

## List of publications 1990-2010

### Research Monographs:

1. Schneider, G., Baringhaus, K. H. *Molecular Design - Concepts and Applications*. Wiley-VCH, Weinheim, **2008**.
2. Schneider, G., So, S. S. *Adaptive Systems In Drug Design*. Landes Bioscience: Georgetown, **2002**.

### Edited Collective Volumes:

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).
3. Böhm, H. J., Schneider, G. (Eds) *Protein-Ligand Interaction – From Molecular Recognition to Drug Design*. Wiley-VCH, Weinheim, **2003**.
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**.

### Peer-reviewed Papers:

1. Reisen, F., Weisel, M., Kriegl, J. M., Schneider, G. Self-organizing fuzzy graphs for structure-based comparison of protein pockets. *J. Proteome Res.*, **2010**, 9, 6498-6510.
2. Alamuri, P., Löwer, M., Hiss, J. A., Himpl, S. D., Schneider, G., Mobley, H. L. T. Adhesion, invasion, and agglutination mediated by two trimeric autotransporters in human uropathogen *Proteus mirabilis*. *Infect. Immun.*, **2010**, 78, 4882-4894.
3. Hoy, B., Löwer, M., Weydig, C., Carra, G., Tegtmeyer, N., Geppert, T., Plattner, P., Sewald, N., Backert, S., Schneider, G., Wessler, S. *Helicobacter pylori* HtrA is a new secreted virulence factor that cleaves E-cadherin to disrupt intercellular adhesion. *EMBO Rep.*, **2010**, 11, 798-804.
4. Klenner, A., Hartenfeller, M., Schneider, P., Schneider, G. 'Fuzziness' in pharmacophore-based virtual screening and *de novo* design. *Drug Discov. Today Technol.*, **2010**, 7, e237-e244.
5. Tanrikulu, Y., Kandru, R., Schneider, G., So, W. V., Bitter, H.-M. Missing value estimation for compound-target activity data. *Mol. Inf.*, **2010**, 29, 678-684.
6. Schneider, G. Virtual screening: An endless staircase? *Nat. Rev. Drug Discov.*, **2010**, 9, 273-276.
7. Werner, T., Sander, K., Tanrikulu, Y., Kottke, T., Proschak, E., Stark, H., Schneider, G. In silico characterization of ligand binding modes in the human histamine H<sub>4</sub> receptor and their impact on receptor activation. *ChemBioChem*, **2010**, 11, 1850-1855.
8. Zettl, H., Weggen, S., Schneider, P., Schneider, G. Exploring chemical space of gamma-secretase modulators. *Trends Pharmacol. Sci.*, **2010**, 31, 402-410.
9. Zander, J., Hartenfeller, M., Haehnke, V., Proschak, E., Besier, S., Wichelhaus, T. A., Schneider, G. Non-nucleoside analogs as bacterial thymidine kinase inhibitors identified by multi-step virtual screening. *Chemistry Eur. J.*, **2010**, 16, 9630-9637.
10. Steri, R., Kara, M., Proschak, E., Steinhilber, D., Schneider, G., Schubert-Zsilavecz, M. Antidiabetic sulfonylureas modulate farnesoid X receptor activation and target gene transcription. *Future Med. Chem.*, **2010**, 2, 575-586.
11. Keppner, S., Proschak, E., Kaufmann, M., Stebhardt, K., Schneider, G., Spänkuch, B. Biological implication of freezing Plk1 in its inactive conformation in cancer cells. *Cell Cycle*, **2010**, 9, 761-763.
12. Haehnke, V., Rupp, M., Krier, M., Rippmann, F., Schneider, G. Pharmacophore Alignment Search Tool (PhAST): Influence of canonical atom labeling on similarity searching. *J. Comp. Chem.*, **2010**, 31, 2810-2826.

13. Winiewska, J. M., Jäger, N., Freier, A., Losch, F. O., Wiesmüller, K.-H., Walden, P., Wrede, P., Schneider, G., Hiss, J. A. MHC I stabilizing potential of computer-designed octapeptides. *J. Biomed. Biotechnol.*, **2010**, 396847.
14. Stauch, B., Simon, B., Basile, T., Schneider, G., Malek, N. P., Kalesse, M., Carlomagno, T. Structure and intermolecular interaction of a reversible cyclic peptide inhibitor of the proteasome revealed by a combination of NMR spectroscopy and molecular modeling. *Angew. Chem. Int. Ed.*, **2010**, *49*, 3934-3938.
15. Hiss, J. A., Hartenfeller, M., Schneider, G. Concepts and applications of "natural computing" techniques in de novo drug and peptide design. *Curr. Pharm. Des.*, **2010**, *16*, 1656-1665.
16. Steri, R., Rupp, M., Proschak, E., Schroeter, T., Zettl, H., Hansen, K., Schwarz, O., Müller-Kuhrt, L., Müller, K.-R., Schneider, G., Schubert-Zsilavec, M. Truxillic acid derivatives act as peroxisome proliferator-activated receptor gamma activators. *Bioorg. Med. Chem. Lett.*, **2010**, *20*, 2920-2923.
17. Thieme, T. M., Steri, R., Proschak, E., Paulke, A., Schneider, G., Schubert-Zsilavec, M. Rational design of a subtype selective pirinixic acid derived PPAR $\gamma$  modulator. *Bioorg. Med. Chem. Lett.*, **2010**, *20*, 2469-2473.
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21. Jäger, N., Wisniewskaja, J. M., Hiss, J. A., Losch, F. O., Walden, P., Wrede, P., Schneider, G. Attractors in sequence space: agent-based exploration of MHC I binding peptides. *Mol. Inf.*, **2010**, *29*, 65-74.
22. Schneider, G. From virtual to real screening – Achievements and challenges for similarity searching. *EFMC Yearbook 2009*, **2010**, 33-45.
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