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Akira Hiratake  
  
**12c**



**X:**

$\text{O}-\overset{\text{P}}{\underset{\text{OH}}{\parallel}}-\text{CH}_2-$ 
 $\text{O}-\overset{\text{P}}{\underset{\text{OH}}{\parallel}}-\text{CH}_2-\text{CH}_2-$ 
 $\text{O}-\overset{\text{P}}{\underset{\text{OH}}{\parallel}}-\text{CF}_2-$

$\text{NH}-\overset{\text{O}}{\parallel}=\text{CH}_2-$ 
 $-S-\text{CH}_2-\text{CH}_2-$

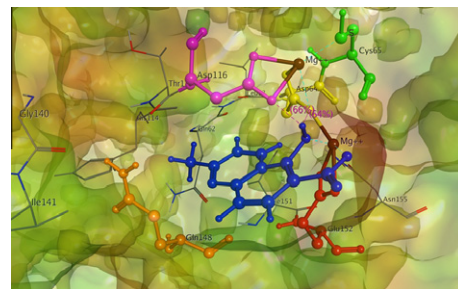
R: H, Et



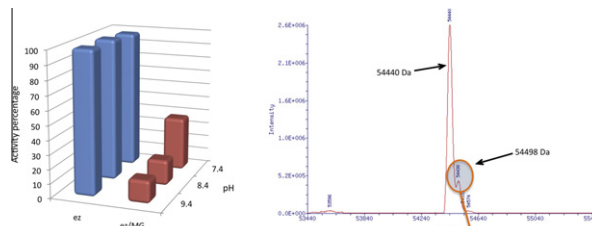
**X-ray and molecular modelling in fragment-based design of three small quinoline scaffolds for HIV integrase inhibitors** pp 1606–1612

Katarzyna Majerz-Maniecka\*, Robert Musiol\*, Agnieszka Skórska-Stania, Dominik Tabak, Pawel Mazur, Barbara J. Oleksyn, Jaroslaw Polanski

Three small molecular scaffolds based on quinoline were characterised in terms of crystal structure and molecular docking into active site of HIV integrase. Selected ligand–protein interactions have been found specific for active compounds.

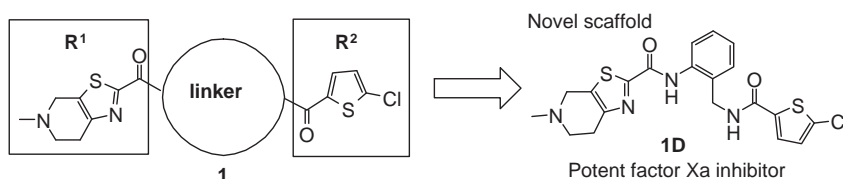
**Enhanced reactivity of Lys182 explains the limited efficacy of biogenic amines in preventing the inactivation of glucose-6-phosphate dehydrogenase by methylglyoxal** pp 1613–1622

Patricio Flores-Morales, Claudio Diema, Marta Vilaseca, Joan Estelrich, F. Javier Luque, Soledad Gutiérrez-Oliva, Alejandro Toro-Labbé, Eduardo Silva\*

**2-Aminomethylphenylamine as a novel scaffold for factor Xa inhibitor**

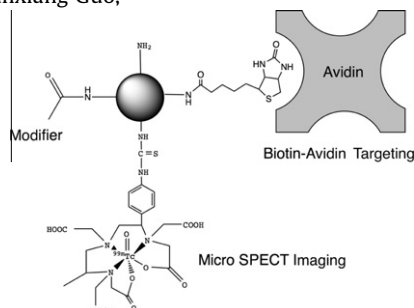
pp 1623–1642

Akiyoshi Mochizuki\*, Tsutomu Nagata, Hideyuki Kanno, Makoto Suzuki, Toshiharu Ohta

**Radiosynthesis, biodistribution and micro-SPECT imaging study of dendrimer–avidin conjugate**

pp 1643–1648

Xiaoping Xu, Yuanqing Zhang, Xudong Wang, Xunxiang Guo, Xuezhong Zhang, Yujin Qi, Yu-Mei Shen\*

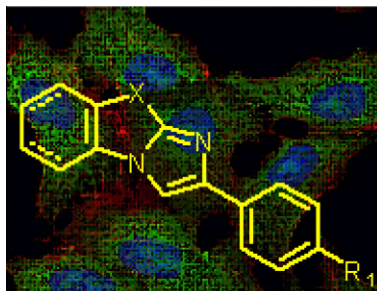


The radiolabeled dendrimer PAMAM–avidin conjugate was successfully prepared and evaluated as potential SPECT imaging agent.

