

REFERENCES AND NOTES

CHAPTER 1

- [1.1] Lodish, M.; Berk, A.; Matsudaira, P.; Kaiser, C. A.; Krieger, M.; Scott, M. P.; Zipursky, S. L.; Darnel, J. (2004) *Molecular cell biology*. (Fifth edn.). W. H. Freeman & Co, New York.
- [1.2] Metzler, D. E. (2001) *Biochemistry: The chemical reaction of living cell*. (2nd edn.). Academic Press. San Diego.
- [1.3] Nelson, D. L.; Cox, M. M. (2004) *Lehninger Principles of biochemistry*. (Fourth edn.). W. H. Freeman & Co, New York.
- [1.4] Stryer, L. (2002) *Biochemistry*. (Fifth edn.). W. H. Freeman & Co, New York.
- [1.5] Garret, R. H.; Grisham, C. M. (1999) *Biochemistry*. (2nd edn.). Thomson Learning, Thomson Corporation, Stamford.
- [1.6] Felix, F., Ed. (1982) *Water a comprehensive treatise*. Plenum Press, New York.
- [1.7] Käiväräinen, A. I. (1985) *Solvent dependent flexibility of proteins and principles of their function*. D. Reidel Publishing Company, Dordrecht.
- [1.8] Arunan, E., *Current Sci.* **2007**, 92, 17-18.
<http://www.iupac.org/projects/2004/2004-026-2-100.html>
- [1.9] Pauling, L. (1939) *The nature of the chemical bond*. Cornell University Press, Ithaca, New York.
- [1.10] Pimentel, G. C.; McClellan, A. L. (1960) *The hydrogen bond*. Freeman, San Francisco.
- [1.11] Jeffrey, G. A.; Saenger, W. (1991) *Hydrogen bonding in biological structures*. Springer-Verlag, Berlin.
- [1.12] Jeffrey, G. A. (1997) *An introduction to hydrogen bonding*. Oxford University Press, New York.
- [1.13] Scheiner, S. (1997) *Hydrogen bonding. A theoretical perspective*. Oxford University Press, Oxford.

- [1.14] Desiraju G. R.; Steiner T. (1999) *The weak hydrogen bond in structural chemistry and biology*. Oxford University Press, Oxford.
- [1.15] Nishio, M.; Hirota, M.; Umezawa, Y. (1998) *The CH/π interaction Evidence, Nature, and Consequences*. Wiley-VCH, Inc, New York.
- [1.16] Gerlt, J. A.; Gassman, P. G., *J. Am. Chem. Soc.* **1993**, 115, 11552-11568.
- [1.17] Cleland, W. W.; Kreevoy, M. M., *Science* **1994**, 264, 1887-1890.
- [1.18] Frey, P. A.; Whitt, S. A.; Tobin, J. B., *Science* **1994**, 264, 1927-1930.
- [1.19] Perrin, C. L.; Nielson, J. B., *Annu. Rev. Phys. Chem.* **1997**, 48, 511-544.
- [1.20] Cleland, W. W.; Frey, P. A.; Gerlt, J. A., *J. Biol. Chem.* **1998**, 25529-25532.
- [1.21] Viragh, C.; Harris, T. K.; Reddy, P. M.; Massiah, M. A.; Mildvan, A. S.; Kovach, I. M., *Biochemistry* **2000**, 39, 16200-16205.
- [1.22] Kim, K. S.; Oh, K. S.; Lee, J. Y., *Proc. Natl. Acad. Sci. USA* **2000**, 97, 6373-6378.
- [1.23] Frey, P. A., *Magn. Reson. Chem.* **2001**, 39, S190-S198.
- [1.24] Massiah, M. A.; Viragh, C.; Reddy, P. M.; Kovach, I. M.; Johnson, J.; Rosenberry, T. L.; Mildvan, A. S., *Biochemistry* **2001**, 40, 5682-5690.
- [1.25] Kim, K. S.; Kim, D.; Lee, J. Y.; Tarakeshwar, P.; Oh, K. S., *Biochemistry* **2002**, 41, 5300-5306.
- [1.26] Dean, N. E.; Miller, J. E.; Halkides, C. J.; Messina, M., *J. Chem. Inf. Model.* **2003**, 43, 554-559.
- [1.27] Poi, M. J.; Tomaszewski, J. W.; Yuan, C.; Dunlap, C. A.; Andersen, N. H.; Gelb, M. H.; Tsai, M. D., *J. Mol. Biol.* **2003**, 329, 997-1009.
- [1.28] Schutz, C. N.; Warshel, A., *Proteins* **2004**, 55, 711-723.
- [1.29] Shokhen, M.; Albeck, A., *Proteins* **2004**, 54, 468-477.
- [1.30] Anderson, S.; Crosson, S.; Moffat, K., *Acta. Crystallogr. Sect. D* **2004**, 60, 1008-1016.
- [1.31] Zhao, L.; Liao, H.; Tsai, M. D., *J. Biol. Chem.* **2004**, 279, 31995-32000.
- [1.32] Wohlfahrt, G., *Proteins* **2005**, 58, 396-406.
- [1.33] Kraut, D. A.; Sigala, P. A.; Pybus, B.; Liu, C. W.; Ringe, D.; Petsko, G. A.; Herschlag, D., *PLOS Biology* **2006**, 4, 501-519.

