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## List of Publications

### Editorial Work

#### Editor:

2002-2009 *QSAR & Combinatorial Science* (Wiley-VCH)  
2010 – *Molecular Informatics* (Wiley-VCH)

#### Editorial Board Member:

- *ChemBioChem*
- *Current Chemical Biology*
- *Molecules*
- *Future Medicinal Chemistry*
- *Chemistry Central Journal*
- *Open Medicinal Chemistry Journal*
- *Open Structural Biology Journal*
- *Open Structural Biology Reviews*
- *Open Cell Development and Biology Journal*

#### Special Journal Issues:

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

#### Edited books:

1. Böhm, H.-J. and Schneider, G. (Eds) (2003) *Protein-Ligand Interaction – From Molecular Recognition to Drug Design*. Wiley-VCH: Weinheim, New York.
2. Böhm, H.-J. and Schneider, G. (Eds) (2000) *Virtual Screening for Bioactive Molecules*. Wiley-VCH: Weinheim, New York.
3. Wrede, P. and Schneider, G. (Eds) (1994) *Concepts in Protein Engineering and Design*. Walter-de-Gruyter: Berlin, New York.

### Textbooks

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

## Peer-reviewed Original Articles & Reviews

1. Stauch, B., Hofmann, H., Perkovic, M., Weisel, M., Kopietz, F., Cichutek, K., Münk, C. and Schneider, G. (2009) Model structure of APOBEC3C reveals a binding pocket modulating ribonucleic acid interaction required for encapsidation. **Proc. Natl. Acad. Sci. USA** 106, 12079-12084.
2. Keppner, S., Proschak, E., Schneider, G. and Spänkuch, U. (2009) Effects of Plk1 inhibition by a novel type II inhibitor identified via virtual screening. **ChemMedChem**, accepted.
3. Spork, S., Hiss, J., Sommer, M., Kooij, T.W.A., Chu, T., Schneider, G. and Przyborski, J. (2009) An unusual ERAD-like complex is targeted to the apicoplast of *Plasmodium falciparum*. **Eukaryotic Cell**, accepted.
4. Noeske, T., Trifanova, D., Kauss, V., Renner, S., Parsons, C.G., Schneider, G. and Weil, T. (2009) Synergism of virtual screening and medicinal chemistry: Identification and optimization of allosteric antagonists of metabotropic glutamate receptor 1. **Bioorg. Med. Chem.** 17, 5708-5715.
5. 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. and Werz, O. (2009) Identification of human cathepsin G as a functional target of boswellic acids from the anti-inflammatory remedy frankincense. **J. Immunol.**, accepted.
6. 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. and Werz, O. (2009) Hyperforin is a novel type of 5-lipoxygenase inhibitor with high efficacy in vivo. **Cell. Mol. Life Sci.** 66, 2759-2771.
7. 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. and Koehl, U. (2009) Multivariate analyses of immune reconstitution in children following allogenic stem cell transplantation: Risk-estimation based on age-matched leukocyte subpopulation. **Bone Marrow Transpl.**, accepted.
8. Sander, K., Kottke, T., Proschak, E., Tanrikulu, Y., Schneider, E., Seifert, R., Schneider, G. and Stark, H. (2009) Lead