**Synthesis and biological evaluation of imidazolo[2,1-*b*]benzothiazole derivatives, as potential p53 inhibitors**

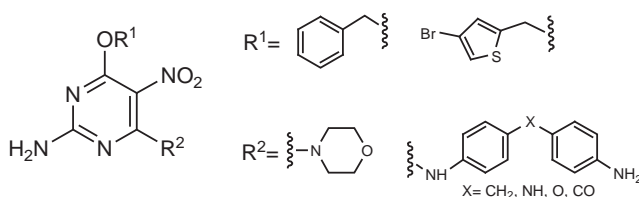
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Michael S. Christodoulou, Francesco Colombo, Daniele Passarella\*, Gabriella Ieronimo, Valentina Zuco, Michelandrea De Cesare, Franco Zunino\*

**Towards more specific O<sup>6</sup>-methylguanine-DNA methyltransferase (MGMT) inactivators**

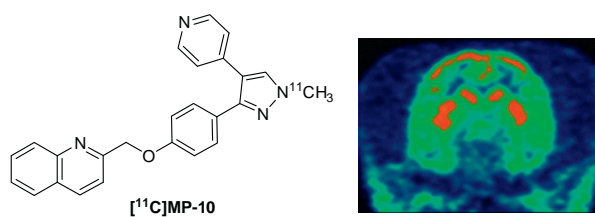
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Sergio Lopez, Geoffrey P. Margison, R. Stanley McElhinney, Alessandra Cordeiro, T. Brian H. McMurry, Isabel Rozas\*

**Radiosynthesis and in vivo evaluation of [<sup>11</sup>C]MP-10 as a PET probe for imaging PDE10A in rodent and non-human primate brain**

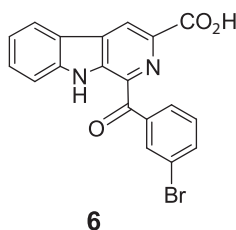
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Structure and microPET image of [<sup>11</sup>C]MP-10**Synthesis, in vitro anti-inflammatory and cytotoxic evaluation, and mechanism of action studies of 1-benzoyl- $\beta$ -carboline and 1-benzoyl-3-carboxy- $\beta$ -carboline derivatives**

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Mei-Lin Yang, Ping-Chung Kuo, Tsong-Long Hwang, Wen-Fei Chiou, Keduo Qian, Chin-Yu Lai, Kuo-Hsiung Lee\*, Tian-Shung Wu\*

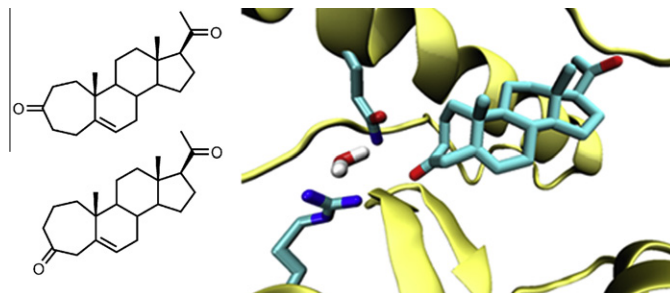


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**Biological activity and ligand binding mode to the progesterone receptor of A-homo analogues of progesterone**

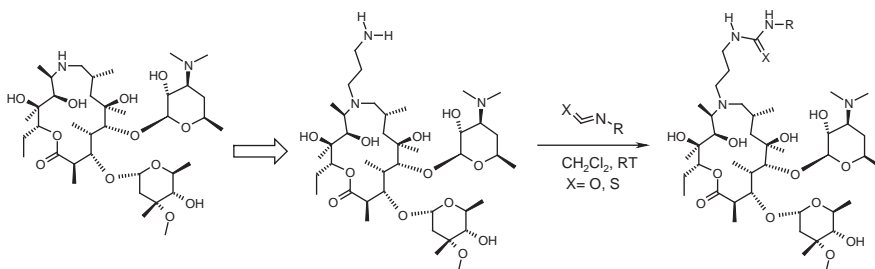
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Lautaro D. Alvarez, María V. Dansey, Marcelo A. Martí, Paola Y. Bertucci, Pablo H. Di Chenna, Adalí Pecci, Gerardo Burton\*

