



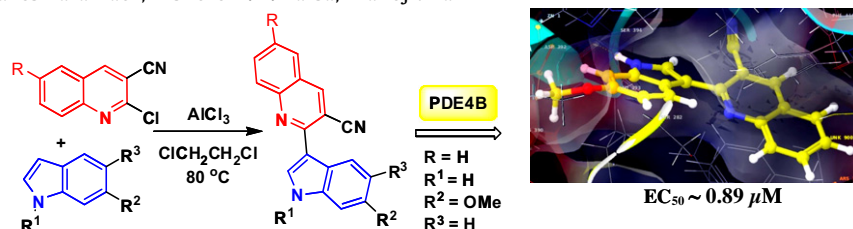
Bioorganic & Medicinal Chemistry Volume 20, Issue 7, 2012

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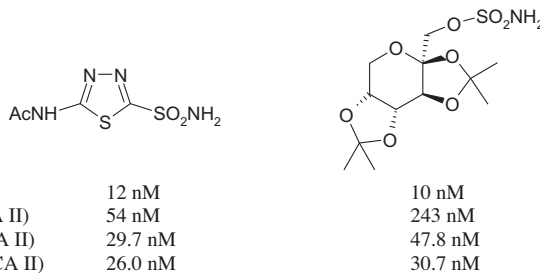
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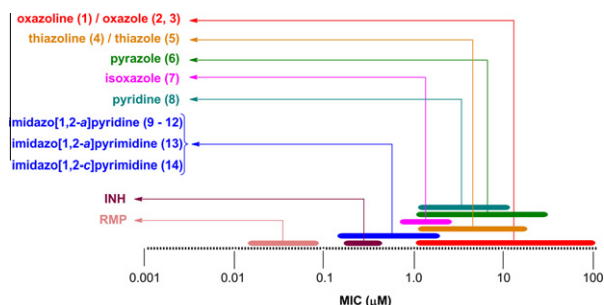
Mutation of active site residues Asn67 to Ile, Gln92 to Val and Leu204 to Ser in human carbonic anhydrase II: Influences on the catalytic activity and affinity for inhibitors pp 2208–2213

Sumeyye Turkoglu, Alfonso Maresca, Meltem Alper, Feray Kockar, Semra Işık, Selma Sinan, Ozen Ozensoy, Oktay Arslan, Claudiu T. Supuran*



Generation and exploration of new classes of antitubercular agents: The optimization of oxazolines, oxazoles, thiazolines, thiazoles to imidazo[1,2-*a*]pyridines and isomeric 5,6-fused scaffolds pp 2214–2220

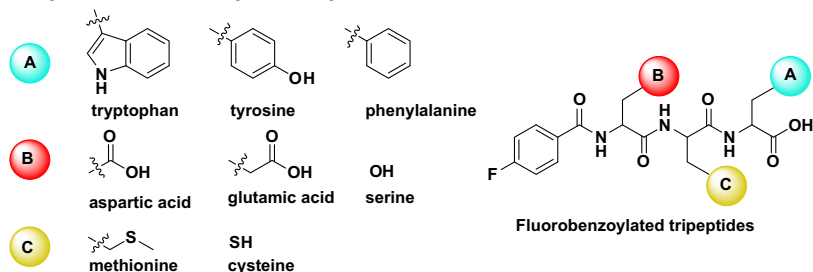
Garrett C. Moraski, Lowell D. Markley, Mayland Chang, Sanghyun Cho, Scott G. Franzblau, Chang Hwa Hwang, Helena Boshoff, Marvin J. Miller*



Synthesis and evaluation of fluorobenzoylated di- and tripeptides as inhibitors of cyclooxygenase-2 (COX-2)

pp 2221–2226

Sai Kiran Sharma, Baker Jawabrah Al-Hourani, Melinda Wuest, Jonathan Y. Mane, Jack Tuszyński, Vickie Baracos, Mavanur Suresh, Frank Wuest*

