

List of Publications 1990-2009

Monographs:

1. Schneider, G., Baringhaus, K. H. *Molecular Design - Concepts and Applications*. Wiley-VCH, Weinheim, **2008**.
2. Böhm, H.-J., Schneider, G. (Eds) *Protein-Ligand Interaction – From Molecular Recognition to Drug Design*. Wiley-VCH, Weinheim, **2003**.
3. Schneider, G., So, S. S. *Adaptive Systems In Drug Design*. Landes Bioscience: Georgetown, **2002**.
4. Böhm, H.-J., Schneider, G. (Eds) *Virtual Screening for Bioactive Molecules*. Wiley-VCH, Weinheim, **2000**.
5. Wrede, P., Schneider, G. (Eds) *Concepts in Protein Engineering and Design*. Walter-de-Gruyter, Berlin, New York, **1994**.

Special Journal Issues:

1. Glen, R., Schneider, G. (Eds) Challenges in Virtual Screening. *QSAR Comb. Sci.* **2006**, 25(12).
2. Schneider, G., Downs, G. (Eds) Machine Learning Methods in QSAR Modeling. *QSAR Comb. Sci.* **2003**, 22(5).

Peer-reviewed Papers:

1. Stauch, B., Hofmann, H., Perkovic, M., Weisel, M., Kopietz, F., Cichutek, K., Münk, C., Schneider, G. Model structure of APOBEC3C reveals a binding pocket modulating ribonucleic acid interaction required for encapsidation. *Proc. Natl. Acad. Sci. USA*, **2009**, 106, 12079-12084.
2. Krüger, B., Weil, T., Schneider, G. Comparative virtual screening and novelty detection for NMDA Glycine(B) antagonists. *J. Comp. Aided Mol. Des.*, **2009**, 23, 869-881.
3. Esser, J., Rakonjac, M., Hofmann, B., Fischer, L., Provost, P., Schneider, G., Steinhilber, D., Samuelsson, B., Rådmark, O. Coactosin-like protein functions as a stabilizing chaperone for 5-lipoxygenase: role of tryptophan 102. *Biochem. J.*, **2009**, 425, 265-274.
4. Sander, K., Kottke, T., Tanrikulu, Y., Proschak, E., Weitzel, L., Schneider, E. H., Seifert, R., Schneider, G., Stark, H. 2,4-diaminopyrimidines as histamine H4 receptor ligands – scaffold optimization and pharmacological characterization. *Bioorg. Med. Chem.*, **2009**, 17, 7186-7196.
5. Hiss, J. A., Schneider, G. Domain organization of long autotransporter signal sequences. *Bioinform. Biol. Insights*, **2009**, 3, 189-204.
6. Keppner, S., Proschak, E., Schneider, G., Spänkuch, U. Identification and validation of a potent type II inhibitor of inactive polo-like kinase. *ChemMedChem*, **2009**, 4, 1806-1809.
7. Spork, S., Hiss, J., Sommer, M., Kooij, T. W. A., Chu, T., Schneider, G., Przyborski, J. An unusual ERAD-like complex is targeted to the apicoplast of *Plasmodium falciparum*. *Eukaryot. Cell*, **2009**, 8, 1134-1145.
8. Noeske, T., Trifanova, D., Kauss, V., Renner, S., Parsons, C. G., Schneider, G., Weil, T. Synergism of virtual screening and medicinal chemistry: Identification and optimization of allosteric antagonists of metabotropic glutamate receptor 1. *Bioorg. Med. Chem.*, **2009**, 17, 5708-5715.
9. Tausch, L., Siemoneit, U., Henkel, A., Poseckel, D., Kather, N., Franke, L., Hofmann, B., Schneider, G., Angioni, C., Geisslinger, G., Skarke, C., Holtmeier, W., Beckhaus, T., Karas, M., Jauch, J., Werz, O. Identification of human cathepsin G as a functional target of boswellic acids from the anti-inflammatory remedy frankincense. *J. Immunol.*, **2009**, 183, 3433-3442.