**An automated, polymer-assisted strategy for the preparation of urea and thiourea derivatives of 15-membered azalides as potential antimalarial chemotherapeutics**

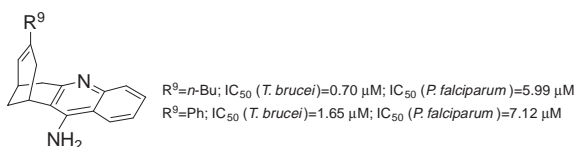
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Antun Hutinec\*, Renata Rupčić, Dinko Žiher, Kirsten S. Smith, Wilbur Milhous, William Ellis, Colin Ohrt, Zrinka Ivezić Schönfeld

**Huprines as a new family of dual acting trypanocidal–antiplasmodial agents**

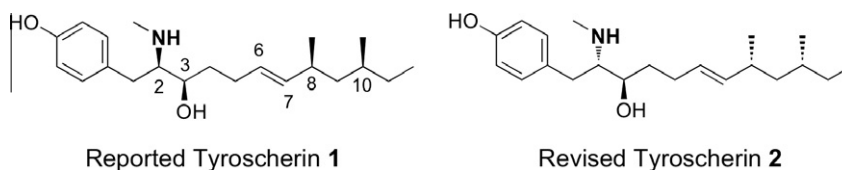
pp 1702–1707

Julien Defaux, Marta Sala, Xavier Formosa, Carles Galdeano, Martin C. Taylor, Waleed A. A. Alobaid, John M. Kelly, Colin W. Wright, Pelayo Camps, Diego Muñoz-Torrero\*

**Unexpected stereochemical tolerance for the biological activity of tyroscherin**

pp 1708–1713

Hyun Seop Tae, John Hines, Ashley R. Schneekloth, Craig M. Crews\*



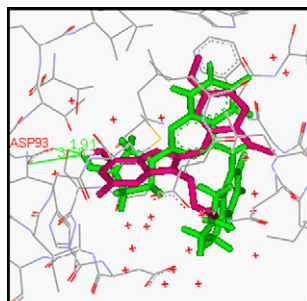
Our concise, unified syntheses of the 15 diastereomers and key analogs of tyroscherin afforded a comprehensive biological analysis of this natural product.



**Structure based design of heat shock protein 90 inhibitors acting as anticancer agents**

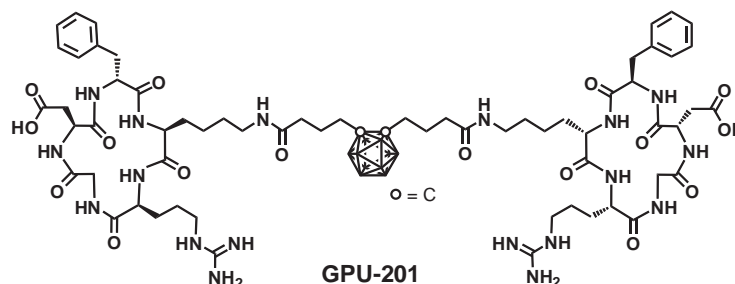
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Munikumar Reddy Doddareddy, Dhanaji Achyut Rao Thorat, Seon Hee Seo, Tae-Joon Hong, Yong Seo Cho, Ji-Sook Hahn, Ae Nim Pae\*

**Synthesis and evaluation of cyclic RGD-boron cluster conjugates to develop tumor-selective boron carriers for boron neutron capture therapy**

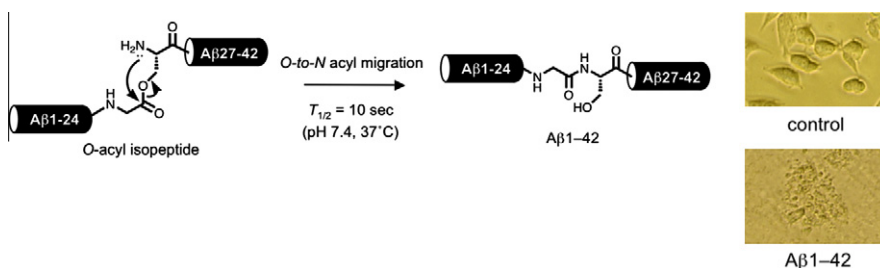
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Sadaaki Kimura, Shin-ichiro Masunaga, Tomohiro Harada, Yasuo Kawamura, Satoshi Ueda, Kensuke Okuda, Hideko Nagasawa\*

