Das virtuelle Labor - Computersimulationen von Molekülen

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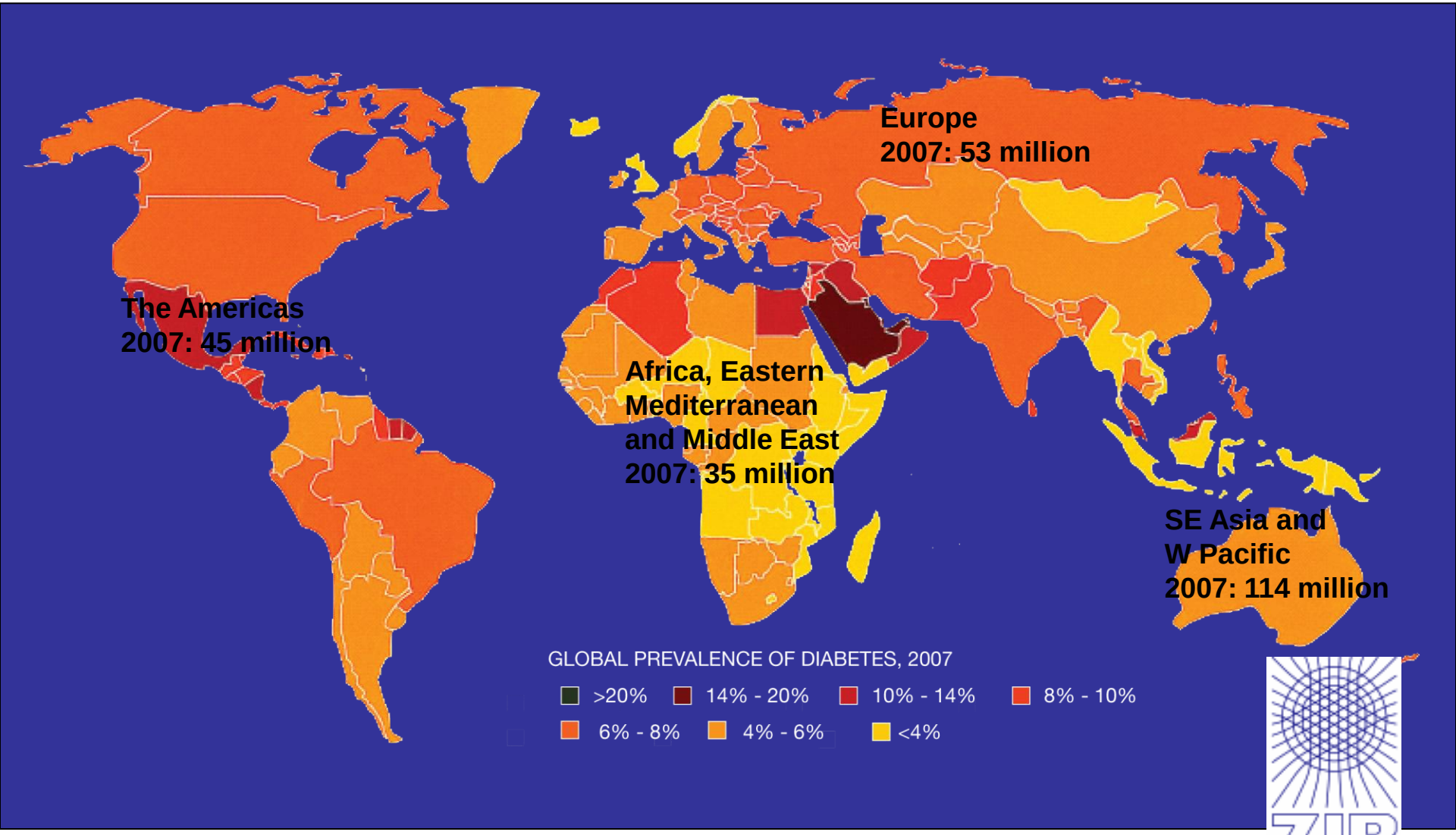
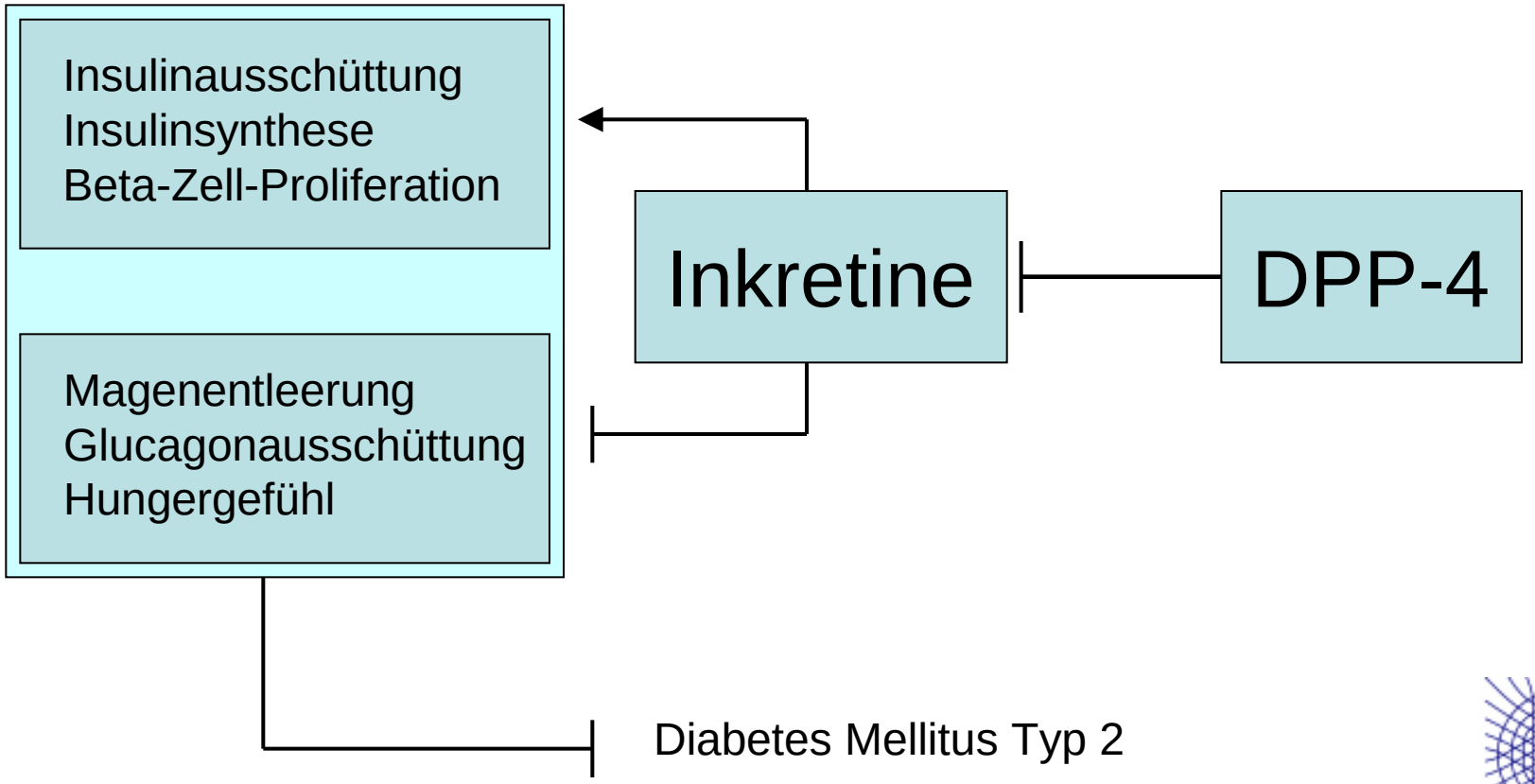
5. Juni 2010
Berlin
LNdW 2010

