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Symposium-in-Print

The Chemistry Biology Interface

Edited by:

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Chemical Biology Core Facility, Chemical Biology Department, RIKEN Advanced Science Institute, Hirosawa 2-1, Wako-shi, Saitama, Japan

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Chemical Genomics Research Group, Chemical Biology Department, RIKEN Advanced Science Institute, Hirosawa 2-1, Wako-shi, Saitama, Japan

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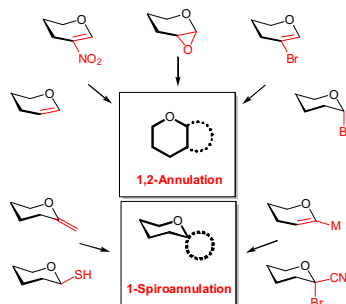
Hiroyuki Osada*, Makoto Muroi, Minoru Yoshida

Chemical approach to bioactive compounds

Syntheses of 1,2-annulated and 1-spiroannulated carbohydrate derivatives: Recent developments

pp 1846–1856

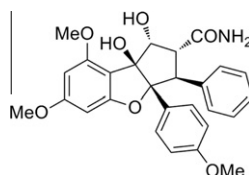
Shahid I. Awan, Daniel B. Werz*



Recent advances in the biology and chemistry of the flavaglines

pp 1857–1864

Nigel Ribeiro, Frédéric Thuaud, Canan Nebigil, Laurent Désaubry*

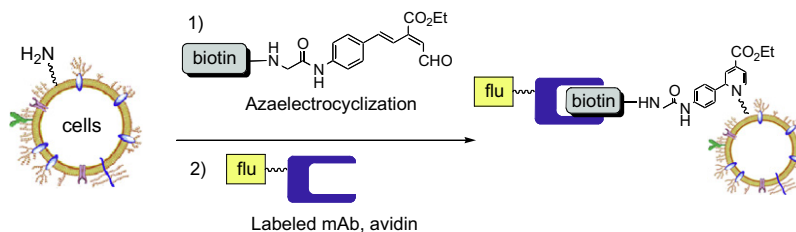


The flavaglines are a family of plant natural products that display potent anticancer and neuroprotective activities. This review summarizes recent synthetic approaches and the current status of the pharmacological properties of this unique class of natural products.

Cell surface biotinylation by azaelectrocyclization: Easy-handling and versatile approach for living cell labeling

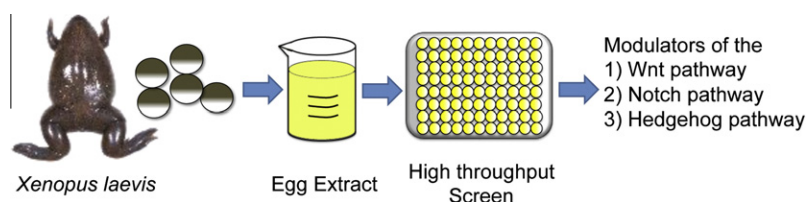
pp 1865–1868

Katsunori Tanaka*, Satomi Yokoi, Koji Morimoto, Takayuki Iwata, Yuka Nakamoto, Kaori Nakayama, Koichi Koyama, Takeshi Fujiwara, Koichi Fukase*

**Screening of bioactive compounds****Screening for small molecule inhibitors of embryonic pathways: Sometimes you gotta crack a few eggs**

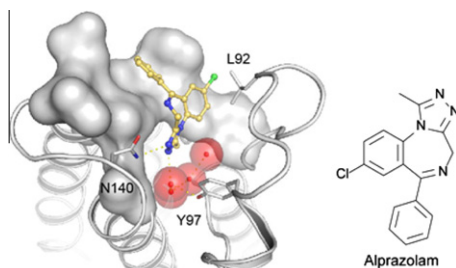
pp 1869–1877

Brian I. Hang, Curtis A. Thorne, David J. Robbins, Stacey S. Huppert, Laura A. Lee, Ethan Lee*

