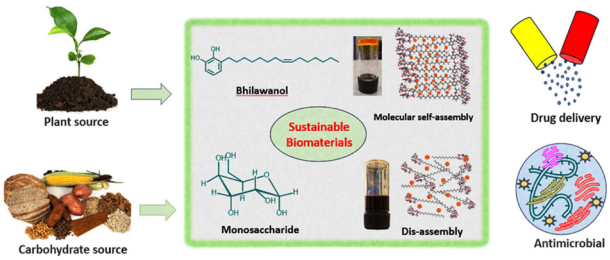
RESEARCH ARTICLES

1715

Biocompatible glycolipid derived from bhilawanol as an antibiofilm agent and a promising platform for drug delivery

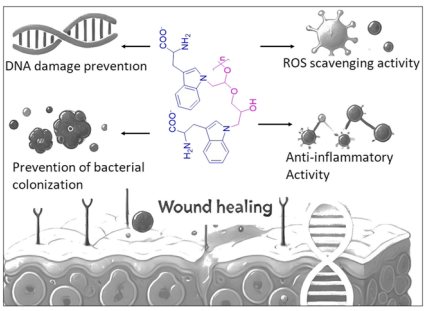
Tohira Banoo, Abhijit Ghosh, Priyasha Mishra, Sanhita Roy and Subbiah Nagarajan*



1729

***N*-Glycidyl D-tryptophan ether-based ointment with anti-infective, anti-inflammatory, and wound-healing properties**

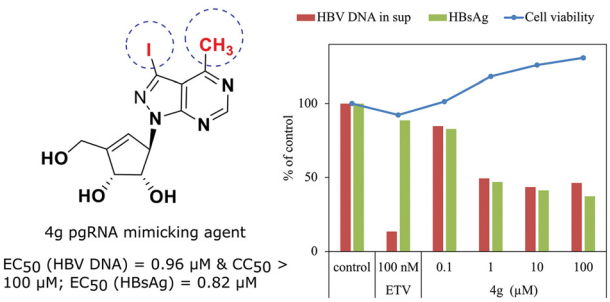
Denial Mahata, Malabendu Jana, Suresh K. Mondal, Sounik Manna, Arundhuti Jana, Anirban Chakraborty, Ananta K. Ghosh, Ranadhir Chakraborty, Tapas K. Hazra and Santi M. Mandal*



1740

Pyrazolo[3,4-*d*]pyrimidine-based neplanocin analogues identified as potential *de novo* pharmacophores for dual-target HBV inhibition

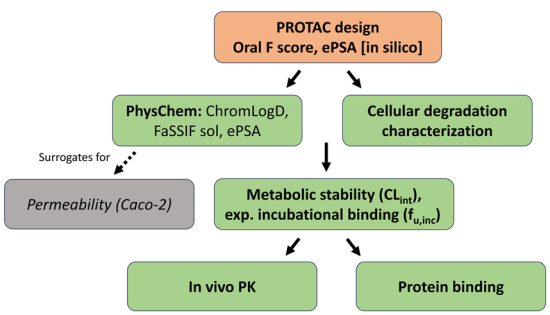
Mohan Kasula,* Masaaki Toyama, Ramakrishnamraju Samunuri, Ashok Kumar Jha, Mika Okamoto, Masanori Baba and Ashoke Sharon*



1746

***In vitro* and *in vivo* ADME of heterobifunctional degraders: a tailored approach to optimize DMPK properties of PROTACs©**

Christine Katharina Maurer, Zhizhou Fang, Christina Schindler, Gianna Pohl, Fouzia Machrouhi-Porcher, Marc Lecomte, Carl Petersson and Heide Marika Duevel*



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RESEARCH ARTICLES

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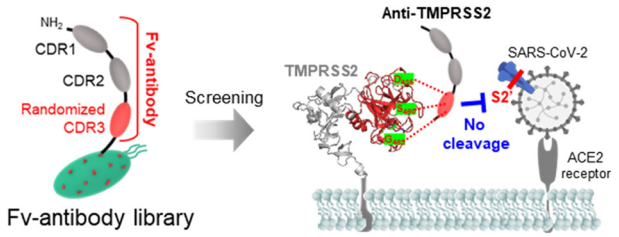
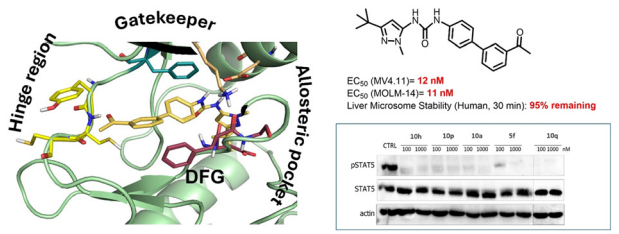


Transmembrane protease serine 2 (TMPRSS2) inhibitors screened from an Fv-antibody library for preventing SARS-CoV-2 infection