References and Notes

- [1.34] Das, A.; Prashar, V.; Mahale, S; Serre, L.; Ferrer, J.-L.; Hosur, M. V., *Proc. Natl. Acad. Sci. USA* **2006**, 103, 18464-18469.
- [1.35] Baker, E. N.; Hubbard, R. E., *Progr. Biophys. Mol. Biol.* **1984**, 44, 97-179.
- [1.36] Sutor, D. J., *Journal of the Chemical Society* **1963**, 1105-1110.
- [1.37] Shefter, E.; Trueblood, K. N., *Acta Crystallographica* **1965**, 18, 1067-1077.
- [1.38] Sundaralingam, M., *Acta Crystallographica* **1966**, 21, 495-505.
- [1.39] Ramachandran, G. N.; Sasisekharan, V., *Biochim. Biophys. Acta.* **1965**, 109, 314-316.
- [1.40] Ramachandran, G. N.; Sasisekharan, V.; Ramakrishnan, C. *Biochim. Biophys. Acta.* **1966**, 112, 168-170.
- [1.41] Derewenda, Z. S.; Lee, L.; Derewenda, U., *J. Mol. Biol.* **1995**, 252, 248-262.
- [1.42] Bella, J.; Berman, H., *J. Mol. Biol.* **1996**, 264, 734-42.
- [1.43] Scheiner, S.; Gu, Y.; Kar, T., *Journal of Molecular Structure (Theochem)* **2000**, 500, 441-452.
- [1.44] Aravinda, S.; Shamala, N.; Pramanik, A.; Das, C.; Balaram, P., *Biochem. Biophys. Res. Commun.* **2000**, 273, 933-936.
- [1.45] Thakur, A. K.; Kishore, R., *Biopolymers* **2000**, 53, 447-454.
- [1.46] Senes A.; Belandia, I. U.; Engelman, D. M., *Proc. Natl. Acad. Sci. USA* **2001**, 98, 9056-9061.
- [1.47] Scheiner, S.; Kar, T.; Gu, Y., *J. Biol. Chem.* **2001**, 276, 9832-9837.
- [1.48] Weiss, M. S.; Brandl, M.; Sühnel, J.; Pal, D.; Hilgenfeld, R., *Trends Biochem. Sci.* **2001**, 26, 521-523.
- [1.49] Adams, A.; Guss, J. M.; Denny, W. A.; Wakelin, L. P., *Nucleic Acids Res.* **2002**, 30, 719-725.
- [1.50] Chamberlain, A. K.; Bowie, J. U., *J. Mol. Biol.* **2002**, 322, 497-503.
- [1.51] Jiang, L.; Lai, L., *J. Biol. Chem.* **2002**, 277, 37732-37740.
- [1.52] Babu, M. M.; Singh, S. K.; Balaram, P., *J. Mol. Biol.* **2002**, 322, 871-880.
- [1.53] Aravinda, S.; Shamala, N.; Bandyopadhyay, A.; Balaram, P., *J. Am. Chem. Soc.* **2003**, 125, 15065-15075.
- [1.54] Bhattacharyya, R.; Chakrabarti, P., *J. Mol. Biol.* **2003**, 331, 925-940.