**Benzodiazepines and benzotriazepines as protein interaction inhibitors targeting bromodomains of the BET family**

pp 1878–1886

Panagis Filippakopoulos, Sarah Picaud, Oleg Fedorov, Marco Keller, Matthias Wrobel, Olaf Morgenstern, Franz Bracher*, Stefan Knapp*

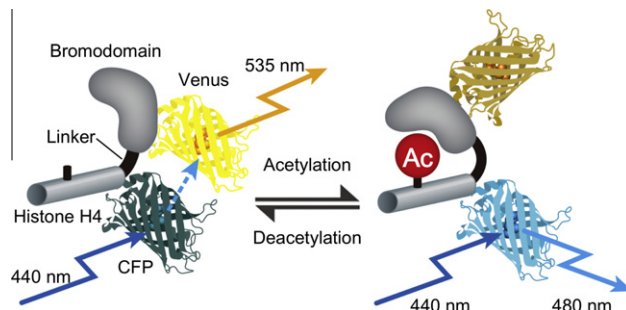


A number of triazolo-benzodiazepines including drugs such as alprazolam have been developed as protein interaction inhibitors that target bromodomains of the BET family.

**Development of live-cell imaging probes for monitoring histone modifications**

pp 1887–1892

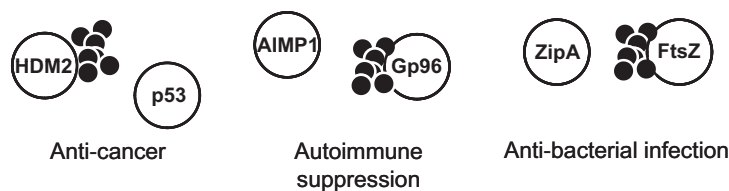
Kazuki Sasaki, Akihiro Ito*, Minoru Yoshida



Chemical modulators working at pharmacological interface of target proteins

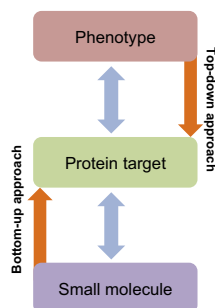
pp 1893–1901

Young Ho Jeon, Jin Young Lee, Sunghoon Kim*

**Target identification of bioactive compounds****Identification and validation of protein targets of bioactive small molecules**

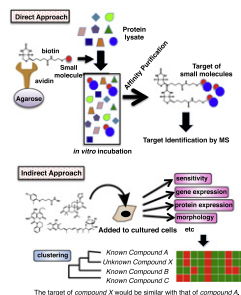
pp 1902–1909

Denis V. Titov, Jun O. Liu*

**Target identification of bioactive compounds**

pp 1910–1921

Etsu Tashiro, Masaya Imoto*

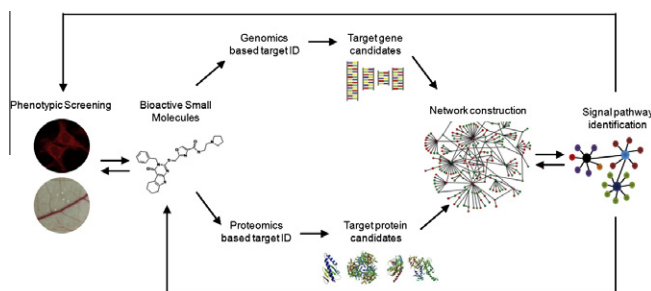


The target of compound X would be similar with that of compound A.

Identification and validation of bioactive small molecule target through phenotypic screening