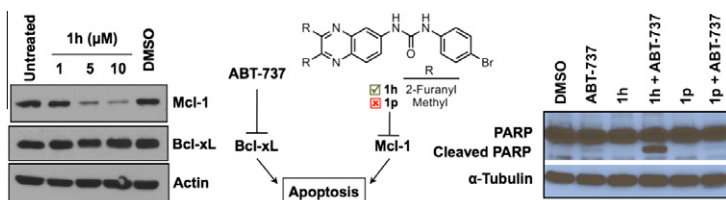


A series of fluorobenzoylated di- and tripeptides as potential leads for the development of molecular probes for imaging of COX-2 expression was prepared according to standard Fmoc-based solid-phase peptide synthesis. All peptides were assessed for their COX-2 inhibitory potency and selectivity profile in a fluorescence-based COX binding assay. Fluorobenzoylated tripeptide FB-Phe-Cys-Ser-OH was further used in molecular modeling docking studies to determine the binding mode within the active site of COX-2.

Perturbing pro-survival proteins using quinoxaline derivatives: A structure–activity relationship study

pp 2227–2234

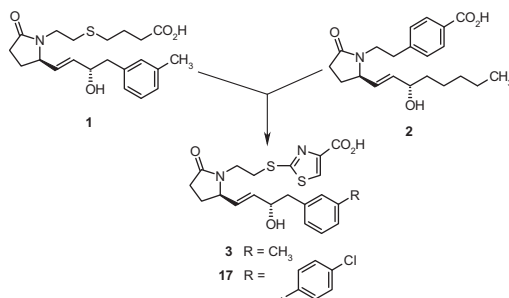
Rajkumar Rajule, Vashti C. Bryant, Hernando Lopez, Xu Luo, Amarnath Natarajan*



Discovery of novel prostaglandin analogs as potent and selective EP2/EP4 dual agonists

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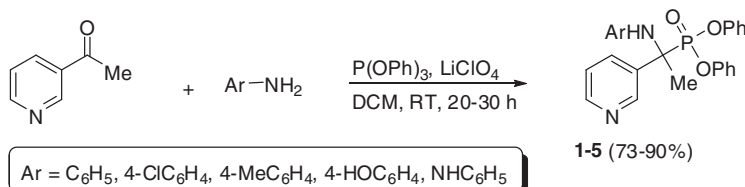
Tohru Kambe*, Toru Maruyama, Yoshihiko Nakai, Hideyuki Yoshida, Hiroji Oida, Takayuki Maruyama, Nobutaka Abe, Akio Nishiura, Hisao Nakai, Masaaki Toda



Synthesis, antimicrobial and anticancer activities of a novel series of diphenyl 1-(pyridin-3-yl)ethylphosphonates

