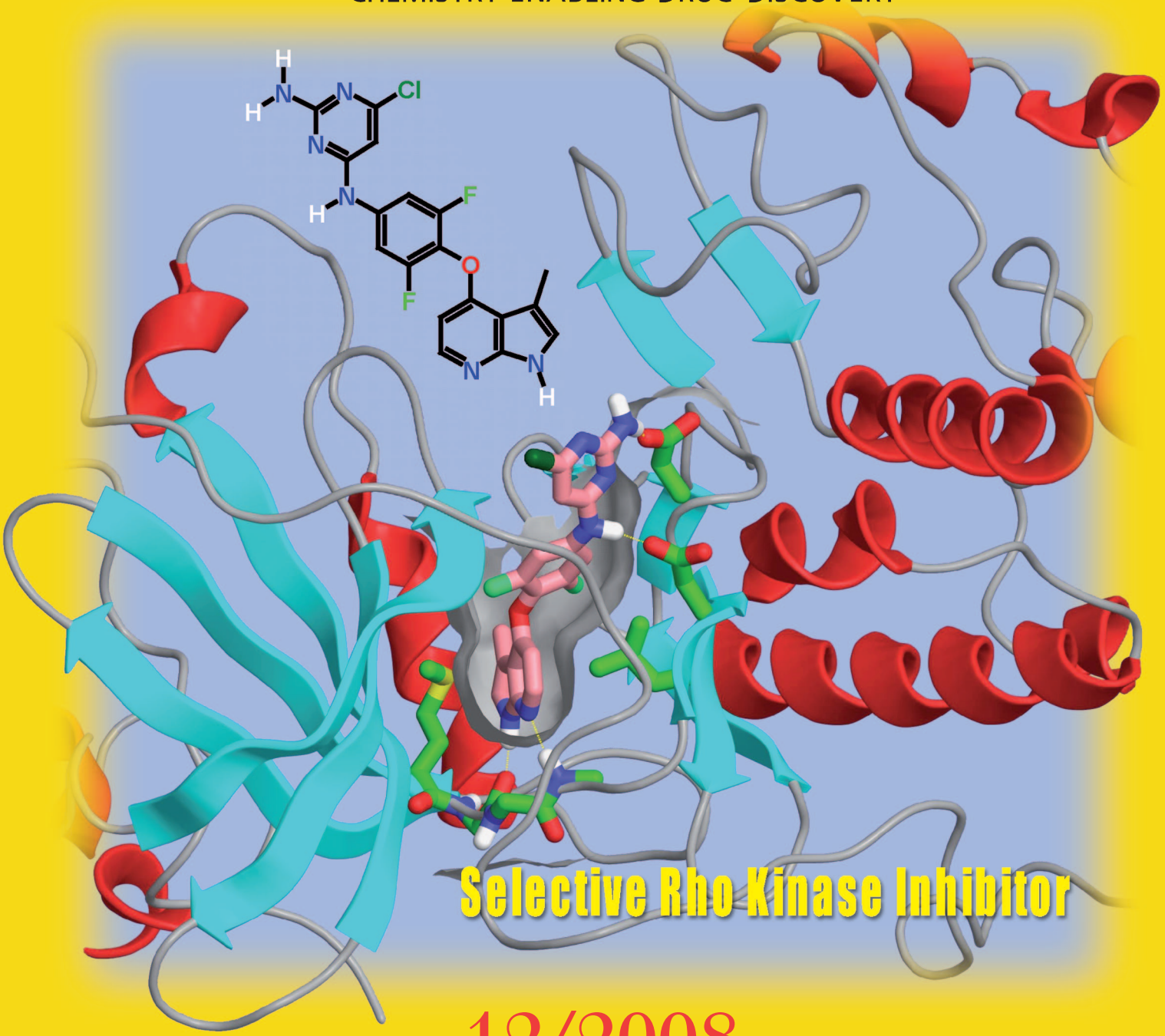
CHEMGX 3 (12) 1797–2004 (2008) · ISSN 1860-7179 · Vol. 3 · No. 12 · December, 2008

CHEMMEDCHEM

CHEMISTRY ENABLING DRUG DISCOVERY



12/2008

Review: Small-Molecule Inhibitors of PDK1
(C. Peifer and D. R. Alessi)
Full Paper: Bicyclic Acetals as Potential Chemotherapeutics
(S. V. Ley)

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Cover Picture

Hartmut Schirok*, Raimund Kast, Santiago Figueroa-Pérez, Samir Bennabi, Mark J. Gnoth, Achim Feurer, Heike Heckroth, Michael Thutewohl, Holger Paulsen, Andreas Knorr, Joachim Hütter, Mario Lobell, Klaus Münter, Volker Geiß, Heimo Ehmke, Dieter Lang, Martin Radtke, Joachim Mittendorf, and Johannes-Peter Stasch

The cover picture shows the 2D chemical structure of Bayer Schering's azaindole-based Rho kinase (ROCK) inhibitor, and also its 3D tube model docked into the ATP binding site of ROCK-1 (X-ray crystallographic structure). The kinase protein is mostly shown as a ribbon diagram with the β-sheet lobe on the left, the hinge region at the bottom, and the α-helical lobe on the right. The gatekeeper methionine and some additional key residues are also shown in tube representation. The depicted inhibitor was identified as a highly selective and orally available ROCK inhibitor, which leads to sustained blood pressure reduction in vivo. For more details, see the Full Paper by H. Schirok et al. on p. 1893 ff.