pp 1922–1928

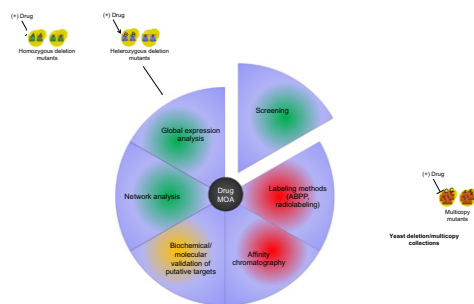
Yoon Sun Cho, Ho Jeong Kwon*



Determining the mode of action of bioactive compounds

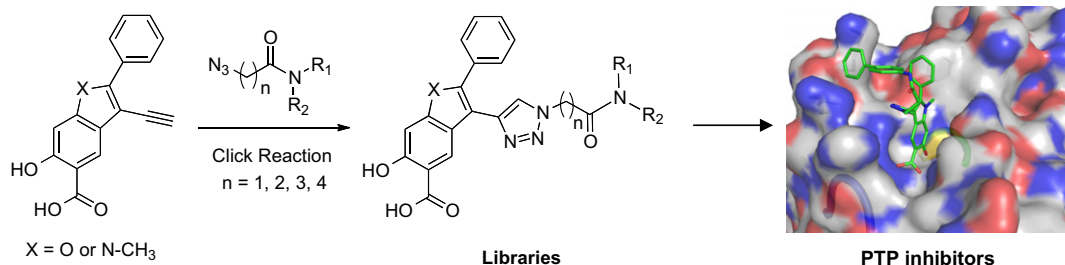
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Marisa A. Azad, Gerard D. Wright*

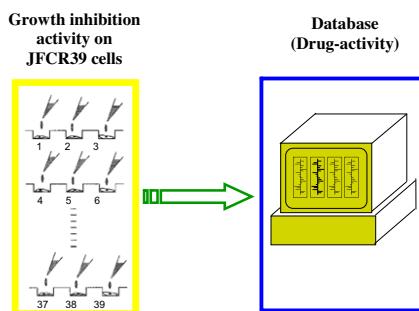
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pp 1940–1946

Yantao He, Li-Fan Zeng, Zhi-Hong Yu, Rongjun He, Sijiu Liu, Zhong-Yin Zhang*

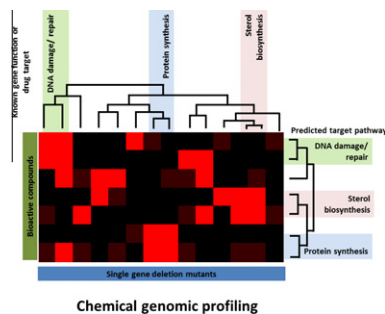
**Profiling of bioactive compounds****JFCR39, a panel of 39 human cancer cell lines, and its application in the discovery and development of anticancer drugs** pp 1947–1951

Dexin Kong, Takao Yamori*

**Chemical-genomic profiling: Systematic analysis of the cellular targets of bioactive molecules**

pp 1952–1960

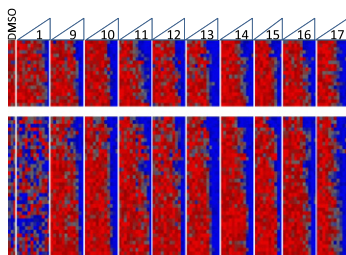
Kerry Andrusiak, Jeff S. Piotrowski, Charles Boone*



Biochemical and transcriptional profiling to triage additional activities in a series of IGF-1R/IR inhibitors

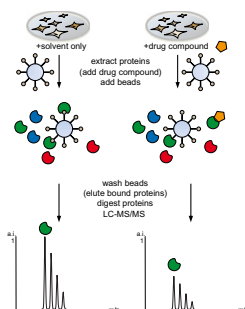
pp 1961–1972

Petra Ross-Macdonald*, Heshani de Silva, Vishal Patel, Amy Truong, Aiqing He, Isaac Neuhaus, Charles Tilford, RuiRu Ji, Nathan Siemers, Ann Greer, Joan Carboni, Marco Gottardis, Krista Menard, Frank Lee, Marco Dodier, David Frennesson, Anthony Sampognaro, Mark Saulnier, George Trainor, Dolatrai Vyas, Kurt Zimmermann, Mark Wittman