Beispiel: Diabetes Mellitus II

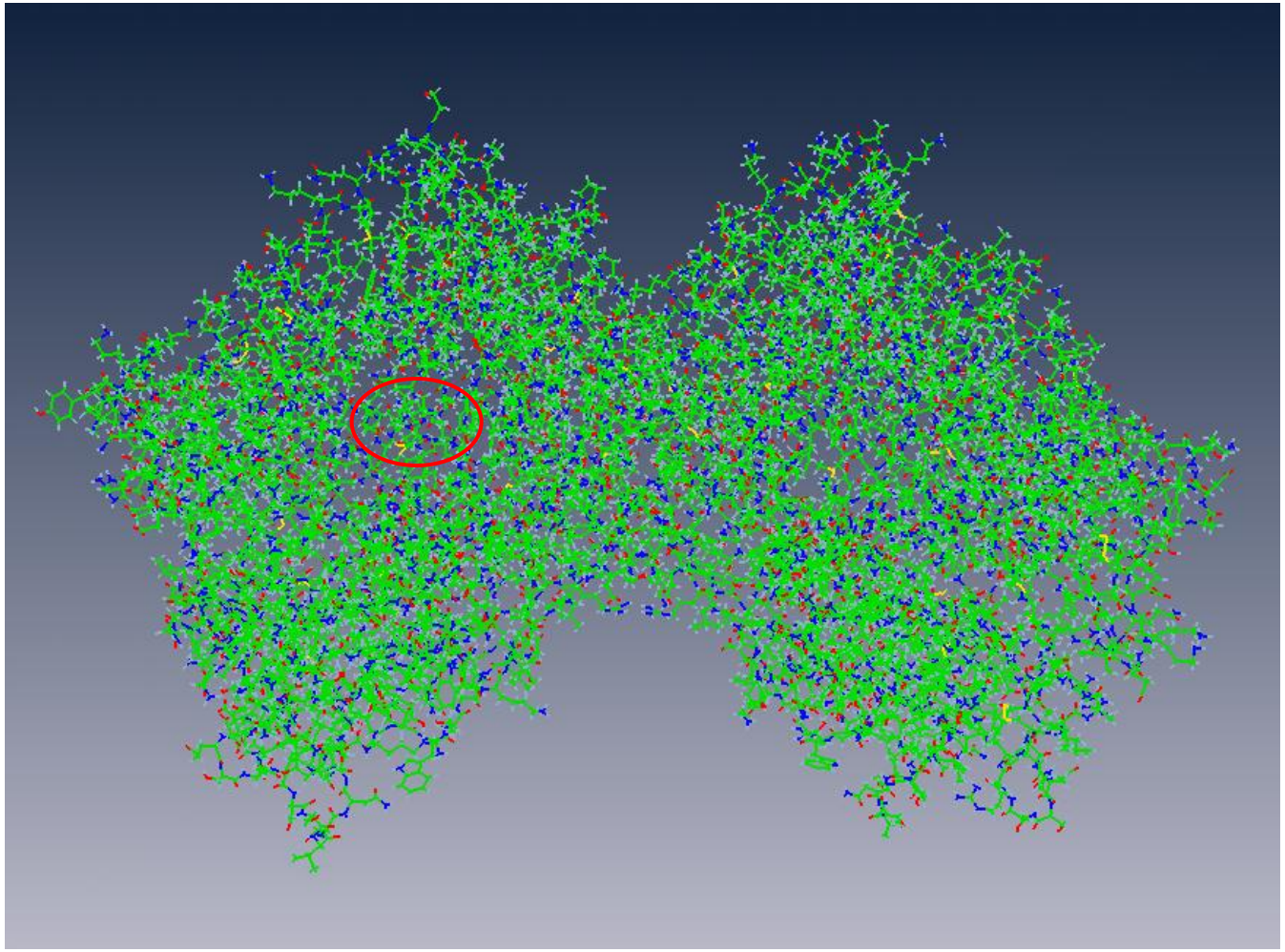


Quelle: International Diabetes Federation. *Diabetes Atlas.* 2nd ed. 2003; 3rd ed. 2006.