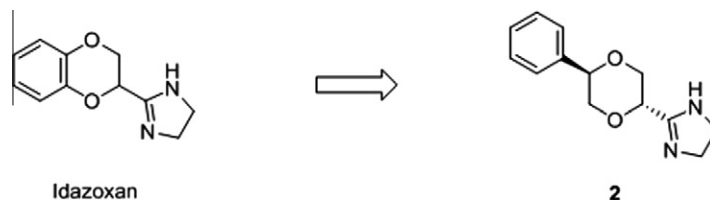
pp 2252–2258

Mohamed F. Abdel-Megeed, Badr E. Badr, Mohamed M. Azaam, Gamal A. El-Hiti*



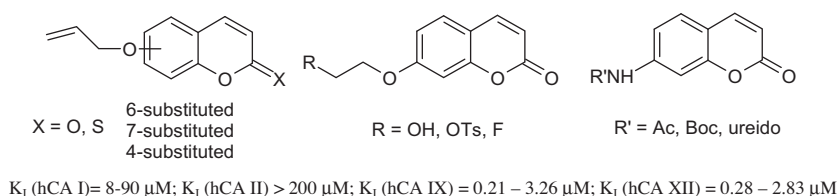
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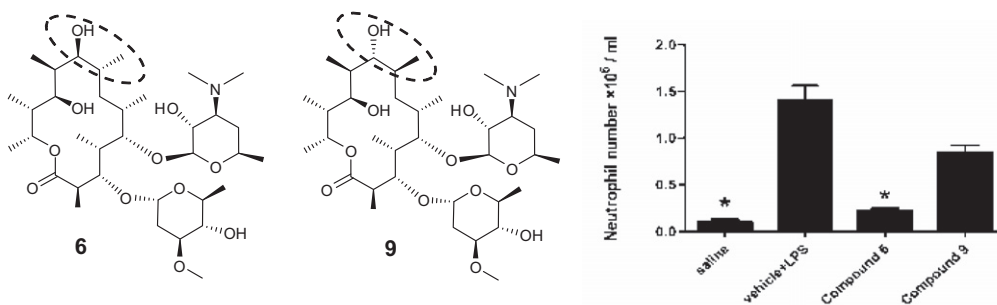
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Fabrizio Carta, Alfonso Maresca, Andrea Scozzafava, Claudiu T. Supuran*



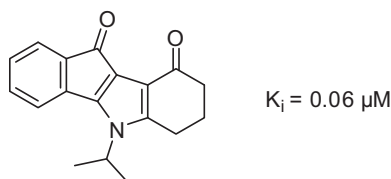
Impact of stereochemistry on the biological activity of novel oleandomycin derivatives pp 2274–2281

Jurica Bauer, Mark Vine, Ilija Čorić, Martina Bosnar, Ivanka Pašalić, Gordana Turkalj, Gorjana Lazarevski, Ognjen Čulić, Goran Kragol*



Indeno[1,2-*b*]indole derivatives as a novel class of potent human protein kinase CK2 inhibitors pp 2282–2289

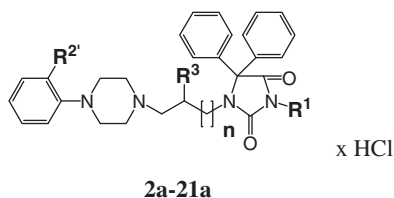
Claas Hundsdörfer, Hans-Jörg Hemmerling, Claudia Götz, Frank Totzke, Patrick Bednarski, Marc Le Borgne, Joachim Jose*



Antiarrhythmic properties of phenylpiperazine derivatives of phenytoin with α_1 -adrenoceptor affinities

pp 2290–2303

Jadwiga Handzlik, Marek Bajda, Małgorzata Zygmunt, Dorota Maciąg, Małgorzata Dybała, Marek Bednarski, Barbara Filipek, Barbara Malawska, Katarzyna Kieć-Kononowicz*

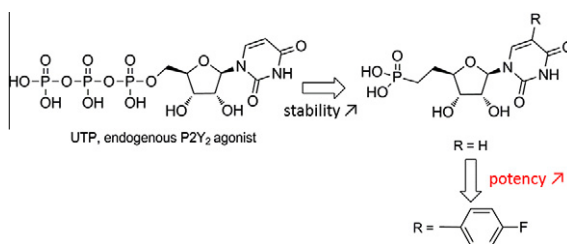


Association between α_1 -adrenoceptor affinities, hERG K⁺-antagonistic properties and antiarrhythmic activities for a series of phenylpiperazine derivatives of phenytoin (**2a–21a**) was investigated. Traditional- or microwave-aided syntheses were carried out.