**Chemoproteomic approaches to drug target identification and drug profiling**

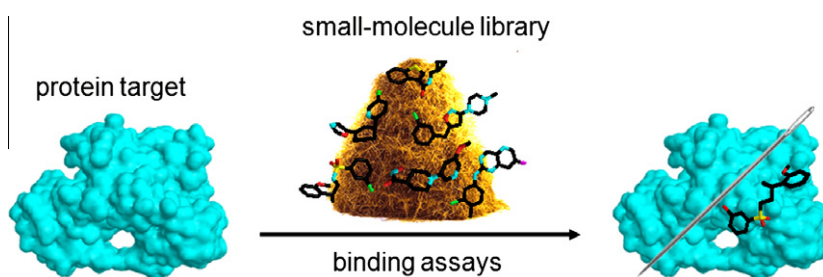
pp 1973–1978

Marcus Bantscheff, Gerard Drewes*

**Novel approach to bioactive compounds****Unbiased binding assays for discovering small-molecule probes and drugs**

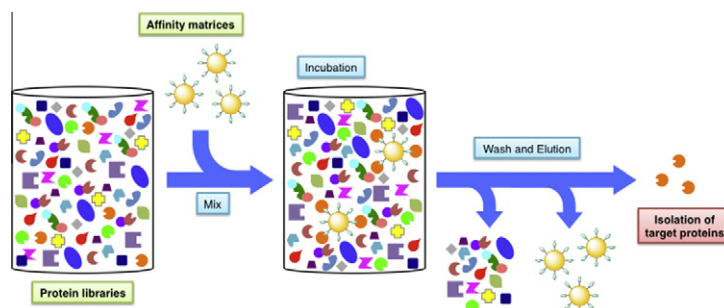
pp 1979–1989

Melissa M. Kemp, Michel Weïwer, Angela N. Koehler*

**Tools and methodologies capable of isolating and identifying a target molecule for a bioactive compound**

pp 1990–2001

Satoshi Sakamoto, Mamoru Hatakeyama, Takumi Ito, Hiroshi Handa*

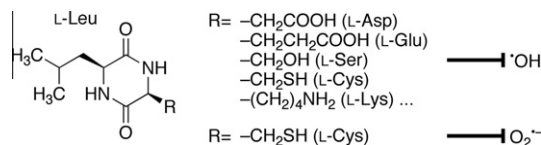


REGULAR ARTICLES

Cyclic dipeptides exhibit potency for scavenging radicals

pp 2002–2009

Tadashi Furukawa, Takashi Akutagawa, Hitomi Funatani, Toshikazu Uchida, Yoshihiro Hotta, Masatake Niwa, Yoshiaki Takaya*

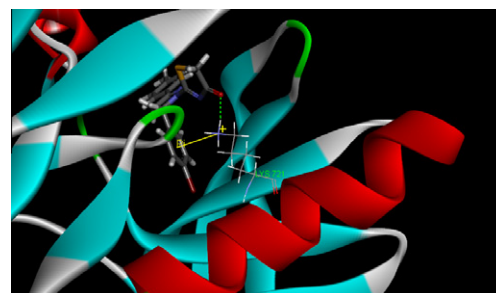


Design, synthesis and biological evaluation of pyrazolyl-thiazolinone derivatives as potential EGFR and HER-2 kinase inhibitors

pp 2010–2018

Ke-Ming Qiu, Hai-Hong Wang, Li-Ming Wang, Yin Luo, Xian-Hui Yang, Xiao-Ming Wang*, Hai-Liang Zhu*

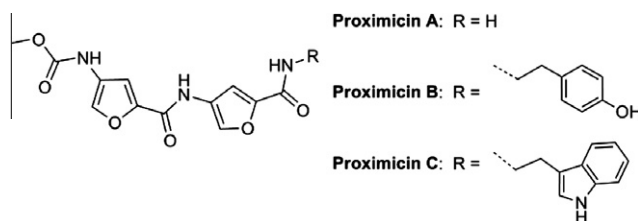
A series of pyrazolyl-thiazolinone derivatives (**E1–E36**) have been designed and synthesized and their biological activities were also evaluated as potential EGFR and HER-2 kinase inhibitors. Thirty-four of the 36 compounds were reported for the first time. Among them, compound 2-(5-(4-bromophenyl)-3-*p*-tolyl-4,5-dihydro-1*H*-pyrazol-1-yl)thiazol-4(5*H*)-one (**E28**) displayed the most potent inhibitory activity ($\text{IC}_{50} = 0.24 \mu\text{M}$ for EGFR and $\text{IC}_{50} = 1.07 \mu\text{M}$ for HER-2). Antiproliferative assay results indicated that compound **E28** owned high antiproliferative activity against MCF-7, B16-F10 and HCT-116 in vitro, with IC_{50} value of 0.30, 0.54, and $0.70 \mu\text{M}$, respectively. Docking simulation was further performed to position compound **E28** into the EGFR active site to determine the probable binding model. Based on the preliminary results, compound **E28** with potent inhibitory activity in tumor growth would be a potential anticancer agent.



