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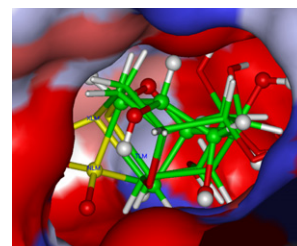
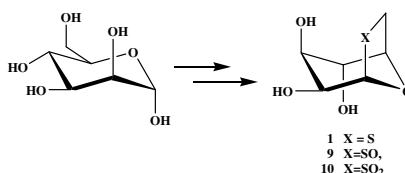
ARTICLES

Conformationally locked thiosugars as potent α -mannosidase inhibitors: Synthesis, biochemical and docking studies

pp 5659–5665

K. Sivapriya, S. Hariharaputran, V. L. Suhas,
N. Chandra and S. Chandrasekaran*

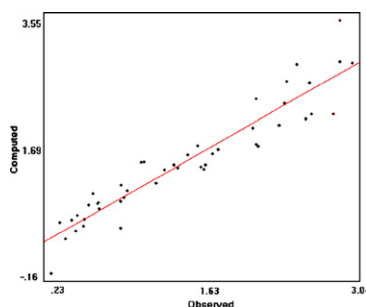
We report here, the synthesis of a series of novel thiosugar derivatives derived from D-mannose and studies of their inhibition against α -mannosidase (jack bean). The sulfone derivative **10** proved to be the best inhibitor with a K_i value of 350 nM.



QSAR studies for the inhibition of the transmembrane isozymes XII and XIV of human carbonic anhydrase with a series of sulfonamides

pp 5666–5671

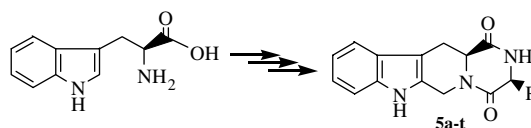
Laszlo Tarko and Claudiu T. Supuran*



A new class of anti-thrombosis hexahydropyrazino-[1',2':1,6]pyrido-[3,4-b]-indole-1,4-dions: Design, synthesis, log K determination, and QSAR analysis

pp 5672–5693

Jiawang Liu, Guofeng Wu, Guohui Cui, Wei-Xuan Wang, Ming Zhao,*
Chao Wang, Ziding Zhang* and Shiqi Peng*



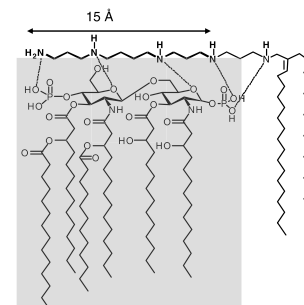
In **5a**, $R_1 = \text{CH}_3$; **5b**, $R = \text{CH}_2\text{C}_6\text{H}_5$; **5c**, $R = \text{CH}(\text{CH}_3)_2$; **5d**, $R = \text{CH}_2\text{OH}$; **5e**, $R = \text{CH}(\text{OH})\text{CH}_3$; **5f**, $R = \text{CH}_2\text{C}_6\text{H}_4\text{-OH-}p$; **5g**, $R = \text{tetrahydropyrrol-2-yl}$; **5h**, $R = \text{CH}_2\text{SH}$; **5i**, $R = \text{CH}_2\text{CH}_2\text{SCH}_3$; **5j**, $R = \text{CH}_2\text{CH}_2\text{CO}_2\text{H}$; **5k**, $R = \text{CH}_2\text{CO}_2\text{H}$; **5l**, $R = 1,3\text{-imidazol-5-methylene}$; **5m**, $R = \text{indol-3-yl-methylene}$; **5n**, $R = \text{CH}_2(\text{CH}_2)_2\text{NHC}(\text{NH}_2)\text{NH}$; **5o**, $R = \text{H}$; **5p**, $R = \text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{NH}_2$; **5q**, $R = \text{CH}_2\text{CH}_2\text{CONH}_2$; **5r**, $R = \text{CH}_2\text{CONH}_2$; **5s**, $R = \text{CH}_2\text{CH}(\text{CH}_3)_2$; **5t**, $R = \text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_3$.