- [1.55] Palsdottir, H.; Lojero, C. G.; Trumpower, B. L.; Hunte, C., *J. Biol. Chem.* **2003**, 278, 31303-31311.
- [1.56] Singh, S. K.; Babu, M. M.; Balaram, P., *Proteins* **2003**, 51, 167-171.
- [1.57] Wieczorek, R.; Dannenberg, J. J., *J. Am. Chem. Soc.* **2003**, 125, 8124-8129.
- [1.58] Braun, P.; Vegh, A. P.; von Jan, M.; Strohmam, B.; Hunter, C. N.; Robert, B.; Scheer, H. *Biochim. Biophys. Acta.* **2003**, 1607, 19-26.
- [1.59] Kang, B. S.; Devedjiev, Y.; Derewenda, U.; Derewenda, Z. S., *J. Mol. Biol.* **2004**, 338, 483-493.
- [1.60] Scheiner, S., *J. Phys. Chem. B Condens. Matter Mater. Surf. Interfaces Biophys.* **2006**, 110, 18670-18679.
- [1.61] Karle, I. L.; Venkateshwarlu, P.; Ranganathan, S., *Biopolymers* **2006**, 84, 502-507.
- [1.62] Thakur, A. K.; Kishore, R., *Biopolymers* **2006**, 81, 440-449.
- [1.63] Loll, B.; Raszewski, G.; Saenger, W.; Biesiadka, J., *J. Mol. Biol.* **2003**, 328, 737-747.
- [1.64] Yohannan, S.; Faham, S.; Yang, D.; Grosfeld, D.; Chamberlain, A. K.; Bowie, J. U., *J. Am. Chem. Soc.* **2004**, 126, 2284-2285.
- [1.65] Brandl, M.; Meyer, M.; Sühnel, J., *J. Biomol. Struct. Dyn.* **2001**, 18, 545-555.
- [1.66] Treger, M.; Westhof, E., *J. Mol. Recognit.* **2001**, 14, 199-214.
- [1.67] Swaminathan, C. P.; Gupta, A.; Surolia, N.; Surolia, A., *J. Biol. Chem.* **2000**, 275, 28483-28487.
- [1.68] Oku, K.; Watanabe, H.; Kubota, M.; Fukuda, S.; Kurimoto, M.; Tsujisaka, Y.; Komori, M.; Inoue, Y.; Sakurai, M., *J. Am. Chem. Soc.* **2003**, 125, 12739-12748.
- [1.69] Rajsekhar, G.; Rao, C. P.; Guionneau, P., *Carbohydr. Res.* **2003**, 338, 801-805.
- [1.70] Baddeley, T. C.; Davidson, I. G.; Glidewell, C.; Low, J. N.; Skakle, J. M.; Wardell, J. L., *Acta. Crystallogr. Sect. B* **2004**, 60, 461-471.
- [1.71] Sujatha, M. S.; Sasidhar, Y. U.; Balaji, P. V., *Biochemistry* **2005**, 44, 8554-8562.

References and Notes

- [1.72] Yates, J. R.; Pham, T. N.; Pickard, C. J.; Mauri, F.; Amado, A. M.; Gil, A. M.; Brown, S. P., *J. Am. Chem. Soc.* **2005**, 127, 10216-10220.
- [1.73] Pandit, S. A.; Bostick, D.; Berkowitz, M. L., *Biophys. J.* **2004**, 86, 1345-1356.
- [1.74] Scheiner, S.; Kar, T., *J. Phys. Chem. B. Condens. Matter. Mater. Surf. Interfaces Biophys.* **2005**, 109, 3681-3689.
- [1.75] Steiner, T.; Koellner, G., *J. Mol. Biol.* **2001**, 305, 535-557.
- [1.76] Brandl, M.; Weiss, M. S.; Jabs, A.; Sühnel, J.; Hilgenfeld, R., *J. Mol. Biol.* **2001**, 307, 357-377.
- [1.77] Scheiner, S.; Kar, T.; Pattanayak, J., *J. Am. Chem. Soc.* **2002**, 124, 13257-13264.
- [1.78] Harigai, M.; Kataoka, M.; Imamoto, Y., *J. Am. Chem. Soc.* **2006**, 128, 10646-10647.
- [1.79] Saraogi, I.; Vijay, V. G.; Das, S.; Sekar, K.; Guru Row T. N., *Crystal Engineering* **2003**, 6, 69-77.
- [1.80] Dougherty, D. D., *Science* **1996**, 271, 163-168.
- [1.81] Ma, J. C.; Dougherty, D. D., *Chem. Rev.* **1997**, 97, 1303-1324.
- [1.82] Zacharias, N.; Dougherty, D. A., *Trends Pharmacol. Sci.* **2002**, 23, 281-287.
- [1.83] Prajapati, R. S.; Sirajuddin, M.; Durani, V.; Sreeramulu, S.; Varadarajan, R., *Biochemistry* **2006**, 45, 15000-15010.
- [1.84] Meyer, E. A.; Castellano, R. K.; Diederich, F., *Angew. Chem. Int. Ed.* **2003**, 42, 1210-1250.
- [1.85] Ouvrard, C., Le Questel, J. -Y.; Berthelot, M.; Laurence, C., *Acta. Crystgra. Sect. B* **2003**, 59, 512-526.
- [1.86] Auffinger, P.; Hays, F. A.; Westhof, E.; Ho, P. S., *Proc. Natl. Acad. Sci. USA* **2004**, 101, 16789-16794.
- [1.87] Kovács, A.; Varga, Z., *Coordination Chem. Reviews* **2006**, 250, 710-727.
- [1.88] Guerra, C. F.; Bickelhaupt, F. M.; Baerends, E. J., *Chemphyschem.* **2004**, 5, 481-487.
- [1.89] Adman, E.; Watenpaugh, K. D.; Jensen, L. H., *Proc. Natl. Acad. Sci. USA* **1975**, 72, 4854-4858.