- identification and optimization of diaminopyrimidines as histamine H<sub>4</sub> receptor ligands. **Inflamm. Res.**, accepted.
9. Schneider, G. (2009) Virtual screening: what are we missing? **MedChemWatch** 7, 3-4.
  10. Rupp, M., Schneider, P. and Schneider, G. (2009) Distance phenomena in high-dimensional chemical descriptor spaces: consequences for similarity-based approaches. **J. Comp. Chem.** 30, 2285-2296.
  11. Löwer, M. and Schneider, G. (2009) Prediction of type III secretion signals in genomes of Gram-negative bacteria. **PLoS ONE** 4, 35917.
  12. Hiss, J. A. and Schneider, G. (2009) Architecture, function and prediction of long signal peptides. **Brief. Bioinform.**, accepted.
  13. Zettl, H., Dittrich, M., Steri, R., Proschak, E., Rau, O., Steinhilber, D., Schneider, G., Lämmerhofer, M. and Schubert-Zsilavecz, M. (2009) Novel pirinixic acids as PPAR $\alpha$  preferential dual PPAR $\alpha$ / $\gamma$  agonists. **QSAR Comb. Sci.** 28, 576-586.
  14. Tanrikulu, Y., Proschak, E., Werner, T., Geppert, T., Todoroff, N., Klenner, A., Kottke, T., Sander, K., Schneider, E., Seifert, R., Stark, H., Clark, T. and Schneider, G. (2009) Homology-model adjustment and ligand screening with a pseudoreceptor of the human histamine H<sub>4</sub> receptor. **ChemMedChem** 4, 820-827.
  15. Koeberle, A., Siemoneit, U., Northoff, H., Hofmann, B., Schneider, G. and Werz, O. (2009) MK-886, an inhibitor of the 5-lipoxygenase-activating protein, inhibits cyclooxygenase-1 activity and suppresses platelet aggregation. **Eur. J. Pharmacol.** 608, 84-90.
  16. Krüger, B., Dietrich, A., Baringhaus, K.-H. and Schneider, G. (2009) Scaffold-hopping potential of fragment-based de novo design: The chances and limits of variation. **Comb. Chem. High-Throughput Screen.** 12, 383-396.
  17. Schneider, G., Tanrikulu, Y. and Schneider, P. (2009) Self-organizing molecular fingerprints: a ligand-based view on druglike chemical space and off-target prediction. **Future Med. Chem.** 1, 213-218.
  18. 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. and Münk, C. (2009) Species-specific inhibition

- of APOBEC3C by the prototype foamy virus protein Bet. **J. Biol. Chem.** 284, 5819-5826.
19. Reisen, F., Schneider, G. and Proschak, E. (2009) ReactionMQL: Line notation for the representation of chemical reactions. **J. Chem. Inf. Model.** 49, 6-12.
  20. Hähnke, V., Hofmann, B., Grgat, T., Proschak, E., Steinhilber, D. and Schneider, G. (2009) PhAST: Pharmacophore Alignment Search Tool. **J. Comput. Chem.** 30, 761-771.
  21. Schneider, P., Tanrikulu, Y. and Schneider, G. (2009) Self-organizing maps in drug discovery: Library design, scaffold-hopping, repurposing. **Curr. Med. Chem.** 16, 258-266.
  22. Weisel, M., Proschak, E., Kriegl, J. M. and Schneider, G. (2009) Form follows function: Shape analysis of protein cavities for receptor-based drug design. **Proteomics** 9, 451-459.
  23. Schneider, G., Hartenfeller, M., Reutlinger, M., Tanrikulu, Y., Proschak, E. and Schneider, P. (2009) Voyages to the (un)known: Adaptive design of bioactive compounds. **Trends Biotechnol.** 27, 18-26.
  24. Altmann, K.-H., Buchner, J., Kessler, H., Diederich, F., Kräutler, B., Lippard, S., Liskamp, R., Müller, K., Samori, B., Schneider, G., Schwalbe, H., Toniolo, C., van Boeckel, C. A. A., Waldmann, H., Walsh, C. T., and Nolan, E. M. (2009) The state of the art in chemical biology. **ChemBioChem** 10, 16-29.
  25. Proschak, E., Zettl, H., Tanrikulu, Y., Weisel, M., Kriegl, J. M., Rau, O., Schubert-Zsilavecz, M. and Schneider, G. (2009) From molecular shape to potent bioactive agents I: Bioisosteric replacement of molecular fragments. **ChemMedChem** 4, 41-44.
  26. Proschak, E., Sander, K., Zettl, H., Tanrikulu, Y., Rau, O., Schneider, P., Schubert-Zsilavecz, M., Stark, H. and Schneider, G. (2009) From molecular shape to potent bioactive agents II: Fragment-based de novo design. **ChemMedChem** 4, 45-48.
  27. Tanrikulu, Y., Rau, O., Schwarz, O., Proschak, E., Siems, K., Müller-Kuhrt, L., Schubert-Zsilavecz, M. and Schneider, G. (2009) Structure-based pharmacophore screening for natural product-derived PPAR $\gamma$  agonists. **ChemBioChem** 10, 75-78.
  28. Meissner, M., Koch, O., Klebe, G. and Schneider, G. (2008) Prediction of turns types in protein structure by machine-learning classifiers. **Proteins** 74, 344-352.