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

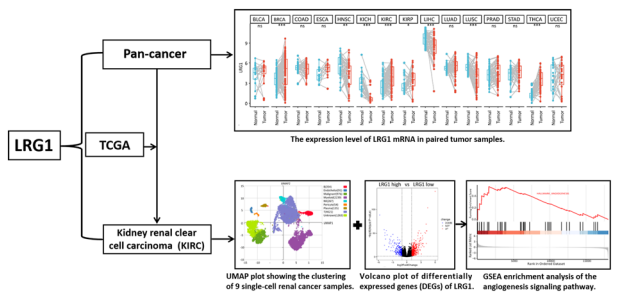
1766



Discovery of selective, metabolically stable pyrazole-based FLT3 inhibitors for the treatment of acute myeloid leukemia

Lorenza Destro, Valentina Crippa, Daniela Gabbia, Marco Roverso, Sara Bogialli, Paolo Zardi, Giovanni Marzaro, Luca Mologni and Alfonso Zambon*

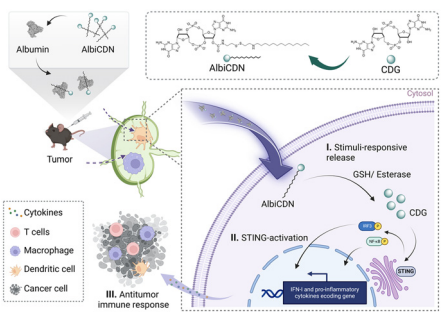
1781



The pan-cancer analysis of LRG1 and its potential role in kidney renal clear cell carcinoma

Ziwen Lei, Shiyu Song, Yizhuo Geng, Bian Liu, Yongzheng Li, Huan Min,* Saiyang Zhang* and Yingqiu Qi*

1797



AlbiCDN: albumin-binding amphiphilic STING agonists augment the immune activity for cancer immunotherapy

Shao-Hua Zhuo, Xi Chen, Lang Zhao, Tian-Yang Wang, Jing-Yun Su, Tao Yang, Lijun Yang, Fei Dong, Yu-Fen Zhao and Yan-Mei Li*

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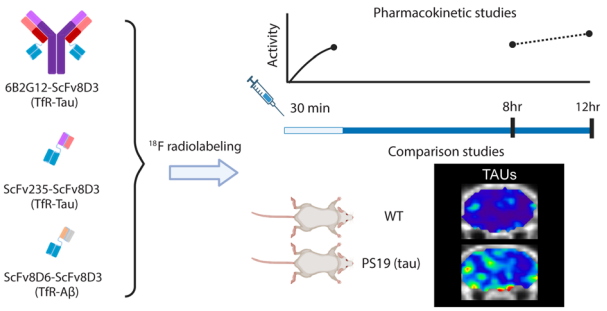
RESEARCH ARTICLES

1808

Feasibility of F-18 radiolabeled brain-penetrable bi-specific antibody radioligands for *in vivo* PET imaging of tauopathy

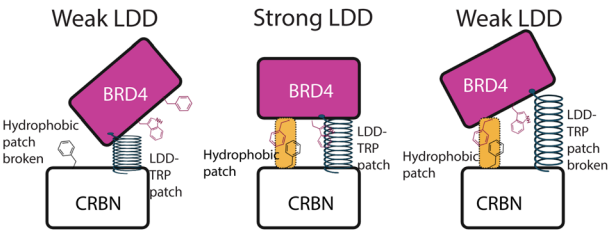
Andrew C. Kelleher, Brandon Richardson, Vinay Kumar Banka, Alex Kazior, Cathy Tan, Sabrina Chan, Rumaish Khastgir, Hao Hu, Zakia Youss, Orin Mishkit and Yu-Shin Ding*



1818

Insights from protein frustration analysis of BRD4–cereblon degrader ternary complexes show separation of strong from weak degraders

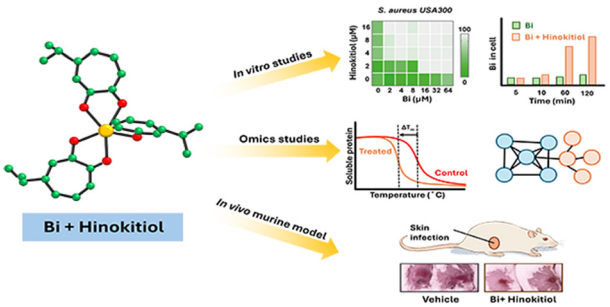
Tianyi Yang, Elizaveta Mukhaleva, Wenyuan Wei, Dahlia Weiss, Ning Ma,* Veerabahu Shanmugasundaram* and Nagarajan Vaidehi*



1829

Hinokitiol potentiates antimicrobial activity of bismuth drugs: a combination therapy for overcoming antimicrobial resistance

Tiffany Ka-Yan Ip, Yuchuan Wang, Suyu Wang, Keyuan Pu, Runming Wang, Bingjie Han, Peng Gao, Yanxuan Xie, Richard Y. Kao, Pak-Leung Ho, Hongyan Li* and Hongzhe Sun*



CORRECTION

1842

Correction: Thiazole-fused androstenone and ethisterone derivatives: potent β- and γ-actin cytoskeleton inhibitors to treat melanoma tumors

Sanjay Adhikary, Subrata Roy, Shailesh Budhathoki, Siam Chowdhury, Abbey Stillwell, Alexei G. Basnakian, Alan Tackett, Nathan Avaritt, Mohamed Milad and Mohammad Abrar Alam*