- [1.90] Ippolito, J. A.; Alexander, R. S.; Christianson, D. W., *J. Mol. Biol.* **1990**, 215, 457-471.
- [1.91] Gregoret, L. M.; Rader, S. D.; Fletterick, R. J.; Cohen, F. E., *Proteins* **1991**, 9, 99-107.
- [1.92] Rajagopal, S.; Vishveshwara, S., *FEBS J.* **2005**, 272, 1819-1832.
- [1.93] Rossmann, M. G.; Arnold, E., Eds. (**2001**) *International tables for crystallography Vol F. Crystallography of biological macromolecules*. Kluwer Academic Publishers, Dordrecht.
- [1.94] Hamilton, W. C.; Ibers, J. A. (**1968**) *Hydrogen bonding in solids*. W. A. Benjamin, New York.
- [1.95] Jeffrey, G. A. (**1992**) Accurate crystal structure analysis by neutron diffraction. In *Accurate molecular structures*. Domenicano, A.; Hargittai, I. Eds., Oxford University Press, Oxford, pp. 270-298.
- [1.96] Gutberlet, T.; Heinemann, U.; Steiner, M., *Acta. Crystallogra. Sect. D* **2000**, 57, 349-354.
- [1.97] Berstein, F., Koetzle, T., Williams, G., Meyer, E., Brice, M., Rodgers, J., Kennard, O., Shimanouchi, T.; Tasumi M., *J. Mol. Biol.* **1977**, 112, 535-542.
- [1.98] Allen, F. H.; Kennard, O., *Chem. Des. Autom. News* **1993**, 8, 31-37.
<http://www.ccdc.cam.ac.uk/prods/csd/csd.html>
- [1.99] Berman, H. M.; Westbrook, J.; Feng, Z.; Gilliland, G.; Bhat, T. N.; Weissig, H.; Shindyalov, I. N.; Bourne, P. E., *Nucleic Acid Res.* **2000**, 28, 235-242.
<http://www.rcsb.org/pdb>
- [1.100] Murzin, A. G.; Brenner, S. E.; Hubbard, T.; Chothia, C., *J. Mol. Biol.* **1995**, 247, 536-540.
<http://scop.mrc-lmb.cam.ac.uk/scop>
- [1.101] Orengo, C. A.; Michie, A. D.; Jones, S.; Jones, D. T.; Swindells, M. B.; Thornton, J. M., *Structure* **1997**, 5, 1093-1108.
<http://www.cathdb.info/latest/index.html>
- [1.102] Laskowski, R. A., *Nucleic Acids Res.* **2001**, 29, 221-222.
<http://www.ebi.ac.uk/thornton-srv/databases/pdbsum>