Protection from endotoxic shock by EVK-203, a novel alkylpolyamine sequestrant of lipopolysaccharide

pp 5694–5709

Thuan B. Nguyen, Ashok Kumar Adisechan, E. V. K. Suresh Kumar, Rajalakshmi Balakrishna, Matthew R. Kimbrell, Kelly A. Miller, Apurba Datta and Sunil A. David*

EVK-203, a novel alkylpolyamine, binds to the toxic lipid A moiety of bacterial lipopolysaccharide and reduces lethality in a dose-dependent manner in a murine model of lipopolysaccharide-induced shock. The potency and lack of apparent toxicity in the animal model renders EVK-203 an attractive lead in the development of anti-lipopolysaccharide agents for the management of Gram-negative sepsis.

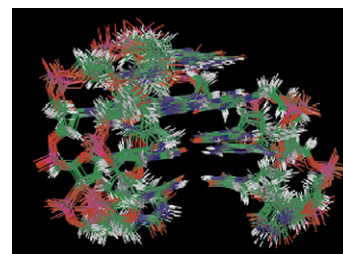


A novel thrombin binding aptamer containing a G-LNA residue

pp 5710–5718

Ada Virno, Antonio Randazzo, Concetta Giancola, Mariarosaria Bucci, Giuseppe Cirino and Luciano Mayol*

In this work, we report the solution structure, the thermodynamic study, and the pharmacological activity of a new modified thrombin binding aptamer (TBA) containing a G-LNA residue.

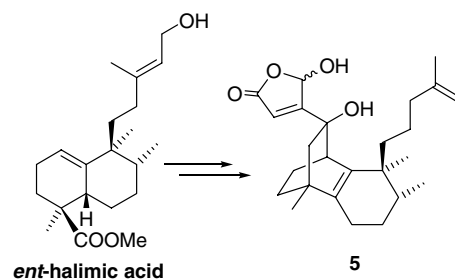


Synthesis of novel antitumoural analogues of dysidiolide from *ent*-halimic acid

pp 5719–5737

I. S. Marcos,* M. A. Escola, R. F. Moro, P. Basabe, D. Diez, F. Sanz, F. Mollinedo, J. de la Iglesia-Vicente, B. G. Sierra and J. G. Urones

Several antitumoural analogues of Dysidiolide have been synthesised starting from *ent*-halimic acid.

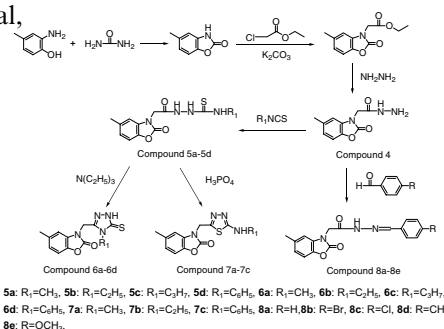


1-Acylthiosemicarbazides, 1,2,4-triazole-5(4*H*)-thiones, 1,3,4-thiadiazoles and hydrazones containing 5-methyl-2-benzoxazolinones: Synthesis, analgesic-anti-inflammatory and antimicrobial activities

pp 5738–5751

Umut Salgın-Gökşen, Nesrin Gökhan-Kelekçi,* Özgür Gökteş, Yavuz Köysal, Ekrem Kılıç, Şamil Işık, Göknuş Aktay and Meral Özalp

A novel series of 1-acylthiosemicarbazides, 1,2,4-triazole-5-thiones, 1,3,4-thiadiazoles and hydrazones containing 5-methyl-2-benzoxazolinones was synthesized and investigated for their antiinflammatory and analgesic activity as well as antimicrobial activity.

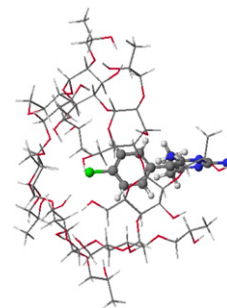


Inclusion complexes of pyrimethamine in 2-hydroxypropyl- β -cyclodextrin: Characterization, phase solubility and molecular modelling

pp 5752–5759

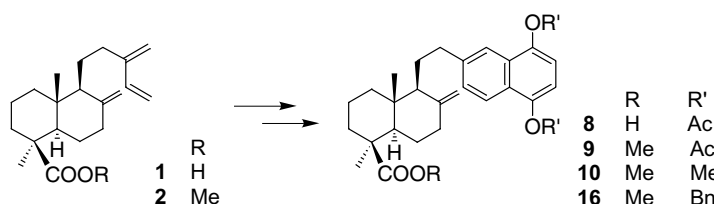
Márcia Valéria Gaspar de Araújo, Elze Kelly Barbosa Vieira, Gilderman Silva Lázaro, Leila de Souza Conegero, Odair Pastor Ferreira, Luís Eduardo Almeida, Ledjane Silva Barreto, Nivan Bezerra da Costa Jr. and Iara F. Gimenez*