Efficient synthesis and biological evaluation of proximicins A, B and C

pp 2019–2024

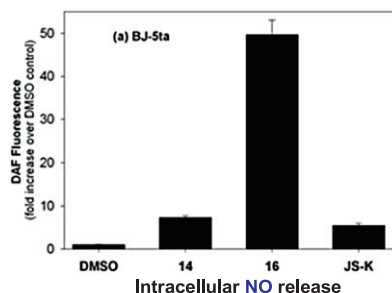
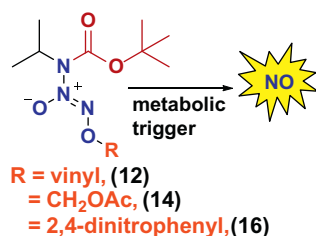
Federico Brucoli*, Antonino Natoli, Preethi Marimuthu, Maria Teresa Borrello, Paul Stapleton, Simon Gibbons, Andreas Schätzlein



Diazeniumdiolated carbamates: A novel class of nitric oxide donors

pp 2025–2029

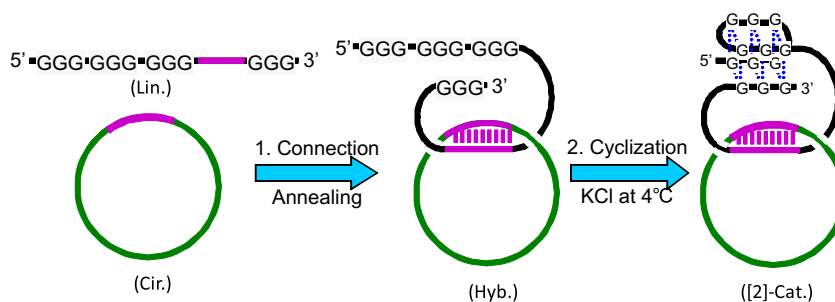
Rahul S. Nandurdikar*, Anna E. Maciag, Zhao Cao, Larry K. Keefer, Joseph E. Saavedra*



Single strand DNA catenane synthesis using the formation of G-quadruplex structure

pp 2030–2034

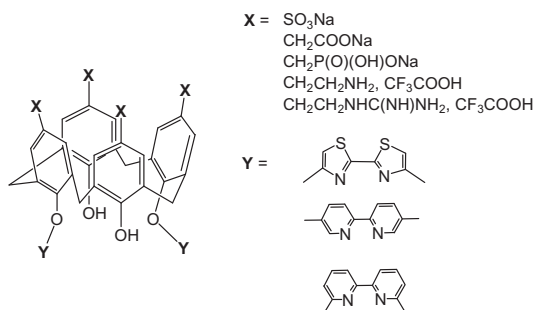
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Anti-mycobacterial activities of some cationic and anionic calix[4]arene derivatives

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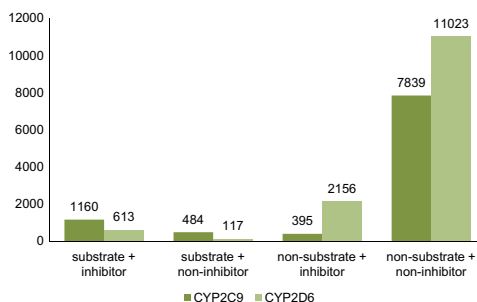
Maxime Mourer, Hugues Massimba Dibama, Patricia Constant, Mamadou Daffé, Jean-Bernard Regnouf-de-Vains*