References and Notes

- [1.103] Chakrabarti, P.; Pal, D., *Progr. Biophys. Mol. Biol.* **2001**, 76, 1-102.
- [1.104] Porter, C. T.; Bartlett, G. J.; Thornton, J. M., *Nucleic Acid Res.* **2004**, 32, D129-D133.
- [1.105] McDonald, I. K.; Thornton, J. M., *J. Mol. Biol.* **1994**, 238, 777-793.
- [1.106] Lindauer, K.; Bendic, C.; Sühnel, J., *Comput. Appl. Biosci.* **1996**, 12, 281-289.
- [1.107] Word, J. M.; Lovell, S. C.; Richardson, J. S.; Richardson, D. C., *J. Mol. Biol.* **1999**, 285, 1735-1747.
- [1.108] Collaborative computational project, number 4., *Acta. Crystallogra. Sect. D* **1994**, 50, 760-763.
- [1.109] Sobolev, V.; Sorokine, A.; Prilusky, J.; Abola, E. E.; Edelman, M., *Bioinformatics* **1999**, 15, 327-332.
- [1.110] Babu, M. M., *Nucleic Acid Res.* **2003**, 31, 3345-3348.
- [1.111] Tiwari, A.; Panigrahi, S. K.; Desiraju, G. R., *HBAT: A complete package for analysing strong and weak hydrogen bonds in macromolecular crystal structures. (communicated)*
- [1.112] Glusker, J. P.; Lewis, M.; Rossi, M. (**1994**) *Crystal structure analysis for chemists and biologists*. VCH, New York.
- [1.113] Böhm, H. -J.; Klebe, G., *Angew. Chem. Int. Ed.* **1996**, 35, 2588-2614.
- [1.114] Gohlke, H.; Klebe, G., *Angew. Chem. Int. Ed.* **2002**, 41, 2644-2676.
- [1.115] Klaholz, B.; Moras, D., *Structure* **2002**, 10, 1197-1204.
- [1.116] Pierce, A. C.; Sandretto, K. L.; Bemis, G. W., *Proteins* **2002**, 49, 567-576.
- [1.117] Pierce, A. C.; ter Haar, E.; Binch, H. M.; Kay, D. P.; Patel, S. R.; Li, P., *J. Med. Chem.* **2005**, 48, 1278-1281.
- [1.118] Denessiouk, K. A.; Johnson, M. S., *J. Mol. Biol.* **2003**, 333, 1025-1043.
- [1.119] Sarkhel, S.; Desiraju, G. R., *Proteins* **2004**, 54, 247-259.
- [1.120] Cashin, A. L.; Petersson, E. J.; Lester, H. A.; Dougherty, D. A., *J. Am. Chem. Soc.* **2005**, 127, 350-356.
- [1.121] Aparna, V.; Rambabu, G.; Panigrahi, S. K.; Sarma, J. A. R. P.; Desiraju, G. R., *J. Chem. Inf. Model.* **2005**, 45, 725-738.

CHAPTER 2

- [2.1] Berman, H. M.; Westbrook, J.; Feng, Z.; Gilliland, G.; Bhat, T. N.; Weissig, H.; Shindyalov, I. N.; Bourne, P. E., *Nucleic Acid Res.* **2000**, 28, 235-242.
<http://www.rcsb.org/pdb>
- [2.2] Desiraju, G. R.; Steiner T. (1999) *The weak hydrogen bond in structural chemistry and biology*. Oxford University Press, Oxford.
- [2.3] Steiner, T.; Koellner, G., *J. Mol. Biol.* **2001**, 305, 535-557.
- [2.4] Xantheas, S. S., *Chem. Phy.* **2000**, 258, 225-231.
- [2.5] Auffinger, P.; Hays, F. A.; Westhof, E.; Ho, P. S., *Proc. Natl. Acad. Sci. USA* **2004**, 101, 16789-16794.
- [2.6] McDonald, I. K.; Thornton, J. M., *J. Mol. Biol.* **1994**, 238, 777-793.
- [2.7] Lindauer, K.; Bendic, C.; Sühnel, J., *Comput. Appl. Biosci.* **1996**, 12, 281-289.
- [2.8] Collaborative computational project, number 4. *Acta. Crystallogra. Sect. D* **1994**, 50, 760-763.
- [2.9] Sobolev, V.; Sorokine, A.; Prilusky, J.; Abola, E. E.; Edelman, M., *Bioinformatics* **1999**, 15, 327-332.
- [2.10] Babu, M. M., *Nucleic Acid Res.* **2003**, 31, 3345-3348.
- [2.11] PERL (www.perl.org)/TK(www.tcl.tk).
- [2.12] Graphviz - Graph Visualization Software: www.graphviz.org.
- [2.13] Brandl, M.; Weiss, M. S.; Jabs, A.; Sühnel, J.; Hilgenfeld, R., *J. Mol. Biol.* **2001**, 307, 357-377.
- [2.14] Koellner, G.; Kryger, G.; Millard, C. B.; Silman, I.; Sussman, J. L.; Steiner T., *J. Mol. Biol.* **2000**, 296, 713-735.
- [2.15] Klaholz, B.; Moras, D., *Structure* **2002**, 10, 1197-1204.
- [2.16] Sarkhel, S.; Desiraju, G. R., *Proteins* **2004**, 54, 247-259.