A 1:1 inclusion complex of pyrimethamine with hydroxypropyl β -cyclodextrin was prepared, characterized and modelled by AM1 method. Phase solubility and stoichiometry of the system was carried out by standard methods.

**New cytotoxic diterpenynaphthohydroquinone derivatives obtained from a natural diterpenoid**

pp 5760–5774

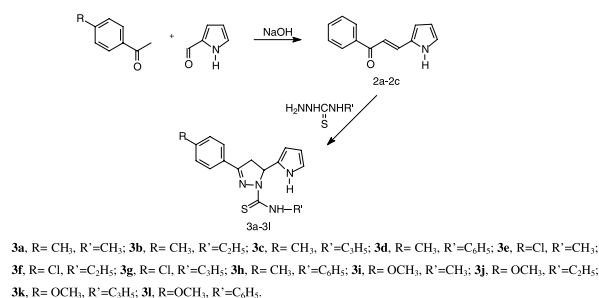
José M. Miguel del Corral,* M. Angeles Castro, M. Lucena Rodríguez, Pablo Chamorro, Carmen Cuevas and Arturo San Feliciano

**A new therapeutic approach in Alzheimer disease: Some novel pyrazole derivatives as dual MAO-B inhibitors and antiinflammatory analgesics**

pp 5775–5786

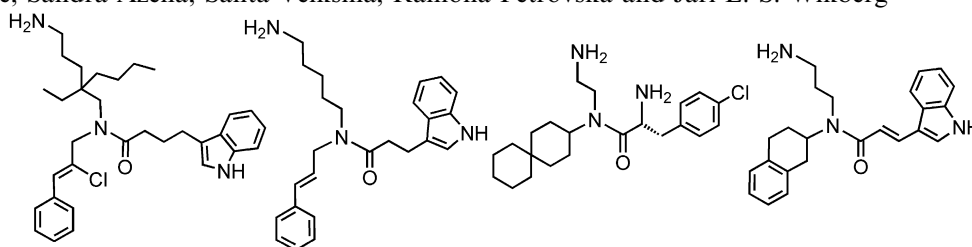
Nesrin Gökhan-Kelekçi,* Samiye Yabanoğlu, Esra Küpeli, Umut Salgın, Özen Özgen, Gülberk Uçar, Erdem Yeşilada, Engin Kendi, Akgül Yeşilada and A. Altan Bilgin

A novel series of pyrazole derivatives was synthesized and investigated for the inhibition of MAO-A and MAO-B. The compounds were also evaluated for their antiinflammatory and analgesic activity as well as ulcerogenic risk.

**Design and synthesis of a library of tertiary amides: Evaluation as mimetics of the melanocortins' active core**

pp 5787–5810

Felikss Mutulis, Jana Kreicberga, Sviatlana Yahorava, Ilze Mutule, Larisa Borisova-Jan, Aleh Yahorau, Ruta Muceniece, Sandra Azena, Santa Veiksina, Ramona Petrovska and Jarl E. S. Wikberg*



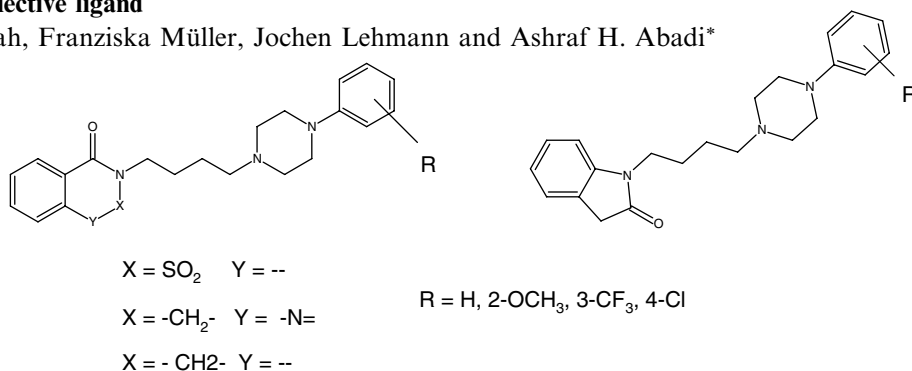
Two hundred and ten substances have been synthesized and tested, reaching submicromolar affinity.