Identification of cytochrome P450 2D6 and 2C9 substrates and inhibitors by QSAR analysis

pp 2042–2053

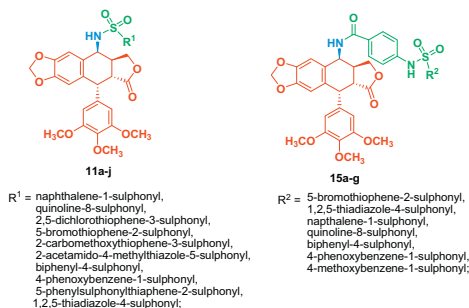
Svava Ósk Jónsdóttir*, Tine Ringsted, Nikolai G. Nikolov, Marianne Dybdahl, Eva Bay Wedebye, Jay R. Niemelä



Synthesis and biological evaluation of 4β-sulphonamido and 4β-[(4'-sulphonamido)benzamide]podophyllotoxins as DNA topoisomerase-IIα and apoptosis inducing agents

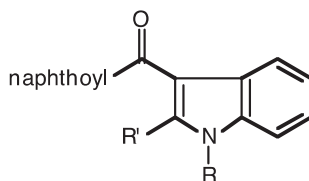
pp 2054–2066

Ahmed Kamal*, Paidakula Suresh, M. Janaki Ramaiah, Adla Mallareddy, Syed Imthiaji, S.N. C. V. L. Pushpavalli, A. Lavanya, Manika Pal-Bhadra*



Synthesis and pharmacology of 1-alkyl-3-(1-naphthoyl)indoles: Steric and electronic effects of 4- and 8-halogenated naphthoyl substituents pp 2067–2081

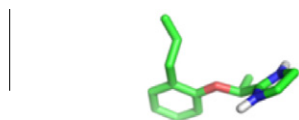
Jenny L. Wiley, Valerie J. Smith, Jianhong Chen, Billy R. Martin, John W. Huffman*



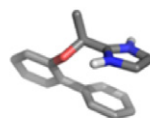
The synthesis and pharmacology of 1-alkyl-3-(4-halo-1-naphthoyl)indoles and 1-alkyl-3-(8-halo-1-naphthoyl)indoles ($R = C_3H_7$ and C_5H_{11} , $R' = H$ and CH_3) is described. Three of these compounds have useful selectivity for the CB_2 receptor.

Might the observed α_{2A} -adrenoreceptor agonism or antagonism of allyphenylene analogues be ascribed to different molecular conformations? pp 2082–2090

Eleonora Diamanti, Fabio Del Bello, Giuseppe Carbonara, Antonio Carrieri, Giuseppe Fracchiolla, Mario Giannella, Valerio Mammoli, Alessandro Piergentili, Katariina Pohjanoksa, Wilma Quaglia, Mika Scheinin, Maria Pigini*



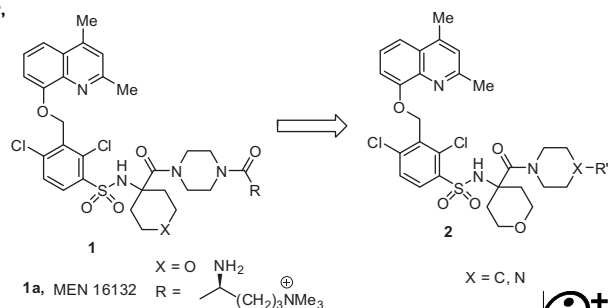
Extended conformation (allyphenylene)



Folded conformation (biphenylene)

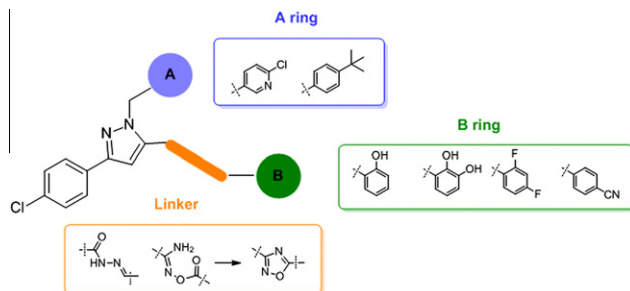
Design and synthesis of novel sulfonamide-containing bradykinin hB_2 receptor antagonists. Synthesis and structure-relationships of α,α -tetrahydropyranylglycine pp 2091–2100