Therapieansatz



DPP-IV



AmiraMol: Johannes Schmidt-Ehrenberg, D. Baum, H.-Ch. Hege, 2002

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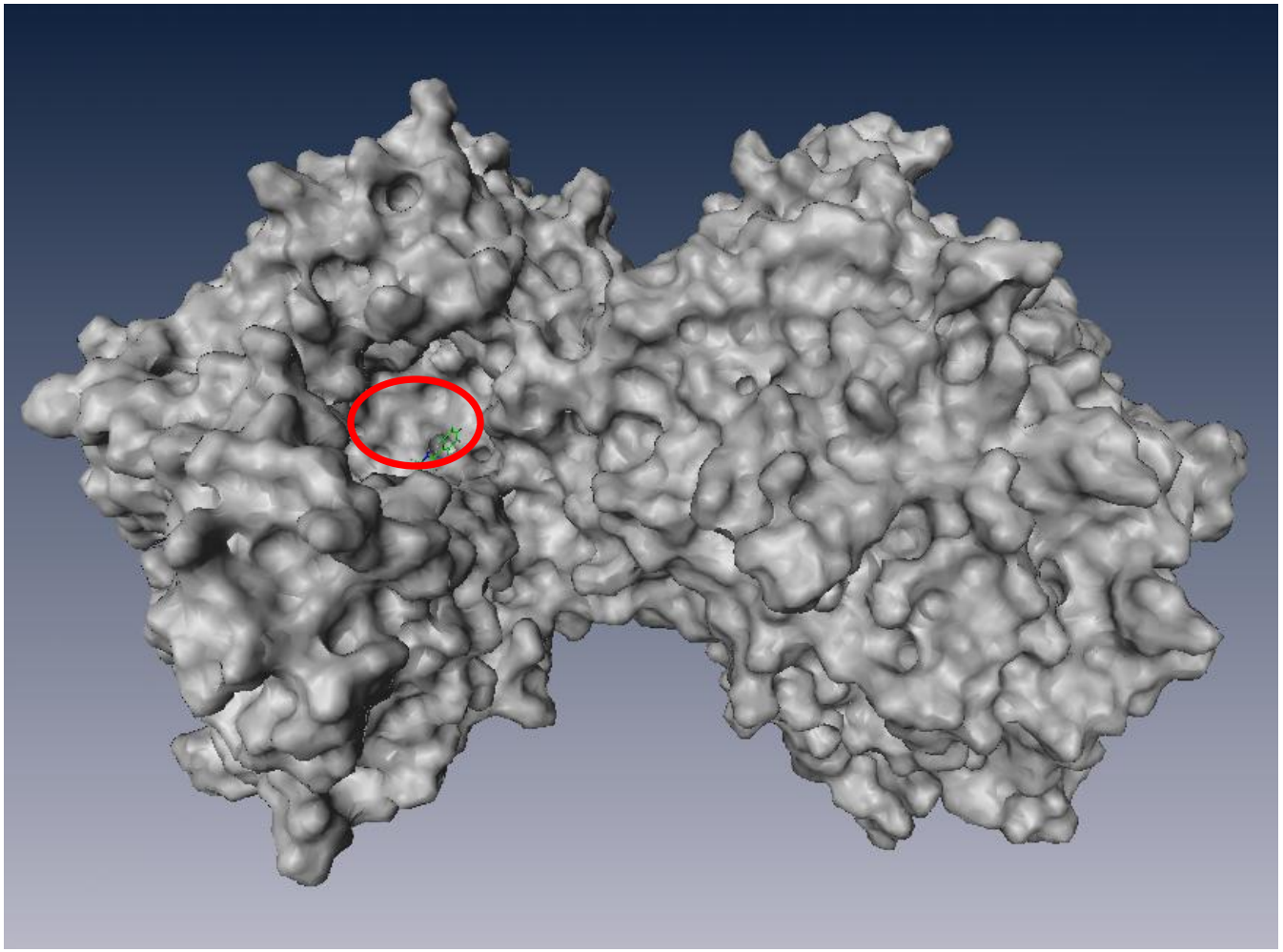
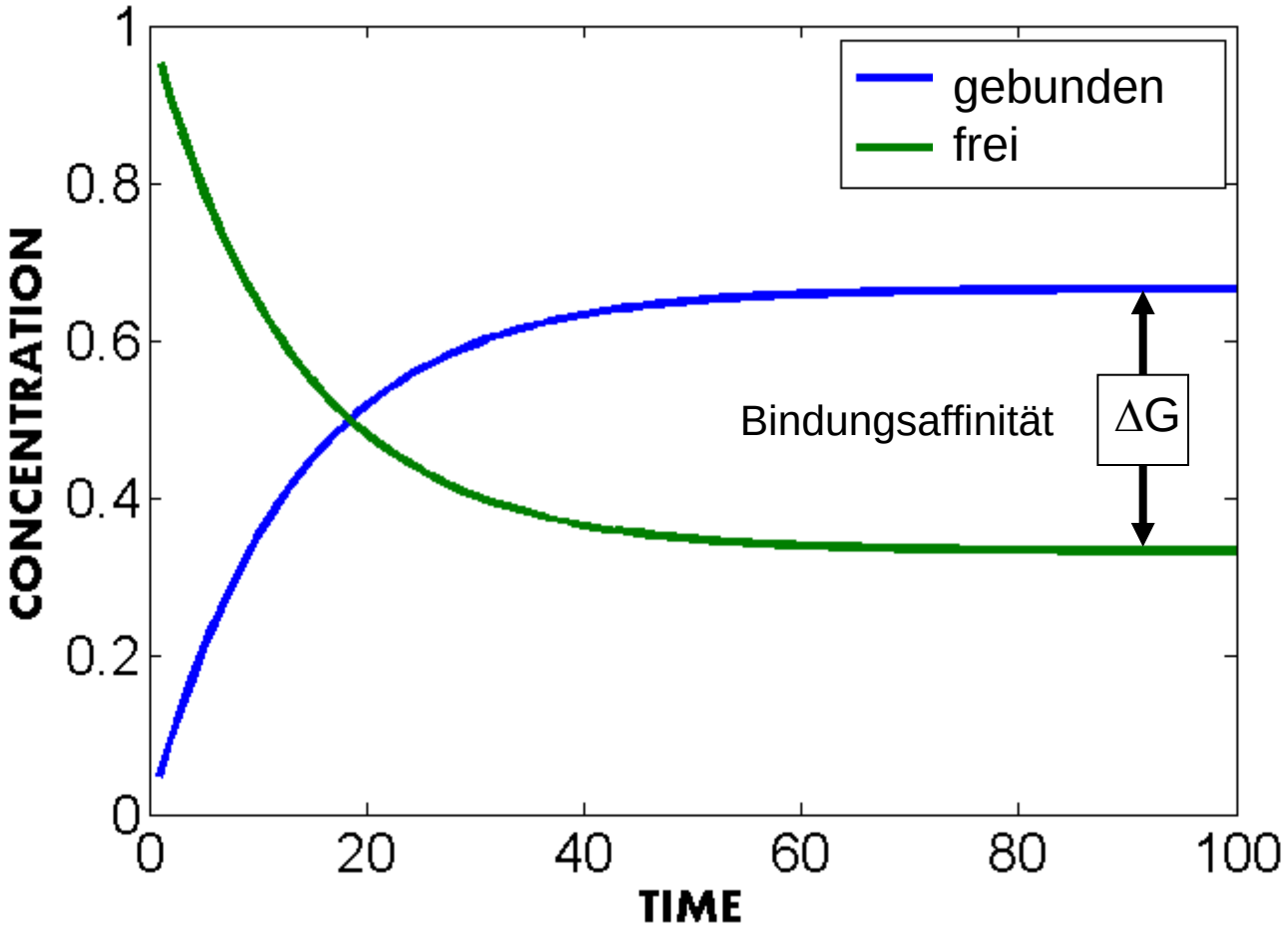
DPP-IV