Synthesis of novel lactam derivatives and their evaluation as ligands for the dopamine receptors, leading to a D₄-selective ligand

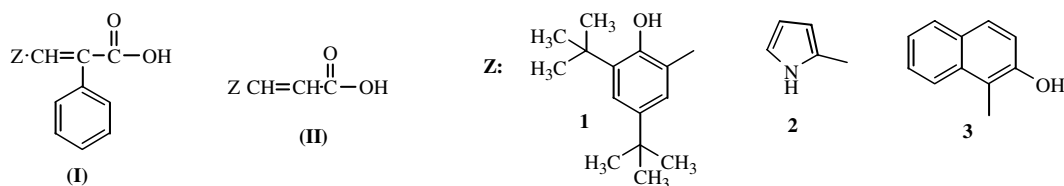
pp 5811–5818

Fadi M. Awadallah, Franziska Müller, Jochen Lehmann and Ashraf H. Abadi*


Synthesis and pharmacochemochemical evaluation of novel aryl-acetic acid inhibitors of lipoxygenase, antioxidants, and anti-inflammatory agents

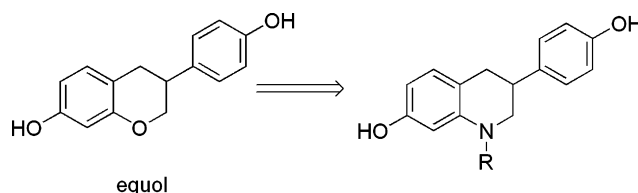
pp 5819–5827

E. Pontiki and D. Hadjipavlou-Litina*

Synthesis, anti-inflammatory, lipoxygenase inhibition, and antioxidant activities of compounds of the type **I** and **II** are reported.
Aza analogues of equol: Novel ligands for estrogen receptor β

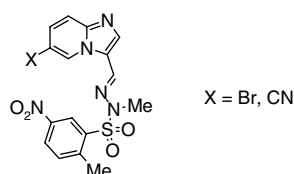
pp 5828–5836

Wuhong Chen, Zhaohu Lin, Mengmeng Ning, Chunhao Yang,* Xueming Yan, Yuyuan Xie, Xu Shen and Ming-Wei Wang*


Synthesis and biological evaluation of sulfonylhydrazone-substituted imidazo[1,2-a]pyridines as novel PI3 kinase p110 α inhibitors

pp 5837–5844

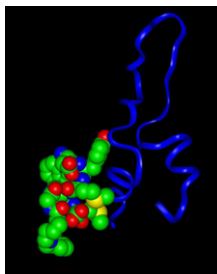
Masahiko Hayakawa,* Ken-ichi Kawaguchi, Hiroyuki Kaizawa, Tomonobu Koizumi, Takahide Ohishi, Mayumi Yamano, Minoru Okada, Mitsuaki Ohta, Shin-ichi Tsukamoto, Florence I. Raynaud, Peter Parker, Paul Workman and Michael D. Waterfield



Synthesis and biological evaluation of cyclic and branched peptide analogues as ligands for cholecystokinin type 1 receptor

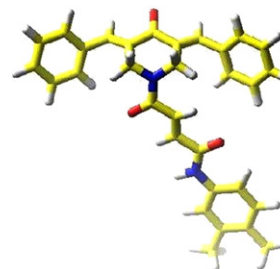
pp 5845–5853

Stefania De Luca, Antonia De Capua, Michele Saviano, Raffaella Della Moglie,
Luigi Aloj, Laura Tarallo, Carlo Pedone and Giancarlo Morelli*

***E,E,E*-1-(4-Arylamino-4-oxo-2-butenoyl)-3,5-bis(arylidene)-4-piperidones: A topographical study of some novel potent cytotoxins**

