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## HIGHLIGHTS

GR Ligands: Can We Improve the Established Drugs?

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## ORIGINAL CONTRIBUTIONS

FLEXNOVO: Structure-Based Searching in Large Fragment Spaces

Jörg Degen, Matthias Rarey\*

Synthesis and Activity of Carbazole Derivatives Against *Mycobacterium tuberculosis*

Taylor A. Choi, Regina Czerwonka, Wolfgang Fröhner, Micha P. Krah, Kethiri R. Reddy, Scott G. Franzblau,\* Hans-Joachim Knölker\*

Permeability of Phospholipid Vesicles to the Tumor Antigen Epitope gp100<sub>280-288</sub>

Antonella Cavazza, Mario Marini, Giulio C. Spagnoli, Michel Adamina, L. Giorgio Roda\*

Phosphopeptide Ligands of the SHP-1 N-SH2 Domain: Effects on Binding and Stimulation of Phosphatase Activity

Kornelia Hampel, Ina Kaufhold, Martin Zacharias, Frank D. Böhmer, Diana Imhof\*

The Predicted 3D Structures of the Human M1 Muscarinic Acetylcholine Receptor with Agonist or Antagonist Bound

Joyce Yao-chun Peng, Nagarajan Vaidehi,\* Spencer E. Hall, William A. Goddard III\*

Improving Potency, Selectivity, and Water Solubility of Adenosine A<sub>1</sub> Receptor Antagonists: Xanthines Modified at Position 3 and Related Pyrimido[1,2,3-*cd*]purinediones

Stefanie Weyler, Friederike Fülle, Martina Diekmann, Britta Schumacher, Sonja Hinz, Karl-Norbert Klotz, Christa E. Müller\*

Automated Protein-Ligand Crystallography for Structure-Based Drug Design

Wijnand T. M. Mooij,\* Michael J. Hartshorn, Ian J. Tickle, Andrew J. Sharff, Marcel L. Verdonk, Harren Jhoti

Integrated Approach Using Protein and Ligand Information to Analyze Selectivity- and Affinity-Determining Features of Carbonic Anhydrase Isozymes

Alexander Hillebrecht, Claudiu T. Supuran, Gerhard Klebe\*

Design, Synthesis, and In Vivo Efficacy of Glycine Transporter-1 (GlyT1) Inhibitors Derived from a Series of [4-Phenyl-1-(propylsulfonyl)pi-peridin-4-yl] methyl benzamides

Craig W. Lindsley,\* Zhijian Zhao, William H. Leister, Julie O'Brien, Wei Lemaire, David L. Williams, Jr., Tsing-Bau Chen, Raymond S. L. Chang, Maryann Burno, Marlene A. Jacobson, Cyrille Sur, Gene G. Kinney, Douglas J. Pettibone, Philip R. Tiller, Sheri Smith, Nancy N. Tsou, Mark E. Duggan, P. Jeffrey Conn, George D. Hartman

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