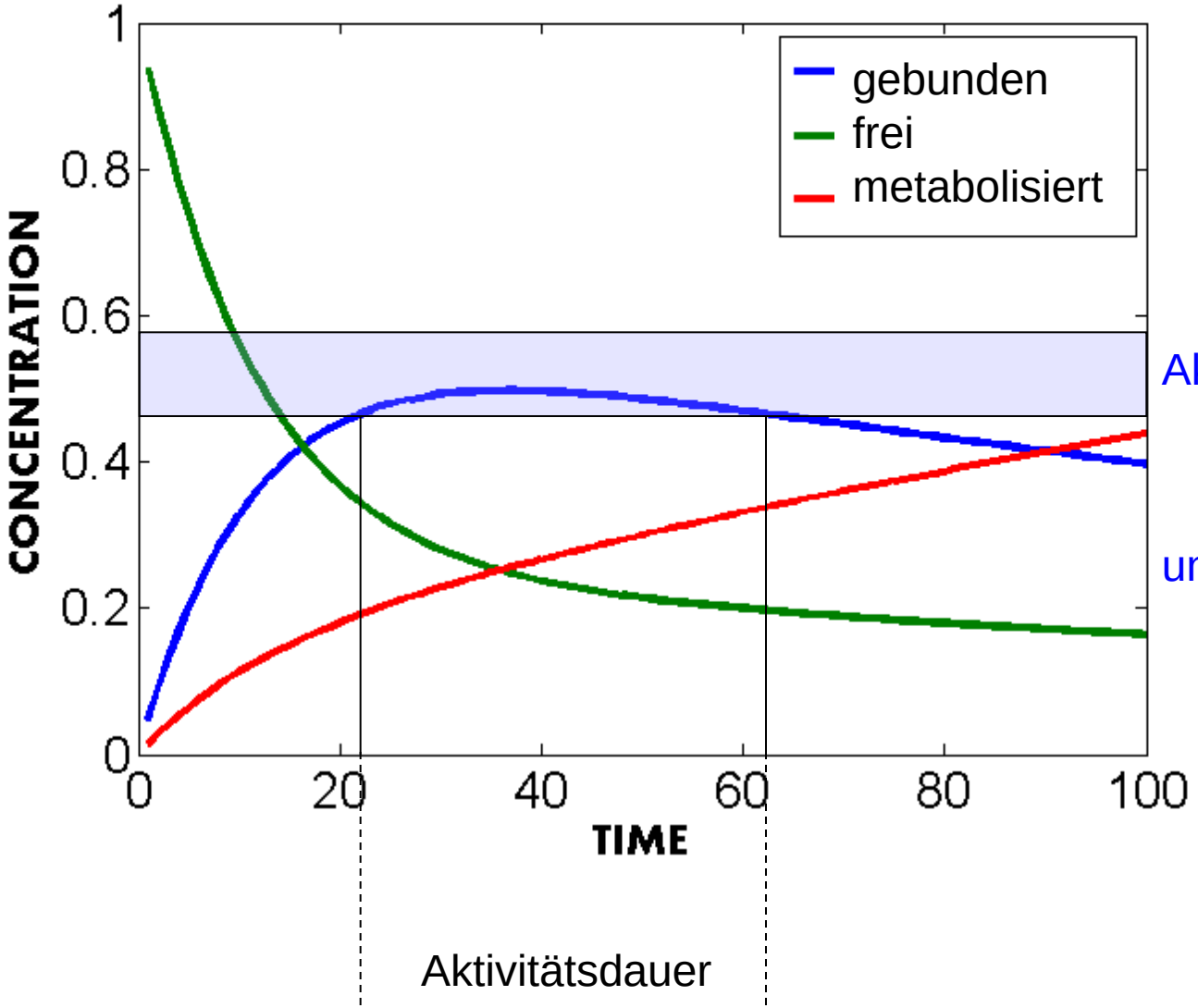


Suche nach dem Schlüssel…

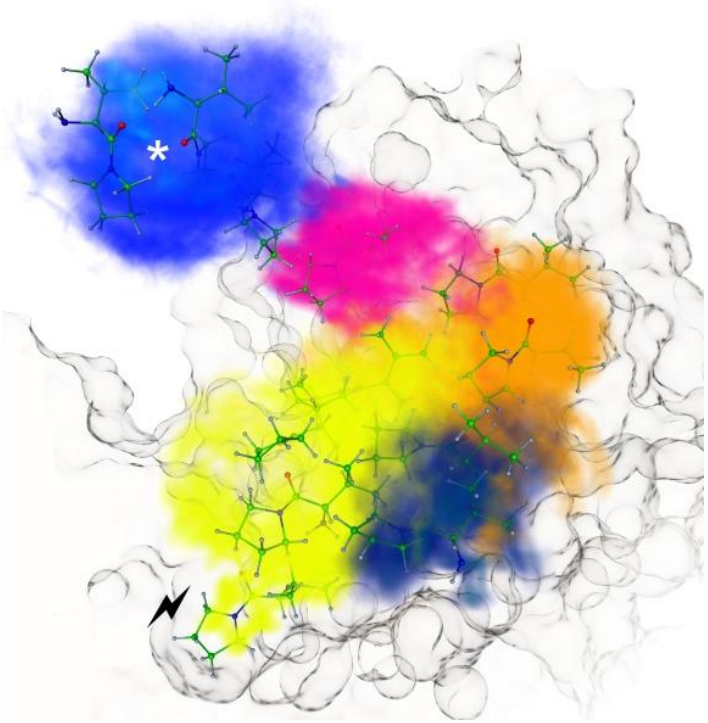
Bindungsaffinität

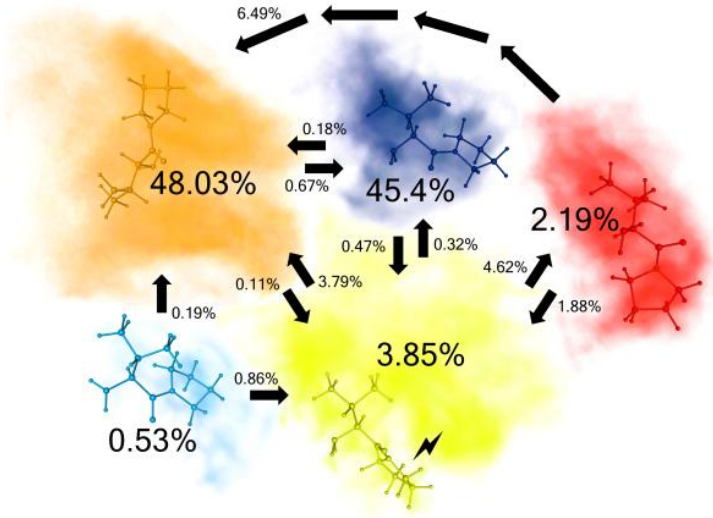