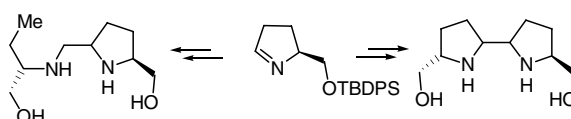
pp 5854–5865

Amitabh Jha,* Chandrani Mukherjee, Ashok K. Prasad, Virinder S. Parmar,
Erik De Clercq, Jan Balzarini, James P. Stables, Elias K. Manavathu,
Anuraag Shrivastav, Rajendra K. Sharma, Kurt H. Nienaber,
Gordon A. Zello and Jonathan R. Dimmock

**Synthesis and biological evaluation of conformationally constrained analogues of the antitubercular agent ethambutol**

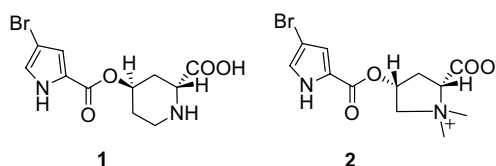
pp 5866–5876

Vanessa Faugeron, Yves Génisson,* Yahya Salma, Patricia Constant and Michel Baltas

**Damipepolin and damituricin, novel bioactive bromopyrrole alkaloids from the Mediterranean sponge *Axinella damicornis***

pp 5877–5887

Anna Aiello, Ernesto Fattorusso,* Antonella Giordano, Marialuisa Menna,
Werner E. G. Müller, Sanja Perović-Ottstadt and Heinz C. Schröder



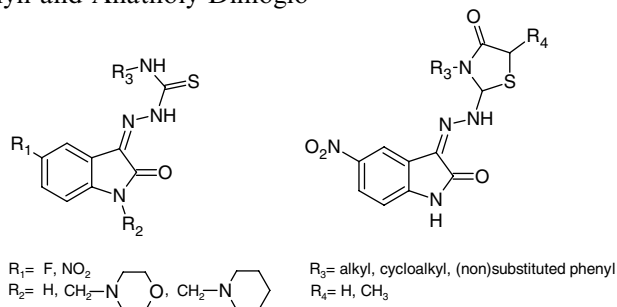
Damipepolin (**1**) and damituricin (**2**) were isolated from the Mediterranean sponge *Axinella damicornis*. These compounds were found to display a modulating effect of the serotonin receptor activity in vitro.



Synthesis and structure–antituberculosis activity relationship of 1*H*-indole-2,3-dione derivatives

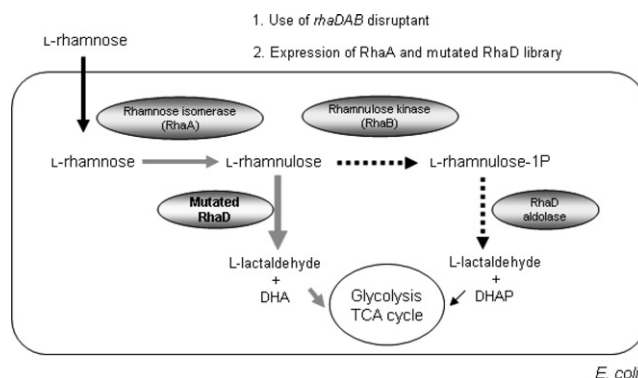
pp 5888–5904

Nilgün Karalı,* Aysel Gürsoy, Fatma Kandemirli, Nathaly Shvets, F. Betül Kaynak, Süheyla Özbey, Vasyi Kovalishyn and Anatholy Dimoglo

**In vivo selection for the directed evolution of L-rhamnulose aldolase from L-rhamnulose-1-phosphate aldolase (RhaD)**

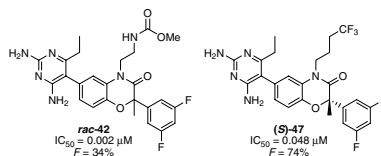
pp 5905–5911

Masakazu Sugiyama, Zhangyong Hong, William A. Greenberg and Chi-Huey Wong*

**Rational design of 6-(2,4-diaminopyrimidinyl)-1,4-benzoxazin-3-ones as small molecule renin inhibitors**

pp 5912–5949

Noel A. Powell,* Fred L. Ciske, Cuiman Cai, Daniel D. Holsworth, Ken Mennen, Chad A. Van Huis, Mehran Jalaie, Jacqueline Day, Michelle Mastronardi, Pat McConnell, Igor Mochalkin, Erli Zhang, Michael J. Ryan, John Bryant, Wendy Collard, Suzie Ferreira, Chungang Gu, Roxane Collins and Jeremy J. Edmunds