CHAPTER 3

- [3.1] Glusker, J. P. (1998) Directional aspects of intermolecular interactions. In *Topics in current chemistry: Design of organic solids*. Weber, E., Ed., Springer-Verlag, Berlin and Heidelberg, pp. 1-56.
- [3.2] Kortemme, T.; Morozov, A. V.; Baker, D., *J. Mol. Biol.* **2003**, 326, 1239-1259.
- [3.3] Allocati, N.; Masulli, M.; Pietracupa, M.; Federici, L.; Di Ilio, C., *Biochem. J.* **2006**, 394, 11-17.
- [3.4] Shokhen, M.; Albeck, A., *Proteins* **2004**, 54, 468-477.
- [3.5] Bledsoe, R. K.; Madauss, K. P.; Holt, J. A.; Apolito, C. J.; Lambert, M. H.; Pearce, K. H.; Stanley, T. B.; Stewart, E. L.; Trump, R. P.; Willson, T. M.; Williams, S. P., *J. Biol. Chem.* **2005**, 280, 31283-31293.
- [3.6] Baker, E. N.; Hubbard, R. E., *Progr. Biophys. Mol. Biol.* **1984**, 44, 97-179.
- [3.7] Jeffrey, G. A.; Saenger, W. (1991) *Hydrogen bonding in biological structures*. Springer-Verlag, Berlin.
- [3.8] Glusker, J. P., *Acta. Crystallogra. Sect. D* **1995**, 51, 418-427.
- [3.9] Wahl, M. C.; Rao, S. T.; Sundaralingam, M., *Nat. Struct. Biol.* **1996**, 3, 24-31.
- [3.10] Derewenda, Z. S.; Derewenda, U.; Kobos, P. M., *J. Mol. Biol.* **1994**, 241, 83-93.
- [3.11] Fabiola, G. F.; Krishnaswamy, S.; Nagarajan, V.; Pattabhi, V., *Acta. Crystallogra. Sect. D* **1997**, 53, 316-320.
- [3.12] Thomas, A.; Benhabiles, N.; Meurisse, R.; Ngwabije, R.; Brasseur, R., *Proteins* **2001**, 43, 37-44.
- [3.13] Steiner, T.; Koellner, G., *J. Mol. Biol.* **2001**, 305, 535-557.
- [3.14] Scheiner, S.; Kar, T.; Gu, Y., *J. Biol. Chem.* **2001**, 276, 9832-9837.
- [3.15] Jiang, L.; Lai, L., *J. Biol. Chem.* **2002**, 277, 37732-37740.
- [3.16] Reddy, C. K.; Das, A.; Jayaram, B., *J. Mol. Biol.* **2001**, 314, 619-632.
- [3.17] Prasad, T.; Prathima, M. N.; Chandra, N., *Bioinformatics* **2003**, 19, 167-168.
- [3.18] Babu, M. M.; Singh, S. K.; Balaram, P., *J. Mol. Biol.* **2002**, 322, 871-880.

