

10/2007

REVIEWS

Overcoming the Inadequacies or Limitations of Experimental Structures as Drug Targets by Using Computational Modeling Tools and Molecular Dynamics Simulations

E. Marco, F. Gago**

HIGHLIGHTS

Crystal Structures of the PBP2 Glycosyltransferase Domain: New Opportunities for Antibacterial Drug Design

*J. Zuegg, W. Meutermans**

SELECTED ORIGINAL CONTRIBUTIONS

Structure–Activity Studies on Suramin Analogues as Inhibitors of NAD⁺-Dependent Histone Deacetylases (Sirtuins)

*J. Trapp, R. Meier, D. Hongwiset, M. U. Kassack, W. Sippl, M. Jung**

N²-Benzyloxycarbonylguan-9-yl Acetic Acid Derivatives as HIV-1 Reverse Transcriptase Non-Nucleoside Inhibitors with Decreased Loss of Potency Against Common Drug-Resistance Mutations.

K. F. Adebambo, S. Zanolli, M. G. Thomas, R. Cancio, N. M. Howarth, G. Maga**

Artesunate and Dihydroartemisinin (DHA): Unusual Decomposition Products Formed under Mild Conditions and Comments on the Fitness of DHA as an Antimalarial Drug

R. K. Haynes, H.-W. Chan, C.-M. Lung, N.-C. Ng, H.-N. Wong, L. Y. Shek, I. D. Williams, A. Cartwright, M. F. Gomes*

Preparation of *N*-Sulfonyl- and *N*-Carbonyl-11-Azaartemisinins with Greatly Enhanced Thermal Stabilities: in vitro Antimalarial Activities

R. K. Haynes, H.-N. Wong, K.-W. Lee, C.-M. Lung, L. Y. Shek, I. D. Williams, S. L. Croft, L. Vivas, L. Ratray, L. Stewart, V. K. W. Wong, B. C. B. Ko*

The Fe²⁺-Mediated Decomposition, PfATP6 Binding, and Antimalarial Activities of Artemisone and Other Artemisinins: The Unlikelihood of C-Centered Radicals as Bioactive Intermediates

R. K. Haynes, W. C. Chan, C.-M. Lung, A.-C. Uhlemann, U. Eckstein, D. Taramelli, S. Parapini, D. Monti, S. Krishna**

Functional Classification of Protein Kinase Binding Sites Using Cavbase

*D. Kuhn, N. Weskamp, E. Hüllermeier, G. Klebe**

Homology Modeling of NR2B Modulatory Domain of NMDA Receptor and Analysis of Ifenprodil Binding.

L. Marinelli, S. Cosconati, T. Steinbrecher, V. Limongelli, A. Bertamino, E. Novellino, D. A. Case*

Naphthyl Tetrone Acids as Multi-Target Inhibitors of Bacterial Peptidoglycan Biosynthesis

T. S. Mansour, C. E. Caufield, B. Rasmussen, R. Chopra, G. Krishnamurthy, K. M. Morris, K. Svenson, J. Bard, C. Smeltzer, S. Naughton, S. Antane, Y. Yang, A. Severin, D. Quagliato, P. J. Petersen, G. Singh*

Design and Synthesis of Cyclopeptide Analogues of the Potent Histone Deacetylase Inhibitor FR235222

L. Gomez-Paloma, I. Bruno, E. Cini, S. Khochbin, M. Rodriguez, M. Taddei, S. Terracciano, K. Sadoul*

Structure–Activity Relationships for a Family of Benzothiophene Selective Estrogen Receptor Modulators Including Raloxifene and Arzoxifene

*C. R. Overk, K.-W. Peng, R. T. Asghodom, I. Kastrati, D. D. Lantvit, Z. Qin, J. Frasor, J. L. Bolton, G. R. J. Thatcher**

Antimalarial Cation-dimers Synthesized in Two Steps from an Inexpensive Starting Material, Isonicotinic Acid

K. Motoshima, Y. Hiwasa, M. Yoshikawa, K. Fujimoto, A. Tai, H. Kakuta, K. Sasaki*

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