**Synthesis and P2Y₂ receptor agonist activities of uridine 5'-phosphonate analogues**

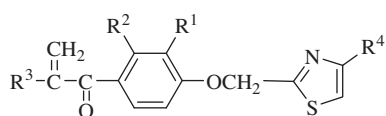
pp 2304–2315

Sara Van Poecke, Matthew O. Barrett, T. Santhosh Kumar, Davy Sinnaeve, José C. Martins, Kenneth A. Jacobson, T. Kendall Harden, Serge Van Calenbergh*

**The synthesis of ethacrynic acid thiazole derivatives as glutathione S-transferase pi inhibitors**

pp 2316–2322

Ting Li, Guyue Liu, Hongcai Li, Xinmei Yang, Yongkui Jing, Guisen Zhao*



R¹=H, Cl or CH₃; R²=Cl or CH₃;

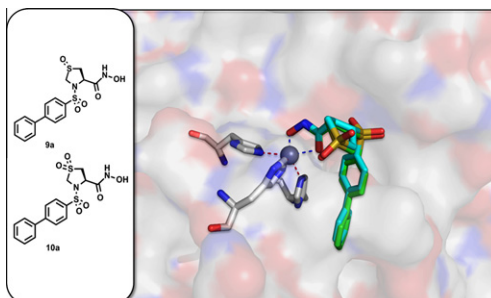
R³= CH₃ or C₂H₅;

R⁴=phenyl, 4-NO₂ phenyl, 2-naphthyl or 4-CF₃ phenyl

**In silico scaffold evaluation and solid phase approach to identify new gelatinase inhibitors**

pp 2323–2337

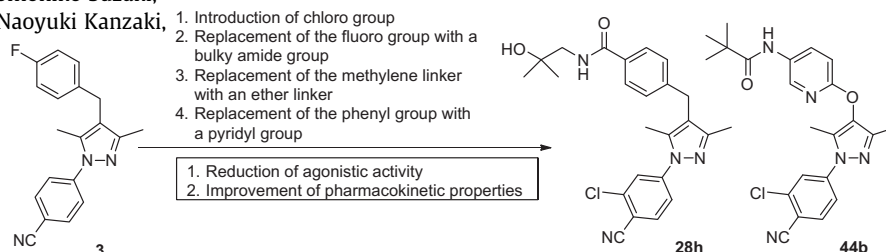
Alessandra Topai*, Perla Breccia, Franco Minissi, Alessandro Padova, Stefano Marini, Ilaria Cerbara



Design, synthesis, and biological evaluation of 4-arylmethyl-1-phenylpyrazole and 4-aryloxy-1-phenylpyrazole derivatives as novel androgen receptor antagonists

pp 2338–2352

Satoshi Yamamoto*, Naoki Tomita, Yuri Suzuki, Tomohiko Suzuki, Tomohiro Kaku, Takahito Hara, Masuo Yamaoka, Naoyuki Kanzaki, Atsushi Hasuoka, Atsuo Baba, Mitsuhiro Ito

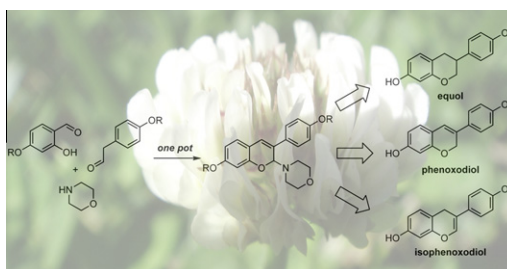


A series of 4-arylmethyl-1-phenylpyrazole and 4-aryloxy-1-phenylpyrazole compounds were designed, synthesized, and evaluated for their potential as novel orally available androgen receptor antagonists therapeutically effective against castration-resistant prostate cancers.