- [3.19] Sarkhel, S.; Desiraju, G. R., *Proteins* **2004**, 54, 247-259.
- [3.20] Berman, H. M.; Westbrook, J.; Feng, Z.; Gilliland, G.; Bhat, T. N.; Weissig, H.; Shindyalov, I. N.; Bourne, P. E., *Nucleic Acid Res.* **2000**, 28, 235-242.
<http://www.rcsb.org/pdb>
- [3.21] Allen, F. H.; Kennard, O., *Chem. Des. Autom. News* **1993**, 8, 31-37.
<http://www.ccdc.cam.ac.uk/prods/csd/csd.html>
- [3.22] Nissink, J. W.; Murray, C.; Hartshorn, M.; Verdonk, M. L.; Cole, J. C.; Taylor, R., *Proteins* **2002**, 49, 457-471.
- [3.23] Kleywegt, G., *Acta. Crystallogra. Sect. D* **2000**, 56, 249-265.
- [3.24] MOE Program, Version 2005, Chemical Computing Inc, Suite 910-1010 Sherbrooke St. W, Montreal, Quebec, Canada, H3A 2R7.
- [3.25] Allinger, N. (1998) Force fields: A brief introduction. In *Encyclopedia of Computational Chemistry*. Schleyer, P. v. R., Ed., John Wiley & Sons, Chicester, UK, Vol 2, pp. 1013-1015. (See also subsequent topics in force field sections).
- [3.26] Word, J. M.; Lovell, S. C.; Richardson, J. S.; Richardson, D. C., *J. Mol. Biol.* **1999**, 285, 1735-1747.
- [3.27] Collaborative computational project, number 4., *Acta. Crystallogra. Sect. D* **1994**, 50, 760-763.
- [3.28] McDonald, I. K.; Thornton, J. M., *J. Mol. Biol.* **1994**, 238, 777-793.
- [3.29] Lindauer, K.; Bendic, C.; Sühnel, J., *Comput. Appl. Biosci.* **1996**, 12, 281-289.
- [3.30] Sobolev, V.; Sorokine, A.; Prilusky, J.; Abola, E. E.; Edelman, M., *Bioinformatics* **1999**, 15, 327-332.
- [3.31] Babu, M. M., *Nucleic Acid Res.* **2003**, 31, 3345-3348.
- [3.32] Brandl, M.; Weiss, M. S.; Jabs, A.; Sühnel, J.; Hilgenfeld, R., *J. Mol. Biol.* **2001**, 307, 357-377.
- [3.33] Koellner, G.; Kryger, G.; Millard, C. B.; Silman, I.; Sussman, J. L.; Steiner, T., *J. Mol. Biol.* **2000**, 296, 713-735.
- [3.34] Auffinger, P.; Hays, F. A.; Westhof, E.; Ho, P. S., *Proc. Natl. Acad. Sci. USA* **2004**, 101, 16789-16794.

References and Notes

- [3.35] Klaholz, B.; Moras, D., *Structure* **2002**, 10, 1197-1204.
- [3.36] Chakrabarti, P.; Chakrabarti, S., *J. Mol. Biol.* **1998**, 284, 867-873.
- [3.37] Kim, J.; Mao, J.; Gunner, M. R., *J. Mol. Biol.* **2005**, 348, 1283-1298.
- [3.38] Park, S.; Saven, J. G., *Proteins* **2005**, 60, 450-463.
- [3.39] Ippolito, J. A.; Alexander, R. S.; Christianson, D. W., *J. Mol. Biol.* **1990**, 215, 457-471.
- [3.40] Ragone, R., *Protein Sci.* **2001**, 10, 2075-2082.
- [3.41] Desiraju, G. R.; Steiner, T. (1999) *The weak hydrogen bond in structural chemistry and biology*. Oxford University Press, Oxford.
- [3.42] Porter, C. T.; Bartlett, G. J.; Thornton, J. M., *Nucleic Acid Res.* **2004**, 32, D129-D133.
- [3.43] Yan, B. X.; Sun, Y. Q., *J. Biol. Chem.* **1997**, 272, 3190-3194.
- [3.44] Steiner, T., *Acta. Crystallogra. Sect. D* **1995**, 51, 93-97.
- [3.45] Lipinski, C. A.; Lombardo, F.; Dominy, B. W.; Feeney, P. J., *Adv. Drug Del. Rev.* **1997**, 23, 3-25.
- [3.46] Ouvrard, C.; Le Questel, J. -Y.; Berthelot, M.; Laurence, C., *Acta. Crystallogra. Sect. B* **2003**, 59, 512-526.
- [3.47] Kovács, A.; Varga, Z., *Coordination Chem. Reviews* **2006**, 250, 710-727.
- [3.48] Gregoret, L. M.; Rader, S. D.; Fletterick, R. J.; Cohen, F. E., *Proteins* **1991**, 9, 99-107.

CHAPTER 4

- [4.1] Jeffrey, G. A.; Saenger, W. (1991) *Hydrogen bonding in biological structures*. Springer Verlag, Berlin.
- [4.2] Baker, E. N.; Hubbard, R. E., *Progr. Biophys. Mol. Biol.* **1984**, 44, 97-179.
- [4.3] Desiraju, G. R.; Steiner, T. (1999) *The weak hydrogen bond in structural chemistry and biology*. Oxford University Press, Oxford, Chapters 1 and 5.
- [4.4] Sarkhel, S.; Desiraju, G. R., *Proteins* **2004**, 54, 247-259.

