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List of Publications

Peer-reviewed Papers and Book Chapters

1. Zuegge, J., Fechner, U., Roche, O., Parrott, N. J., Engkvist, O. and Schneider, G. (2002) A fast virtual screening filter for cytochrome P450 3A4 inhibition liability of compound libraries. *Quant. Struct. Act. Relat.* **21**, 249-256.

[http://dx.doi.org/10.1002/1521-3838\(200208\)21:3<249::AID-QSAR249>3.0.CO;2-S](http://dx.doi.org/10.1002/1521-3838(200208)21:3<249::AID-QSAR249>3.0.CO;2-S)

2. Byvatov, E., Fechner, U., Sadowski, J. and Schneider, G. (2003) Comparison of support vector machines and artificial neural networks for drug-likeness prediction. *J. Chem. Inf. Comput. Sci.* **43**, 1882-1889.

<http://dx.doi.org/10.1021/ci0341161>

3. Fechner, U., Franke, L., Renner, S., Schneider, P. and Schneider, G. (2003) Comparison of correlation vector methods for ligand-based similarity searching. *J. Comput. Aided Mol. Des.* **17**, 687-698.

<http://dx.doi.org/10.1023/B:JCAM.0000017375.61558.ad>

4. Fechner, U. and Schneider, G. (2004) Optimization of a pharmacophore-based correlation vector descriptor, *QSAR Comb. Sci.* **23**, 19-22.

<http://dx.doi.org/10.1002/qsar.200330855>

5. Fechner, U. and Schneider, G. (2004) Evaluation of distance metrics for ligand based similarity searching, *Chembiochem* **5**, 538-540.

<http://dx.doi.org/10.1002/cbic.200300812>

6. Schneider, G. and Fechner, U. (2004) Advances in the prediction of protein targeting signals, *Proteomics* **4**, 1571-1580.

<http://dx.doi.org/10.1002/pmic.200300786>

7. Paetz, J., Fechner, U., Franke, L., Renner, S., Schneider, P. and Schneider G. (2004) Pharmacophore Feature Selection with a Neuro-Fuzzy System, In: *Proc. of the 4th Europ. Symp. on Intelligent Technologies, Hybrid Systems and their Implementation on Smart Adaptive Systems (EUNITE 2004)*, Aachen, Germany, Hrsg.: Elite Foundation, 179-184, Aachen, Verlag Mainz, Wissenschaftsverlag 2004.

8. Schneider, G., Renner, S. and Fechner, U. (2005) Navigation in chemical space based on correlation-vector representations of molecules, In: *The Chemical Theatre of Biological Systems* (Hicks, M., Kettner, K.; Eds.), Proceedings of the Beilstein-Institut Symposium 2004, Logos Verlag, Berlin, pp 197-218.

<http://www.beilstein-institut.de/bozen2004/proceedings/Schneider/Schneider.pdf>

9. Schneider, G. and Fechner U. (2005) Computer-based *de novo* design of drug-like molecules, *Nature Rev. Drug Discov.* **4**, 649-663.

<http://dx.doi.org/10.1038/nrd1799>

10. Fechner, U., Paetz, J. and Schneider, G. (2005) Comparison of Three Holographic Fingerprint Descriptors and their Binary Counterparts, *QSAR Comb. Sci.* 24, 961-967.
<http://dx.doi.org/10.1002/qsar.200530118>
11. Renner, S., Fechner, U. and Schneider, G. (2005) Alignment-free pharmacophore patterns – A correlation-vector approach. In: *Pharmacophores and Pharmacophore Searches* (Langer, T. and Hoffmann, E.; Eds), Wiley-VCH, Weinheim, pp. 49-80.
12. 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.
<http://dx.doi.org/10.1021/ci0503560>
13. 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.
<http://dx.doi.org/10.2174/138620706777452375>
14. Proschak, E., Wegner, J. K., Schüller, A., Schneider, G. and Fechner, U. (2007) Molecular Query Language (MQL) - A Context-Free Grammar for Substructure Matching, *J. Chem. Inf. Model.*, 47, 295-301.
<http://dx.doi.org/10.1021/ci600305h>
15. 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.
<http://dx.doi.org/10.1021/ci6005307>
16. Schüller, A., Suhartono, M., Fechner, U., Tanrikulu, Y., Breitung, S., Scheffer, U., Göbel, M. W. and Schneider, G. (2007) The concept of template-based de novo design from drug-derived molecular fragments and its application to TAR RNA. *J. Comput. Aided Mol. Des.* 22, 59-68.
<http://dx.doi.org/10.1007/s10822-007-9157-4>