Simulation von Bindungsprozessen



Bindungskinetik





A. Bujotzek, 2008

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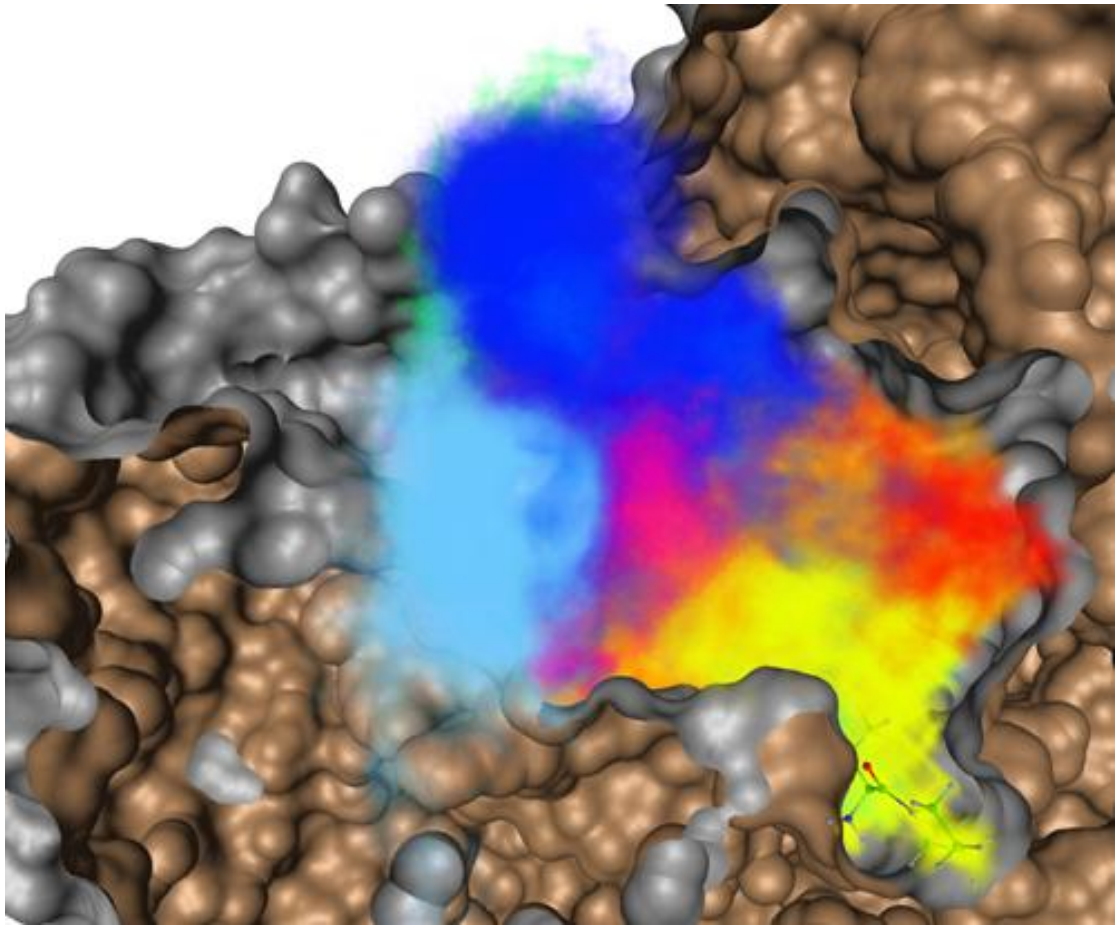
Simulationsansatz