**'Click peptide' using production of monomer A $\beta$  from the O-acetyl isopeptide: Application to assay system of aggregation inhibitors and cellular cytotoxicity**

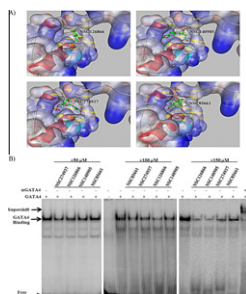
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Youhei Sohma\*, Yuta Hirayama, Atsuhiko Taniguchi, Hidehito Mukai, Yoshiaki Kiso\*

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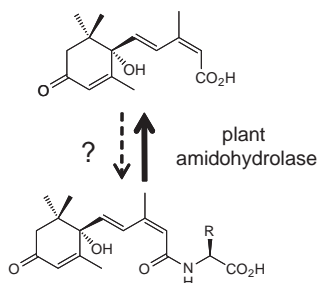
Nehmé El-Hachem, Georges Nemer\*



### Synthesis and biological activity of amino acid conjugates of abscisic acid

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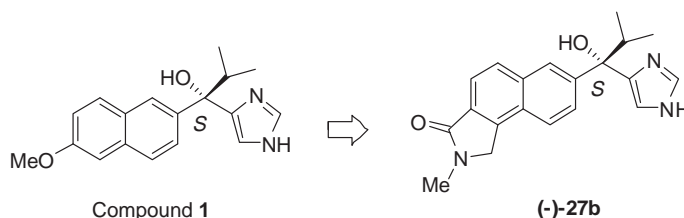
Yasushi Todoroki\*, Kenta Narita, Taku Muramatsu, Hajime Shimomura, Toshiyuki Ohnishi, Masaharu Mizutani, Kotomi Ueno, Nobuhiro Hirai



### 17,20-Lyase inhibitors. Part 4: Design, synthesis and structure–activity relationships of naphthylmethylimidazole derivatives as novel 17,20-lyase inhibitors

pp 1751–1770

Tomohiro Kaku\*, Nobuyuki Matsunaga, Akio Ojida, Toshimasa Tanaka, Takahito Hara, Masuo Yamaoka, Masami Kusaka, Akihiro Tasaka

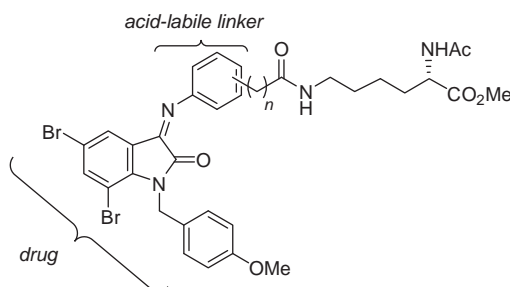


A novel series of naphthylmethylimidazole derivatives and related compounds have been investigated as selective 17,20-lyase inhibitors.

### Synthesis and hydrolytic evaluation of acid-labile imine-linked cytotoxic isatin model systems

pp 1771–1778

Lidia Matesic, Julie M. Locke, Kara L. Vine, Marie Ranson, John B. Bremner, Danielle Skropeta\*

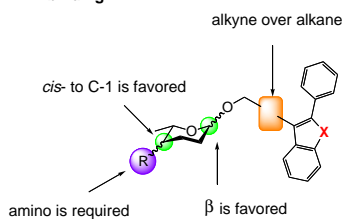


### Structure–activity relationships in glycosylated 2-phenyl-indoles, 2-phenyl-benzo[*b*]thiophenes and 2-phenyl-benzo[*b*]furans as DNA binding and potential antitumor agents

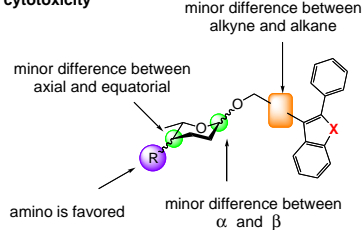
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Wei Shi, Todd L. Lowary\*

#### SAR on DNA binding



#### SAR on cytotoxicity



X = O, S, NTs

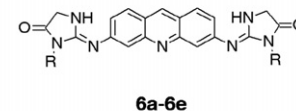
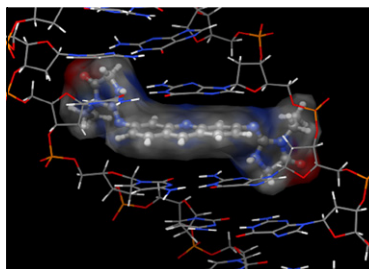