2-Morpholinoisoflav-3-enes as flexible intermediates in the synthesis of phenoxodiol, isophenoxodiol, equol and analogues: Vasorelaxant properties, estrogen receptor binding and Rho/RhoA kinase pathway inhibition

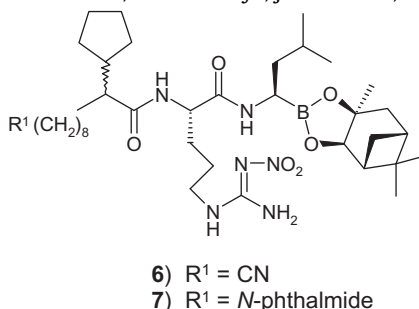
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Andrew J. Tilley, Shannon D. Zanatta, Cheng Xue Qin, In-Kyeom Kim, Young-Mi Seok, Alastair Stewart, Owen L. Woodman, Spencer J. Williams*

**Proteasome inhibitors for cancer therapy**

pp 2362–2368

Mohamed Iqbal, Patricia A. Messina McLaughlin, Derek Dunn, Satish Mallya, Jean Husten, Mark A. Ator, Sankar Chatterjee*

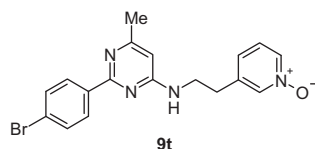


Potent, selective and cell-permeable proteasome inhibitors **6** and **7** displayed activity against various rodent and human tumor cell lines (in vitro).

Synthesis and structure–activity relationship of 4-amino-2-phenylpyrimidine derivatives as a series of novel GPR119 agonists

pp 2369–2375

Kenji Negoro*, Yasuhiro Yonetoku, Tatsuya Maruyama, Shigeru Yoshida, Makoto Takeuchi, Mitsuaki Ohta

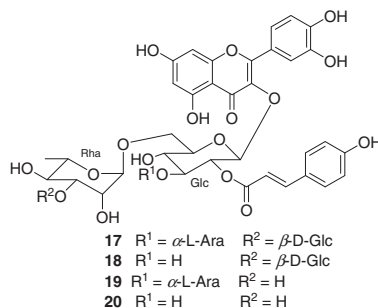


A series of novel 4-amino-2-phenylpyrimidine derivatives were synthesized and evaluated as GPR119 agonists. 2-(4-Bromophenyl)-6-methyl-N-[2-(1-oxido-3-pyridyl)ethyl]pyrimidin-4-amine (**9t**) had potent GPR119 agonistic activity, good potency in vivo, and a good PK profile.

Tea catechins and flavonoids from the leaves of *Camellia sinensis* inhibit yeast alcohol dehydrogenase

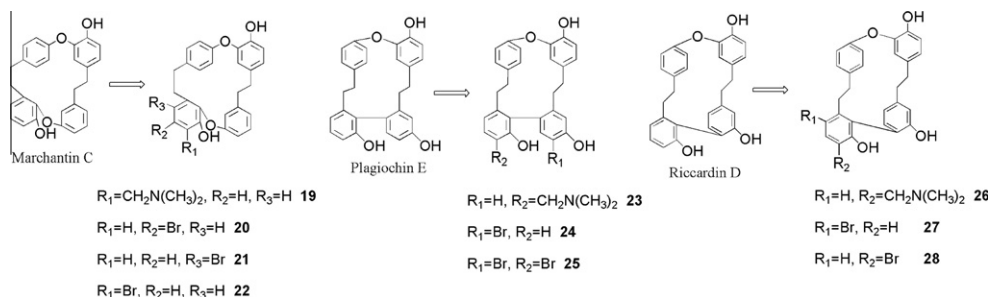
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Md. Maniruzzaman Manir, Jeong Kee Kim, Byeong-Gon Lee, Surk-Sik Moon*

**Synthesis of macrocyclic bisbibenzyl derivatives and their anticancer effects as anti-tubulin agents**

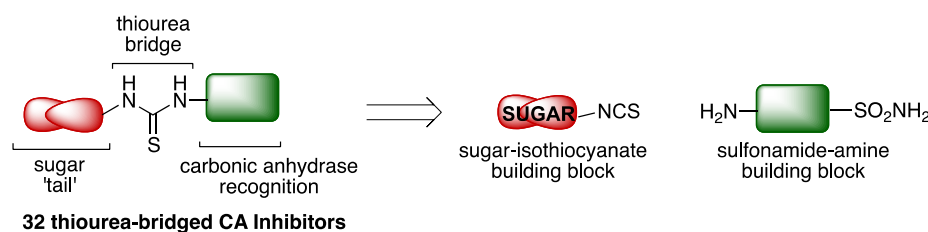
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Juan Jiang, Bin Sun, Yan-yan Wang, Min Cui, Li Zhang, Chang-zhi Cui, Yan-feng Wang, Xi-gong Liu, Hong-xiang Lou*