29. Hofmann, B., Franke, L., Proschak, E., Tanrikulu, Y., Schneider, P., Steinhilber, D. and Schneider, G. (2008) Scaffold-hopping cascade yields potent inhibitors of 5-lipoxygenase. **ChemMedChem** 3, 1535-1538.
30. Löwer, M., Weydig, C., Metzler, D., Reuter, A., Starzinski-Powitz, A., Wessler, S. and Schneider, G. (2008) Prediction of extracellular proteases of the human pathogen *Helicobacter pylori* reveals proteolytic activity of the Hp1018/19 protein HtrA. **PLoS ONE** 3, e3510.
31. Grabowski, K., Baringhaus, K.-H. and Schneider, G. (2008) Scaffold diversity of natural-products: Inspiration for combinatorial library design. **Nat. Prod. Rep.** 25, 892-904.
32. Alig, L., Alsenz, J., Andjelkovic, M., Bendels, S., Bénardeau, A., Bleicher, K., Bourson, A., David-Pierson, P., Guba, W., Hildbrand, S., Kube, D., Lübbers, T., Mayweg, A. V., Narquizian, R., Neidhart, W., Nettekoven, M., Plancher, J. M., Rocha, C., Rogers-Evans, M., Röver, S., Schneider, G., Taylor, S. and Waldmeier, P (2008) Benzodioxoles: Novel cannabinoid-1 receptor inverse agonists for the treatment of obesity. **J. Med. Chem.** 51, 2115-2127.
33. Schüller, A. and Schneider, G. (2008) Identification of hits and lead structure candidates with limited resources by adaptive optimization. **J. Chem. Inf. Model.** 48, 1473-1491.
34. Tanrikulu, Y. and Schneider, G. (2008) Pseudoreceptor models in drug design: Bridging ligand- and receptor-based virtual screening. **Nature Rev. Drug Discov.** 7, 668-677.
35. Hiss, J., Resch, E., Schreiner, A., Meissner, M., Starzinski-Powitz, A. and Schneider, G. (2008) Domain organization of long signal peptides of single-pass integral membrane proteins reveals multiple functional capacity. **PLoS ONE** 3, e2767.
36. Resch, E., Quaiser, S., Quaiser, T., Schneider, G., Starzinski-Powitz, A. and Schreiner, A. (2008) Synergism of shrew-1's signal peptide and transmembrane segment required for plasma membrane localization. **Traffic** 9, 1344-1353.
37. Hartenfeller, M., Proschak, E., Schüller, A. and Schneider, G. (2008) Concept of combinatorial de novo design of druglike molecules by particle swarm optimization. **Chem. Biol. Drug Des.** 72, 16-26.