**Cytotoxic 3,6-bis((imidazolidinone)imino)acridines: Synthesis, DNA binding and molecular modeling**

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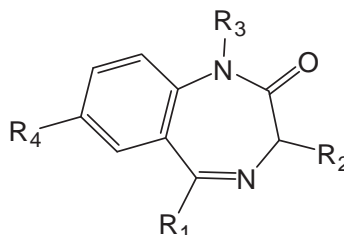
Ladislav Janovec, Mária Kožurková, Danica Sabolová, Ján Ungvarský, Helena Paulíková, Jana Plšíková, Zuzana Vantová, Ján Imrich\*

Synthesis, DNA binding and fragmentation, topoisomerase inhibition, antitumor activity, and modeling of novel 3,6-bis((1-alkyl-5-oxo-imidazolidin-2-ylidene)imino)acridine hydrochlorides **6a–6e** are reported.

**Synthesis and biological evaluation of 1,4-benzodiazepin-2-ones with antitrypanosomal activity**

pp 1802–1815

John Spencer\*, Rajendra P. Rathnam, Alan L. Harvey, Carol J. Clements, Rachel L. Clark, Michael P. Barrett, Pui Ee Wong, Louise Male, Simon J. Coles, Simon P. Mackay



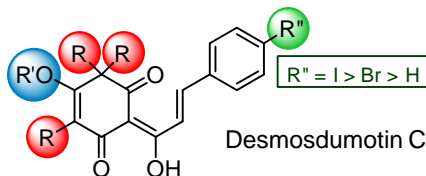
A library of 1,4-benzodiazepines has been synthesized and displays MIC values as low as 0.78  $\mu$ M against *Trypanosoma brucei*.

**Antitumor agents 283. Further elaboration of Desmosdumotin C analogs as potent antitumor agents: Activation of spindle assembly checkpoint as possible mode of action**

pp 1816–1822

Kyoko Nakagawa-Goto\*, Pei-Chi Wu, Kenneth F. Bastow, Shuenn-Chen Yang, Sung-Liang Yu, Hsuan-Yu Chen, Jau-Chen Lin, Masuo Goto, Susan L. Morris-Natschke, Pan-Chyr Yang, Kuo-Hsiung Lee\*

R = Pr > iBu, Bu > Et > Me > Prenyl > iPen



Desmosdumotin C Analogs

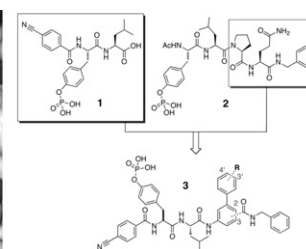
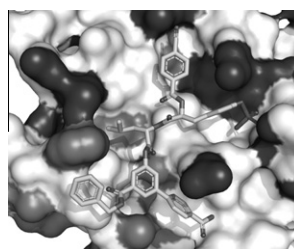
OR' = OPr > OMe > O-iBu > OBu > O-iPen

**Design, synthesis, and in vitro characterization of novel hybrid peptidomimetic inhibitors of STAT3 protein**


pp 1823–1838

Vijay M. Shahani, Peibin Yue, Steven Fletcher, Sumaiya Sharmeen, Mahadeo A. Sukhai, Diana P. Luu, Xiaolei Zhang, Hong Sun, Wei Zhao, Aaron D. Schimmer, James Turkson\*, Patrick T. Gunning\*

A novel family of hybrid peptidomimetic Stat3 inhibitors that bind to STAT3's SH2 domain with a high affinity, disrupt STAT3:phosphopeptide complexation events and inhibit STAT3–STAT3 protein dimerization in vitro and in whole cells containing aberrant STAT3 activity.



\*Corresponding author

 Supplementary data available via ScienceDirect

## COVER

Constructing potent inhibitors of Stat3 protein's SH2 domain: identification of a novel class of hybrid peptidomimetic inhibitor. [Shahani, V. M.; Yue, P.; Fletcher, S.; Sharmeen, S.; Sukhai, M. A.; Luu, D. P.; Zhang, X.; Sun, H.; Zhao, W.; Schimmer, A. D.; Turkson, J.; Gunning, P.T. *Bioorg. Med. Chem.*; **2011**, 19, 1823–1838.]

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