**Design and synthesis of thiourea compounds that inhibit transmembrane anchored carbonic anhydrases**

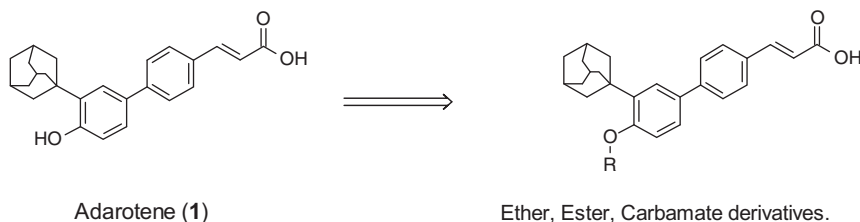
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Janina Moeker, Kanae Teruya, Sabine Rossit, Brendan L. Wilkinson, Marie Lopez, Laurent F. Bornaghi, Alessio Innocenti, Claudiu T. Supuran*, Sally-Ann Poulsen*

**New retinoid derivatives as back-ups of Adarotene**

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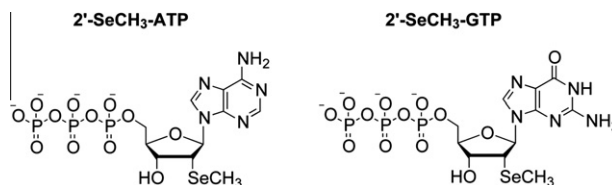
Giuseppe Giannini*, Tiziana Brunetti, Gianfranco Battistuzzi, Domenico Alloatti, Gianandrea Quattrociochi, Maria Grazia Cima, Lucio Merlini, Sabrina Dallavalle, Raffaella Cincinelli, Raffaella Nannei, Loredana Vesci, Federica Bucci, Rosanna Foderà, Mario Berardino Guglielmi, Claudio Pisano, Walter Cabri



The synthesis of 2'-methylseleno adenosine and guanosine 5'-triphosphates

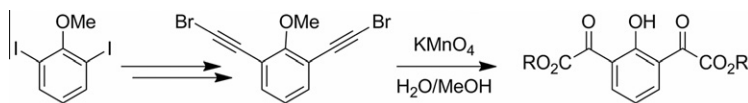
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Tobias Santner, Vanessa Siegmund, Andreas Marx, Ronald Micura*

**1,3-Phenylene bis(ketoacid) derivatives as inhibitors of *Escherichia coli* dihydrodipicolinate synthase**

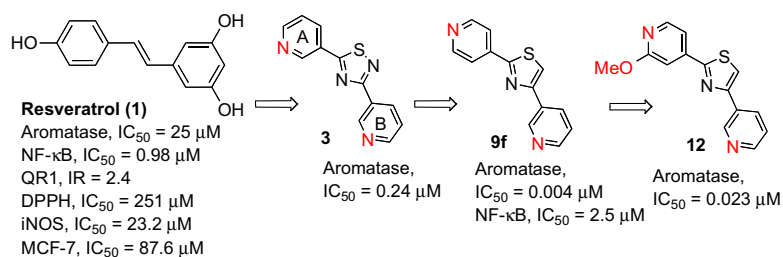
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Berin A. Boughton, Lilian Hor, Juliet A. Gerrard, Craig A. Hutton*