38. Hiss, J. A., Przyborski, J. M., Schwarte, F., Lingelbach, K. and Schneider, G. (2008) The *Plasmodium* export element revisited. **PLoS ONE** 3, e1560.
39. Schüller, A., Suhartono, M., Fechner, U., Tanrikulu, Y., Breitung, S., Scheffer, U., Göbel, M.W. and Schneider, G. (2008) The concept of template-based de novo design from drug-derived molecular fragments and its application to TAR RNA. **J. Comp. Aided Mol. Des.** 22, 59-68.
40. Grabowski, K., Proschak, E., Baringhaus, K.-H., Rau, O., Schubert-Zsilavec, M. and Schneider, G. (2008) Bioisosteric replacement of molecular scaffolds: From natural products to synthetic compounds. **Nat. Prod. Commun.** 3, 1355-1360.
41. Schmuker, M. and Schneider, G. (2007) Processing and classification of chemical data inspired by insect olfaction. **Proc. Natl. Acad. Sci. USA** 104, 20285-20289.
42. Renner, S., Hechenberger, M., Noeske, T., Böcker, A., Jatzke, C., Schmuker, M., Parsons, C. G., Weil, T. and Schneider, G. (2007) Searching for drug scaffolds with 3D pharmacophores and neural network ensembles. **Angew. Chem. Int. Ed.** 46, 5336-5339.
43. Franke, L., Schwarz, O., Müller-Kuhrt, L., Hoernig, C., Fischer, L., George, S., Tanrikulu, Y., Schneider, P., Werz, O., Steinhilber, D. and Schneider, G. (2007) Identification of natural product-derived inhibitors of 5-lipoxygenase activity by ligand-based virtual screening. **J. Med. Chem.** 50, 2640-2646.
44. Proschak, E., Rupp, M., Derksen, S. and Schneider, G. (2007) Shapelets: Possibilities and limitations of shape-based virtual screening. **J. Comp. Chem.** 29, 108-114.
45. Tanrikulu, Y., Nietert, M., Scheffer, U., Proschak, E., Grabowski, K., Schneider, P., Weidlich, M., Karas, M., Göbel, M. and Schneider, G. (2007) Scaffold-hopping by "fuzzy" pharmacophores and application to RNA targets. **ChemBioChem** 8, 1932-1936.
46. Noeske, T., Jirgensons, A., Stachenkovs, I., Renner, S., Jaunzeme, I., Trifanova, D., Hechenberger, M., Bauer, T., Schneider, G., Parsons, C.G. and Weil, T. (2007) Virtual screening for selective allosteric mGluR1 antagonists and structure-activity relationship investigations for coumarine derivatives. **ChemMedChem** 2, 1763-1773.

47. Böcker, A., Sasse, B. C., Nietert, M., Stark, H. and Schneider, G. (2007) GPCR-targeted library design: Novel dopamine D<sub>3</sub> receptor antagonists. **ChemMedChem** 2, 1000-1005.
48. Werz, O., Fischer, L., Hornig, M., Pergola, C., Meindl, N., Franke, L., Tarikulu, Y., Dodt, G., Schneider, G. and Steinhilber, D. (2007) On the molecular mechanism of 5-lipoxygenase product synthesis inhibition by licofelone. **Brit. J. Pharmacol.** 152, 471-480.
49. Siemoneit, U., Hofmann, B., Kather, N., Lamkemeyer, T., Madlung, J., Franke, L., Schneider, G., Jauch, J., Poeckel, D. and Werz, O. (2007) Identification and functional analysis of cyclooxygenase-1 as a molecular target of boswellic acids. **Biochem. Pharmacol.** 75, 503-513.
50. Givehchi, A., Ludwig, V., Boden, O., Krebs, A., Scheffer, U., Göbel, M. and Schneider, G. (2007) Classification and prediction of tripeptides inhibiting HIV-1 Tat/TAR-RNA interaction using a self-organizing map. **Lett. Drug Des. Discov.** 4, 410-416.
51. Byvatov, E., Baringhaus, K.-H., Schneider, G. and Matter, H. (2007) Virtual screening filter for identification of cytochrome P450 2C9 (CYP2C9) inhibitors. **QSAR Comb. Sci.** 26, 618-628.
52. Meissner, M. and Schneider, G. (2007) Protein folding simulation by particle swarm optimization. **Open Struct. Biol. J.** 1, 1-6.
53. Schmuker, M., Schwarte, F., Brück, A., Proschak, E., Tanrikulu, Y., Givehchi, A., Scheiffle, K. and Schneider, G. (2007) SOMMER: Self-organizing maps for education and research. **J. Mol. Model.** 13, 225-228.
54. Grabowski, K. and Schneider, G. (2007) Properties and architecture of drugs and natural products revisited. **Curr. Chem. Biol.** 1, 115-127.
55. Rabal, O., Schneider, G., Borrell, J. I. and Teixidó, J. (2007) Structure-based virtual screening of FGFR inhibitors: Cross-decoys and induced-fit effect. **Biodrugs** 21, 31-45.
56. Schmuker, M., de Bruyne, M., Hähnel, M. and Schneider, G. (2007) Predicting olfactory receptor neuron responses from odorant structure. **Chemistry Central J.** 1, 11.
57. Weisel, M., Proschak, E. and Schneider, G. (2007) PocketPicker: Analysis of ligand binding-sites with shape descriptors. **Chemistry Central J.** 1, 7.