10. Feißt, C., Pergola, C., Rakonjac, M., Rossi, A., Koeberle, A., Dodt, G., Hoffmann, M., Hoernig, C., Fischer, L., Steinhilber, D., Franke, L., Schneider, G., Rådmark, O., Werz, O. Hyperforin is a novel type of 5-lipoxygenase inhibitor with high efficacy in vivo. *Cell. Mol. Life Sci.*, **2009**, *66*, 2759-2771.
11. Koenig, M., Huenecke, S., Salzmann, E., Esser, R., Quaritsch, R., Steinhilber, D., Radeke, H. H., Martin, H., Bader, P., Klingebiel, T., Schwabe, D., Schneider, G., Lehrnbecher, T., Orth, A., Koehl, U. Multivariate analyses of immune reconstitution in children following allogenic stem cell transplantation: Risk-estimation based on age-matched leukocyte subpopulation. *Bone Marrow Transpl.*, **2009**, *45*, 613-621.
12. Rupp, M., Schneider, P., Schneider, G. Distance phenomena in high-dimensional chemical descriptor spaces: consequences for similarity-based approaches. *J. Comp. Chem.*, **2009**, *30*, 2285-2296.
13. Löwer, M., Schneider, G. Prediction of type III secretion signals in genomes of Gram-negative bacteria. *PLoS ONE*, **2009**, *4*, 35917.
14. Hiss, J. A., Schneider, G. Architecture, function and prediction of long signal peptides. *Brief. Bioinform.*, **2009**, *10*, 569-578.
15. Zettl, H., Dittrich, M., Steri, R., Proschak, E., Rau, O., Steinhilber, D., Schneider, G., Lämmerhofer, M., Schubert-Zsilavecz, M. Novel pirinixic acids as PPAR α preferential dual PPAR α / γ agonists. *QSAR Comb. Sci.*, **2009**, *28*, 576-586.
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18. Krüger, B., Dietrich, A., Baringhaus, K.-H., Schneider, G. Scaffold-hopping potential of fragment-based *de novo* design: The chances and limits of variation. *Comb. Chem. High-Throughput Screen.*, **2009**, *12*, 383-396.
19. Schneider, G., Tanrikulu, Y., Schneider, P. Self-organizing molecular fingerprints: a ligand-based view on druglike chemical space and off-target prediction. *Future Med. Chem.*, **2009**, *1*, 213-218.
20. Perković, M., Schmidt, S., Marino, D., Russell, R. A., Stauch, B., Hofmann, H., Kopietz, F., Kloke, B.-P., Zielonka, J., Ströver, H., Hermle, J., Lindemann, D., Pathak, V. K., Schneider, G., Löchelt, M., Cichutek, K., Münk, C. Species-specific inhibition of APOBEC3C by the prototype foamy virus protein Bet. *J. Biol. Chem.*, **2009**, *284*, 5819-5826.
21. Reisen, F., Schneider, G., Proschak, E. ReactionMQL: Line notation for the representation of chemical reactions. *J. Chem. Inf. Model.*, **2009**, *49*, 6-12.
22. Hähnke, V., Hofmann, B., Grgat, T., Proschak, E., Steinhilber, D., Schneider, G. PhAST: Pharmacophore Alignment Search Tool. *J. Comput. Chem.*, **2009**, *30*, 761-771.
23. Schneider, P., Tanrikulu, Y., Schneider, G. Self-organizing maps in drug discovery: Library design, scaffold-hopping, repurposing. *Curr. Med. Chem.*, **2009**, *16*, 258-266.
24. Weisel, M., Proschak, E., Kriegl, J. M., Schneider, G. Form follows function: Shape analysis of protein cavities for receptor-based drug design. *Proteomics*, **2009**, *9*, 451-459.
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28. Proschak, E., Sander, K., Zettl, H., Tanrikulu, Y., Rau, O., Schneider, P., Schubert-Zsilavec, M., Stark, H., Schneider, G. From molecular shape to potent bioactive agents II: Fragment-based *de novo* design. *ChemMedChem*, **2009**, *4*, 45-48.
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