Christopher I. Fincham, Alessandro Bressan, Piero D'Andrea, Alessandro Ettorre, Sandro Giuliani, Sandro Mauro, Stefania Meini, Marielle Paris, Laura Quartara, Cristina Rossi, Antonella Squarcia, Claudio Valenti, Fattori Daniela*, Carlo Alberto Maggi



Synthesis and biological validation of novel pyrazole derivatives with anticancer activity guided by 3D-QSAR analysis pp 2101–2110

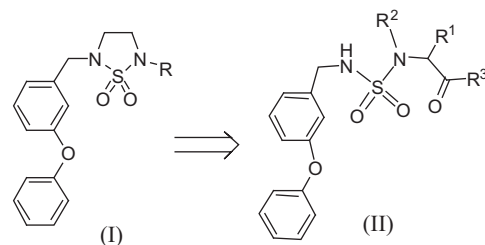
Ines Vujasinović, Andrea Paravić-Radičević, Kata Mlinarić-Majerski, Karmen Brajša, Branimir Bertoša*



Potent norovirus inhibitors based on the acyclic sulfamide scaffold

pp 2111–2118

Dengfeng Dou, Kok-Chuan Tiew, Sivakoteswara Rao Mandadapu, Mallikarjuna Reddy Gunnam, Kevin R. Alliston, Yunjeong Kim, Kyeong-Ok Chang, William C. Groutas*

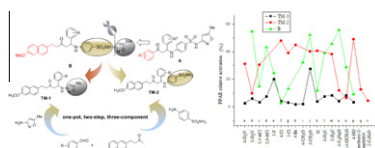


A series of amino acid-derived acyclic sulfamide-based norovirus inhibitors has been synthesized and evaluated using a cell-based replicon system. Several compounds were found to display potent anti-norovirus activity, low toxicity, and good aqueous solubility. These compounds are suitable for further optimization of in vivo potency and ADMET properties.

Synthesis and antidiabetic performance of β -amino ketone containing nabumetone moiety

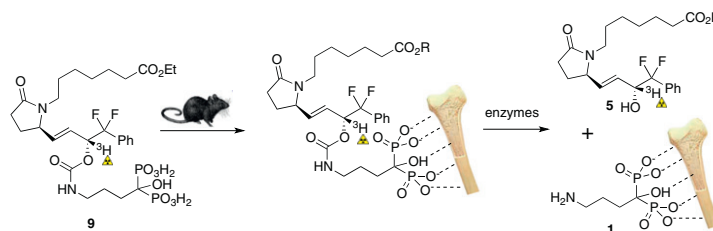
pp 2119–2130

Hang Wang, Ju-fang Yan, Xiao-li Song, Li Fan, Jin Xu, Guang-ming Zhou, Li Jiang*, Da-cheng Yang*

**Design and synthesis of novel bone-targeting dual-action pro-drugs for the treatment and reversal of osteoporosis**

pp 2131–2140

Steve Arns, Romelo Gibe, Anne Moreau, M. Monzur Morshed, Robert N. Young*

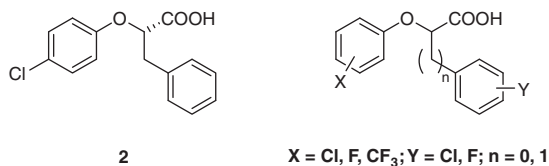


Dual-action pro-drugs (e.g. **9**) target and bind to bone in vivo and slowly release the bone resorption inhibitor, alendronic acid (**1**) and the bone growth stimulant EP4 receptor selective agonist (**5**) in situ.