**Optimization of the aromatase inhibitory activities of pyridylthiazole analogues of resveratrol**

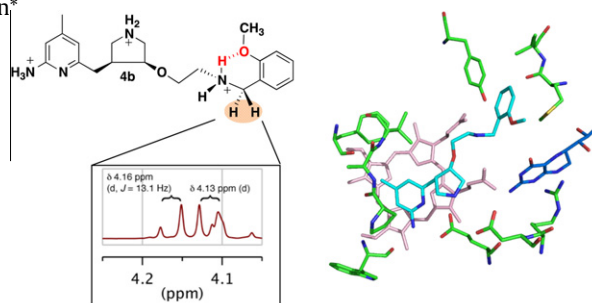
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Abdelrahman S. Mayhoub, Laura Marler, Tamara P. Kondratyuk, Eun-Jung Park, John M. Pezzuto, Mark Cushman*

**Intramolecular hydrogen bonding: A potential strategy for more bioavailable inhibitors of neuronal nitric oxide synthase**

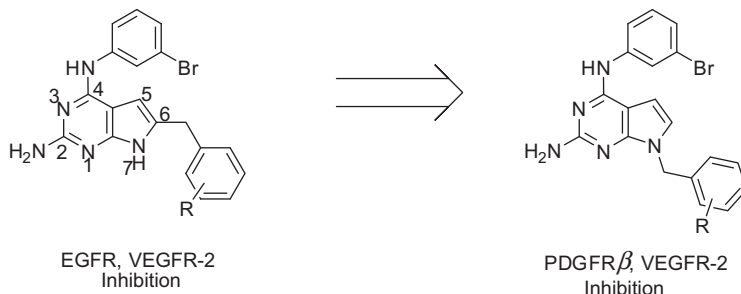
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Kristin Jansen Labby, Fengtian Xue, James M. Kraus, Haitao Ji, Jan Mataka, Huiying Li, Pavel Martásek, Linda J. Roman, Thomas L. Poulos*, Richard B. Silverman*



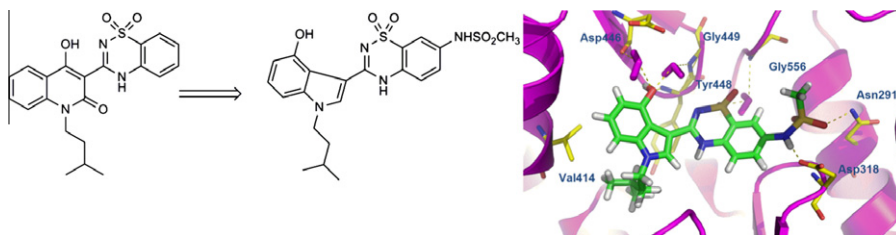
***N*⁴-(3-Bromophenyl)-7-(substituted benzyl) pyrrolo[2,3-*d*]pyrimidines as potent multiple receptor tyrosine kinase inhibitors: Design, synthesis, and in vivo evaluation** pp 2444–2454

Aleem Gangjee*, Nilesh Zaware, Sudhir Raghavan, Jie Yang, Jessica E. Thorpe, Michael A. Ihnat



Integrated structure-based activity prediction model of benzothiadiazines on various genotypes of HCV NS5b polymerase (1a, 1b and 4) and its application in the discovery of new derivatives pp 2455–2478

Mohamed A. H. Ismail*, Dalal A. Abou El Ella, Khaled A. M. Abouzid, Amr H. Mahmoud



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*Corresponding author

Supplementary data available via SciVerse ScienceDirect

COVER

The cover image shows a 2'-methylseleno guanosine 5'-triphosphate, the synthesis of which is described by Santner et al. in this issue. Modified NTPs of this type are potential substrates for engineered RNA polymerases to generate long RNA transcripts for X-ray crystallographic applications. (Background RNA polymerase structure: PDB 2E21) [Santner, T.; Siegmund, V.; Marx, A.; Micura, R. *Bioorg. Med. Chem. Lett.*, **2012**, 20, 2416.]

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