Other Publications

1. Proschak, E., Wegner, J.K., Schneider, G. and Fechner, U. (2005) MQL - Development of a novel substructure query language, *CDK News* 2, 62-64.
<http://prdownloads.sourceforge.net/cdk/cdknews2.3.pdf?download>
2. Fechner, U. and Guha, R. (2006) A Protocol for Descriptor QA, *CDK News* 3, 3-4.
<http://prdownloads.sourceforge.net/cdk/cdknews3.1.pdf?download>
3. Fechner, U. and Grabowski, T. (2006) QA of the XlogP Descriptor, *CDK News* 3, 12-14.
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4. Grabowski, T. and Fechner, U. (2006) QA of the Topological Polar Surface Area Descriptor, *CDK News* 4, 27-31.
<http://prdownloads.sourceforge.net/cdk/cdknews3.2.pdf?download>

Poster Presentations

1. Renner, S., Fechner, U. and Schneider, G. (2004) Correlation Vector Approaches for Ligand-Based Similarity Searching, *3rd Joint Sheffield Conference on Chemoinformatics*, Sheffield, UK, 21st-23rd April, 2004.

<http://cisrg.shef.ac.uk/shef2004/posters.htm#31>

2. Fechner, U., Grabowski, K. and Schneider G. (2004) Design of natural product-like combinatorial libraries, *18. CIC Workshop*, Boppard, Germany, 16th-18th November, 2004.

http://va.gdch.de/wwwdata/abstracts/5264/5264_0026.pdf

3. Fechner, U. and Schneider, G. (2005) "Ultra-fast" ligand-based de novo design using virtual reaction schemes, *7th International Conference on Chemical Structures*, Noordwijkerhout, The Netherlands, 5th-9th June, 2005.

http://www.int-conf-chem-structures.org/html/7th_iccs_red_poster_session.html#P-36

4. Fechner, U. and Bender, A. (2005) BayCATS – Combining the Potency of a Pharmacophore Descriptor with the Power of the Bayes Classifier, *MGMS International Meeting 2005*, Dublin, Ireland, Sept 11th-14th, 2005.

<http://www.tchpc.tcd.ie/MGMS/details/Abstracts.htm>

5. Bender, A. and Fechner, U. (2005) BayCATS – A Novel Pharmacophore-based Compound Classification Approach, *1st German Conference on Chemoinformatics 19. CIC-Workshop 2005*, Goslar, 13th – 15th November, 2005.

https://va.gdch.de/wwwdata/abstracts/5281/5281_0067.pdf

6. Proschak, E., Fechner, U., Wegner, J.K. and Schneider, G. (2005) MQL - Development of a novel stand-alone substructure query language, *1st German Conference on Chemoinformatics 19. CIC-Workshop 2005*, Goslar, 13th – 15th November, 2005.

https://va.gdch.de/wwwdata/abstracts/5281/5281_0003.pdf

7. Guenther, B., Fechner, U., Michels, S., Koller, D., Nietfeld, M., Reschel, U., Zuegge, J. (2006) The Beilstein Chemistry Toolkit: An Overview of its Functionality, *2nd German Conference on Chemoinformatics 20. CIC-Workshop 2006*, Goslar, 12th – 14th November, 2006.

https://va.gdch.de/wwwdata/abstracts/5298/5298_0064.pdf

8. Guenther, B., Fechner, U., Michels, S., Koller, D., Nietfeld, M., Reschel, U., Zuegge, J. (2007) The Beilstein Chemistry Toolkit, *4th Joint Sheffield Conference on Chemoinformatics*, Sheffield, UK, 18th – 20th June, 2007.

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