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# Bioorganic & Medicinal Chemistry Volume 22, Issue 1, 2014 Contents

#### **REVIEWS**

### Natural product based leads to fight against leishmaniasis

Nisha Singh, Bhuwan B. Mishra, Surabhi Bajpai, Rakesh K. Singh\*, Vinod K. Tiwari\*

pp 18-45



### Pyrrolizines: Promising scaffolds for anticancer drugs

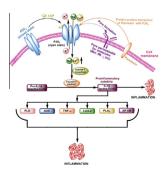
Amany Belal, Bahaa El-Dien M. El-Gendy\*

pp 46-53

#### Purinergic receptor P2X<sub>7</sub>: A novel target for anti-inflammatory therapy

Nisha Mehta, Maninder Kaur, Manjinder Singh, Sukhvir Chand, Bhawna Vyas, Pragati Silakari, Malkeet Singh Bahia, Om Silakari\*

pp 54–88



 $P2X_7$  a ligand gated ion channel plays an important role in IL-1 $\beta$  release and its antagonism play beneficial role in management of many inflammatory and autoimmune disease conditions like rheumatoid arthritis etc.

### ARTICLES

### Design, synthesis and molecular modeling of novel *N*-acylhydrazone derivatives as pyruvate dehydrogenase complex E1 inhibitors

pp 89-94

Jun-Bo He, Ling-Ling Feng, Jing Li, Rui-Juan Tao, Yan-Liang Ren, Jian Wan\*, Hong-Wu He\*

$$\begin{array}{c} NH_2 & CH_3 \\ N=N & N=N \end{array} \begin{array}{c} O \\ N=N$$

### A highly predictive 3D-QSAR model for binding to the voltage-gated sodium channel: Design of potent new ligands

pp 95-104

Predicted IC<sub>50</sub> (nM) Observed IC<sub>50</sub> (nM)

Congxiang Zha, George B. Brown, Wayne J. Brouillette\*

R= 251 129

R= 260 119

A comprehensive comparative molecular field analysis (CoMFA) model for ligand binding to the neuronal voltage-gated sodium channel was developed and used to design very potent (IC $_{50}$  near 100 nM) sodium channel ligands as demonstrated by the following examples.

#### Synthesis and anticancer evaluation of 3-substituted quinolin-4-ones and 2,3-dihydroquinolin-4-ones

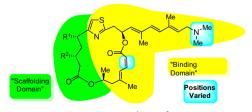
pp 105-115

Santosh Rajput, Christopher R. Gardner, Timothy W. Failes, Greg M. Arndt, David StC. Black, Naresh Kumar\*

MeO 
$$\stackrel{\text{OMe O}}{\underset{\text{H}}{\bigvee}}$$
  $\stackrel{\text{OMe O}}{\underset{\text{NH}_2}{\bigvee}}$   $\stackrel{\text{OMe O}}{\underset$ 

### Second-generation derivatives of the eukaryotic translation initiation inhibitor pateamine A targeting eIF4A as potential pp 116–125 anticancer agents

Woon-Kai Low\*, Jing Li, Mingzhao Zhu, Sai Shilpa Kommaraju, Janki Shah-Mittal, Ken Hull, Jun O. Liu, Daniel Romo\*



Pateamine A (PatA, R<sup>1</sup>=Me; R<sup>2</sup>=NH<sub>2</sub>) Des-methyl, des-amino PatA (R<sup>1</sup>, R<sup>2</sup>= H)



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