58. Rupp, M., Proschak, E. and Schneider, G. (2007) Kernel approach to molecular similarity based on iterative graph similarity. **J. Chem. Inf. Model.** 47, 2280-2286.
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60. Schüller, A., Hähnke, V. and Schneider, G. (2007) SmiLib v2.0: A Java-based tool for rapid combinatorial library enumeration. **QSAR Comb. Sci.** 26, 407-410.
61. Hiß, J., Bredenbeck, A., Losch, F. O., Wrede, P., Walden, P. and Schneider, G. (2007) Design of MHC I stabilizing peptides by agent-based exploration of sequence space. **Prot. Eng. Des. Sel.** 20, 99-108.
62. Fechner, U. and Schneider, G. (2007) Flux (2): Comparison of molecular mutation and crossover operators for ligand-based de novo design. **J. Chem. Inf. Model.** 47, 656-667.
63. Fechner, U. and Schneider, G. (2006) Flux (1): A virtual synthesis scheme for fragment-based de novo design. **J. Chem. Inf. Model.** 46, 699-707.
64. Meissner, M., Schmuker, M. and Schneider, G. (2006) Optimized Particle Swarm Optimization (OPSO) and its application to artificial neural network training. **BMC Bioinformatics** 7, 125-136.
65. Renner, S. and Schneider, G. (2006) Scaffold-hopping potential of ligand-based similarity concepts. **ChemMedChem** 1, 181-185.
66. Noeske, T., Sasse, B.C., Stark, H., Parsons, C.G., Weil, T. and Schneider, G. (2006) Predicting compound selectivity by self-organizing maps: cross-activities of metabotropic glutamate receptor antagonists. **ChemMedChem** 1, 1066-1068.
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68. Schüller, A., Fechner, U., Renner, S., Franke, L., Weber, L. and Schneider, G. (2006) A pseudo-ligand approach to virtual screening. **Comb. Chem. High-Throughput Screen.** 9, 359-364.
69. Böcker, A., Schneider, G. and Teckentrup, A. (2006) NIPALSTREE: A new hierarchical clustering approach for large

- compound libraries and its application to virtual screening. **J. Chem. Inf. Model.** 46, 2220-2229.
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  71. Schneider, G., Schneider, P. and Renner, S. (2006) Scaffold-hopping: How far can you jump? **QSAR Comb. Sci.** 25, 1162-1171.
  72. Schneider, G. and Fechner, U. (2005) Computer-based de novo design of druglike molecules. **Nature Rev. Drug Discov.** 4, 649-663.
  73. Werz, O., Tretiakova, I., Michel, A., Ulke, A., Hörnig, M., Franke, L., Schneider, G., Samuelsson, B., Rådmark, O. and Steinhilber, D. (2005) Caspase-mediated degradation of human 5-lipoxygenase in B-lymphocytic cells. **Proc. Natl. Acad. Sci. USA** 102, 13164-13169.
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  75. Byvatov, E., Sasse, B. C., Stark, H. and Schneider, G. (2005) From virtual to real screening for novel D<sub>3</sub> dopamine receptor ligands. **ChemBioChem** 6, 997-999.
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  78. Böcker, A., Derksen, S., Schmidt, E., Teckentrup, A. and Schneider, G. (2005) A hierarchical clustering approach for large compound libraries. **J. Chem. Inf. Model.** 45, 807-815.
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81. Givehchi, A. and Schneider, G. (2005) Multi-space classification for predicting GPCR ligands. **Mol. Divers.** 9, 371-383.
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  85. Schneider, G. and Fechner, U. (2004) Advances in the prediction of protein targeting signals. **Proteomics** 4, 1571-1580.
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