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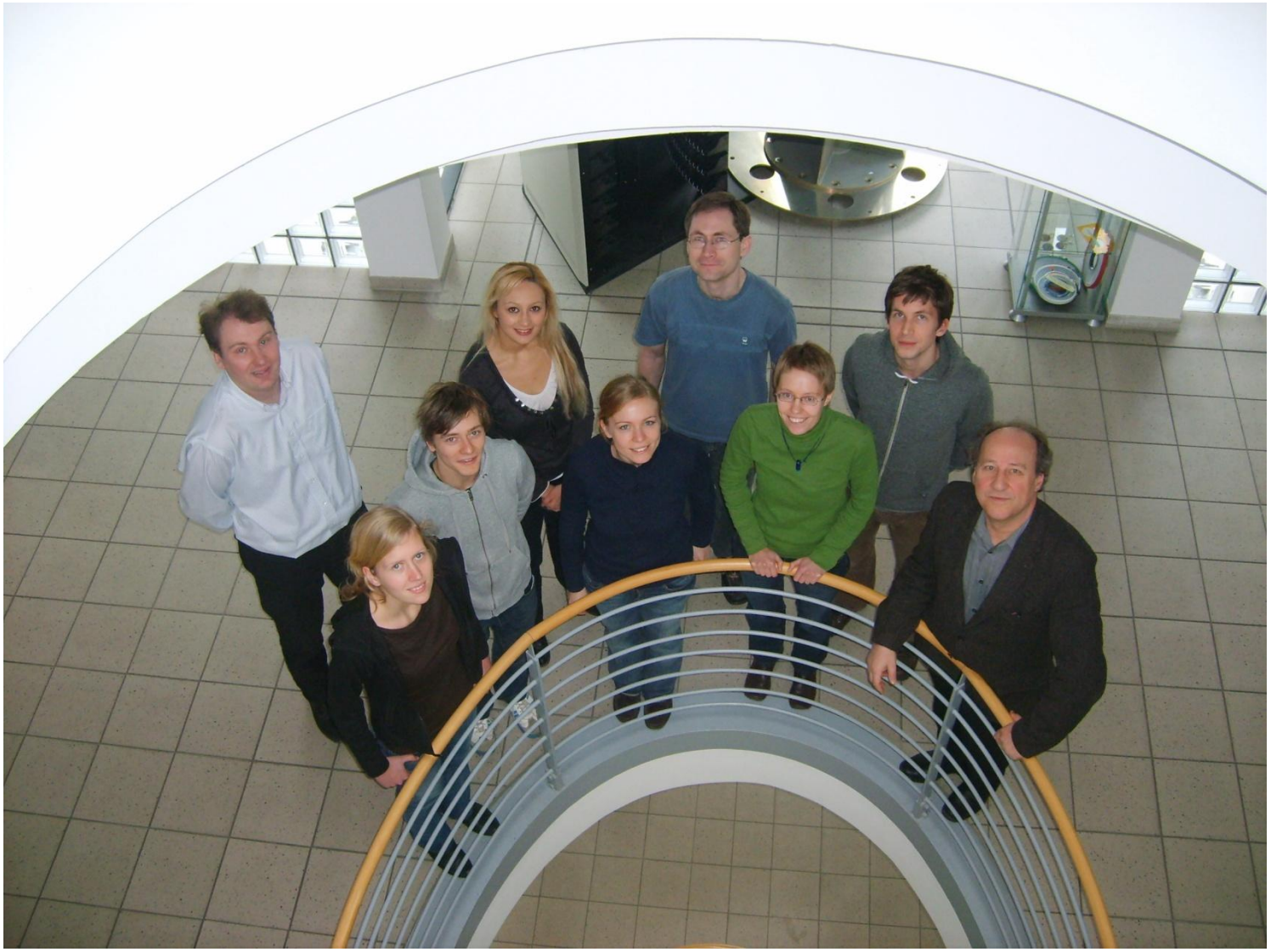
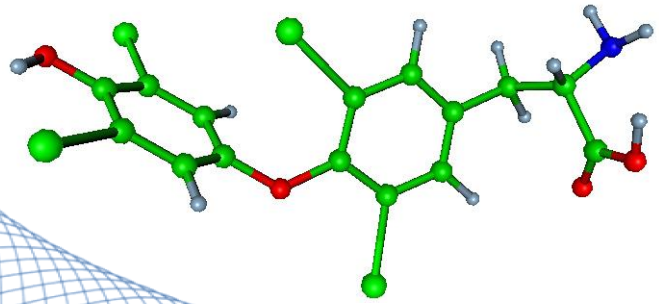
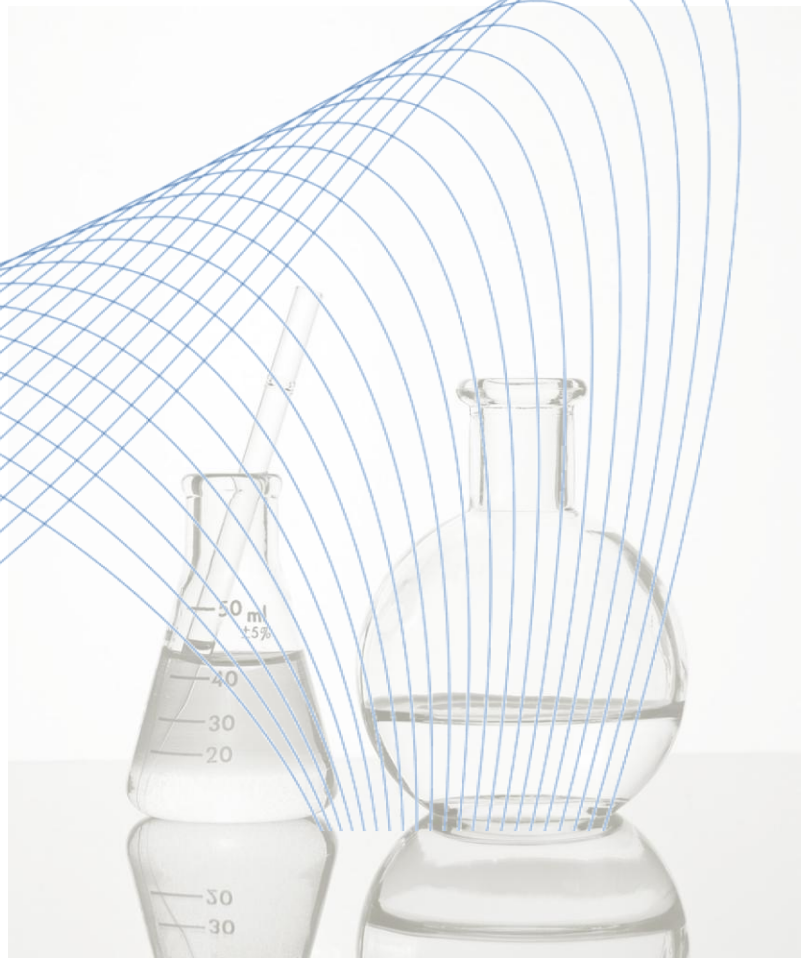
Arbeitsgruppe am ZIB