**Synthesis, biological evaluation and molecular investigation of fluorinated peroxisome proliferator-activated receptors α/γ dual agonists**

pp 2141–2151

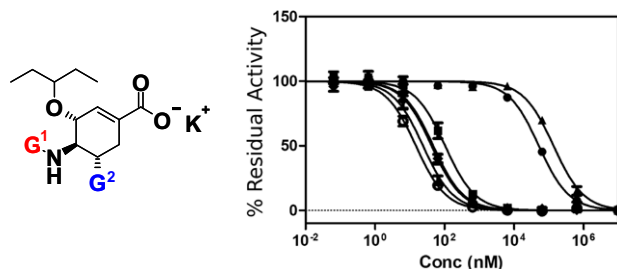
Giuseppe Fracchiolla, Antonio Laghezza, Luca Piemontese, Mariagiovanna Parente, Antonio Lavecchia*, Giorgio Pochetti, Roberta Montanari, Carmen Di Giovanni, Giuseppe Carbonara, Paolo Tortorella, Ettore Novellino, Fulvio Loiodice*



Synthesis and in vitro study of novel neuraminidase inhibitors against avian influenza virus

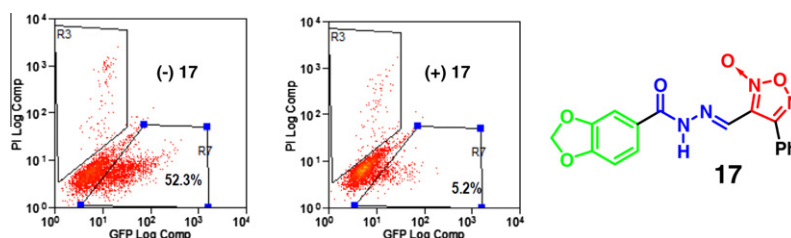
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**Discovery of new orally effective analgesic and anti-inflammatory hybrid furoxanyl *N*-acylhydrazone derivatives**

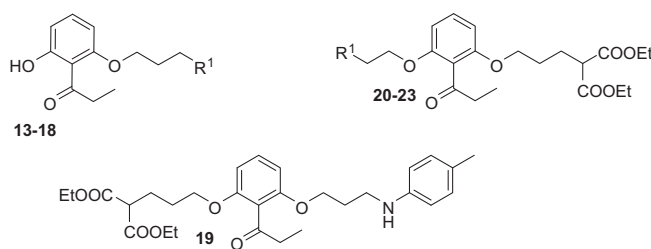
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Paola Hernández, Mauricio Cabrera, María Laura Lavaggi, Laura Celano, Inés Tiscornia, Thiago Rodrigues da Costa, Leonor Thomson, Mariela Bollati-Fogolín, Ana Luisa P. Miranda, Lidia M. Lima, Eliezer J. Barreiro*, Mercedes González*, Hugo Cerecetto*

**Synthesis of propiophenone derivatives as new class of antidiabetic agents reducing body weight in *db/db* mice**

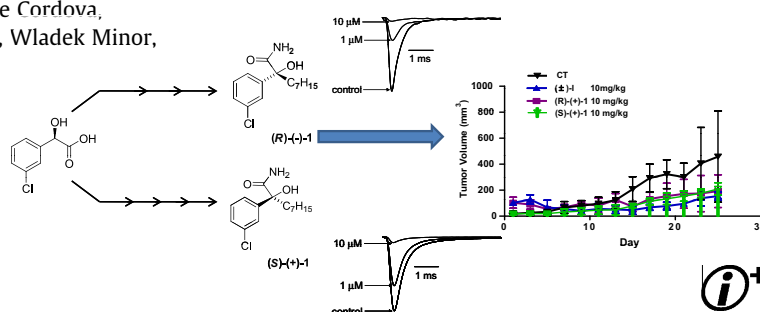
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Atul Kumar*, Siddharth Sharma, Lalit Prakash Gupta, Pervez Ahmad, Swayam Prakash Srivastava, Neha Rahuja, A. K. Tamrakar, Arvind K. Srivastava

**Asymmetric synthesis and evaluation of a hydroxyphenylamide voltage-gated sodium channel blocker in human prostate cancer xenografts**


pp 2180–2188

Gary C. Davis, Yali Kong, Mikell Paige, Zhang Li, Ellen C. Merrick, Todd Hansen, Simeng Suy, Kan Wang, Sivanesan Dakshanamurthy, Antoinette Cordova, Owen B. McManus, Brande S. Williams, Maksymilian Chruszcz, Wladek Minor, Manoj K. Patel, Milton L. Brown*



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*Corresponding author

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