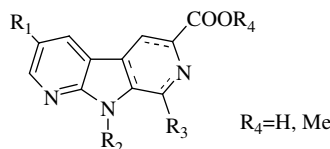


We report the design and synthesis of a series of 6-(2,4-diaminopyrimidinyl)-1,4-benzoxazin-3-ones that are orally bioavailable small molecule inhibitors of renin.

**Synthesis of 3,8,9-trisubstituted-1,7,9-triaza-fluorene-6-carboxylic acid derivatives as a new class of insulin secretagogues**

pp 5950–5964

Rajesh H. Bahekar,* Mukul R. Jain, Pradip A. Jadav, Ashish Goel, Dipam N. Patel, Vijay M. Prajapati, Arun A. Gupta, Honey Modi and Pankaj R. Patel

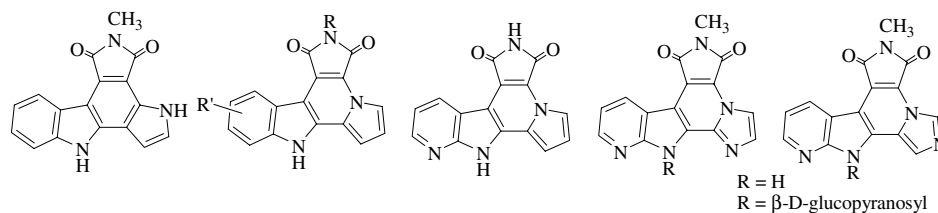


New class of substituted-triaza-fluorene-6-carboxylic acid derivatives were prepared as β -carboline analogs and screened in vitro for glucose-dependent insulinotropic activity.

Synthesis and biological activities of isogranulatimide analogues

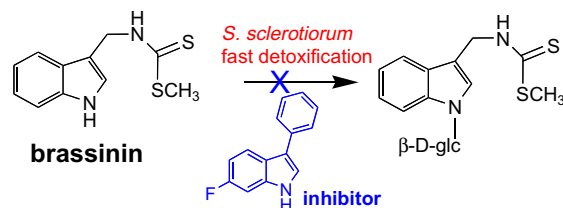
pp 5965–5980

Bernadette Hugon, Fabrice Anizon, Christian Bailly, Roy M. Golsteyn, Alain Pierré, Stéphane Léonce, John Hickman, Bruno Pfeiffer and Michelle Prudhomme*

**Design, synthesis, and evaluation of potential inhibitors of brassinin glucosyltransferase, a phytoalexin detoxifying enzyme from *Sclerotinia sclerotiorum***

pp 5981–5996

M. Soledade C. Pedras* and Mohammad Hossain

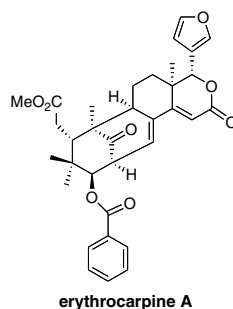


Among potential inhibitors of brassinin detoxification in *Sclerotinia sclerotiorum*, 6-fluoro-3-phenylindole inhibited brassinin glucosylation almost completely, indicating that selective inhibitors of BGT can be developed to control this major plant pathogen.

**Erythrocarpines A–E, new cytotoxic limonoids from *Chisocheton erythrocarpus***

pp 5997–6002

Khalijah Awang,* Chong Soon Lim, Khalit Mohamad, Hiroshi Morita, Yusuke Hirasawa, Koichi Takeya, Odile Thoison and A. Hamid A. Hadi

**OTHER CONTENTS**

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*Corresponding author

Supplementary data available via ScienceDirect

COVER

Terfenadine (an antihistamine pulled from the market in 1997) bound to a model of an open form of the homo-tetrameric pore domain of hERG, produced using Schrödinger's "Induced Fit Docking" technology [Farid, R.; Day, T.; Friesner, R. A.; Pearlstein, R. A. *Bioorg. Med. Chem.* **2006**, *14*, 3160–3173].

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ISSN 0968-0896