http://molConcept.com





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Ausgewählte Publikationen

• **P. Deuflhard, M. Weber:** Robust Perron Cluster Analysis in Conformation Dynamics, *Lin. Alg. App.* 2005, 398c, Special issue on matrices and mathematical biology, 161-184.

• **M. Weber, S. Kube [Röblitz]:** Robust Perron Cluster Analysis for Various Applications in Computational Life Science, in: *Computational Life Sciences: First International Symposium, CompLife 2005, September 25-27, (Ed. M.R. Berthold et al.) Springer, Heidelberg* 2005, 57-66.

• **M. Weber:** Meshless Methods in Conformation Dynamics. Doctoral Thesis, FU Berlin, 2006.

• **A. Guerler, S. Moll, M. Weber, H. Meyer, F. Cordes:** Selection and flexible optimization of binding modes from conformation ensembles. *Biosystems* 92(1):42-48, April 2008.

• **M. Weber, S. Kube [Röblitz]:** Preserving the Markov Property of Reduced Reversible Markov Chains. *Numerical Analysis and Applied Mathematics*, Int. Conf. on Num. Analy. and Appl. Math. 2008, AIP Conference Proceedings, Kos, 1048:593-596, September 2008.

• **S. Röblitz:** Statistical Error Estimation and Grid-free Hierarchical Refinement in Conformation Dynamics. Doctoral Thesis, FU Berlin, 2008.

• **A. Bujotzek, M. Weber:** Efficient Simulation of Ligand-Receptor Binding Processes Using the Conformation Dynamics Approach. Accepted for: *Journal of Bioinformatics and Computational Biology*, April 2009.

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