- [4.5] Panigrahi, S. K.; Desiraju, G. R., *Proteins* **2007**, ASAP, DOI 10.1002/prot.21253.
- [4.6] Auffinger, P.; Hays, F. A.; Westhof, E.; Ho, P. S. *Proc. Natl. Acad. Sci. USA* **2004**, 101, 16789-16794.
- [4.7] Glusker, J. P., *Acta. Crystallogra. Sect. D* **1995**, 51, 418-427.
- [4.8] Bartlett, G. J.; Porter, C. T.; Borkakoti, N.; Thornton, J. M., *J. Mol. Biol.* **2002**, 324, 105-121.
- [4.9] Steiner, T., *Angew. Chem. Int. Ed.* **2002**, 41, 48-76.
- [4.10] Pierce, A. C.; Sandretto, K. L.; Bemis, G. W., *Proteins* **2002**, 49, 567-576.
- [4.11] Pierce, A. C.; ter Haar, E.; Binch, H. M.; Kay, D. P.; Patel, S. R.; Li, P., *J. Med. Chem.* **2005**, 48, 1278-1281.
- [4.12] Cohen, P., *Nature Rev. Drug Discov.* **2002**, 1, 309-315.
- [4.13] Levitzki, A., *Acc. Chem. Res.* **2003**, 36, 462-469.
- [4.14] Bridges, A. J., *Chem. Rev.* **2001**, 101, 2541-2571.
- [4.15] Vieth, M.; Higgs, R. E.; Robertson, D. H.; Shapiro, M.; Gragg, E. A.; Hemmerle, H., *Biochim. Biophys. Acta* **2004**, 1697, 243-257.
- [4.16] Berman, H. M.; Westbrook, J.; Feng, Z.; Gilliland, G.; Bhat, T. N.; Weissig, H.; Shindyalov, I. N.; Bourne, P. E., *Nucleic Acid Res.* **2000**, 28, 235-242.
<http://www.rcsb.org/pdb>
- [4.17] (a) The Protein Kinase Resource, SDSC, UC, San Diego, MC, 2004, www.kinaset.net/pkr
- [4.18] Williams, D. H.; Mitchell, T., *Curr. Opin. Pharmacol.* **2002**, 2, 567-573.
- [4.19] (a) Sugan, Structure and Phylogeny of the Protein Kinases, Salk Institute, La Jolla, CA, 2002, <http://198.202.68.14/human/kinome/phylogeny.html>.
(b) <http://kinasedb.ontology.ims.u-tokyo.ac.jp>. (c) Wang, R.; Fang, X.; Lu, Y.; Yang, C. Y.; Wang, S., *J. Med. Chem.* **2005**, 48, 4111-4119.
www.pdbbind.org
- [4.20] Naumann, T.; Matter, H., *J. Med. Chem.* **2002**, 45, 2366-2378.
- [4.21] Hanks, S. K.; Hunter, T., *FASEB J.* **1995**, 9, 576-596.

References and Notes

- [4.22] Dar, A. C.; Wybenga-Groot, L. E.; Sicheri, F. (2005) The Eukaryotic Protein Kinase Domain. In *Modular Protein Domains*, Cesareni, G.; Gimona, M.; Sudol, M.; Yaffe, M., Eds., Wiley-VCH Verlag GmbH & Co.: KGaA, Chapter 9.
- [4.23] Panigrahi, S. K.; Desiraju, G. R., *Nat. Acad. Sci. Lett. (India)* **2004**, 27, 1-11.
- [4.24] Mao, L.; Wang, Y.; Lie, Y.; Hu, X., *J. Mol. Biol.* **2004**, 336, 787-807.
- [4.25] MOE Program, Version 2006-08 Chemical Computing Inc, Sherbrooke St. W, Montreal, Quebec, Canada, H3A 2R7.
- [4.26] Halgren, T., *J. Comput. Chem.* **1996**, 17, 490-519.
- [4.27] Tiwari, A.; Panigrahi, S. K.; Desiraju, G. R. *HBAT*: A complete package for analysing strong and weak hydrogen bonds in macromolecular crystal structures. (*communicated*)
- [4.28] (a) Thompson, J. D.; Higgins, D. G.; Gibson, T. J., *Nucleic Acids Res.* **1994**, 22, 4673-4680. (b) ClustalW WWW Service at the European Bioinformatics Institute. www.ebi.ac.uk/clustalw.
- [4.29] Williams, M. A.; Goodfellow, J. M.; Thornton, J. M., *Protein Sci.* **1994**, 3, 1224-1235.
- [4.30] Aparna, V.; Rambabu, G.; Panigrahi, S. K.; Sarma, J. A. R. P.; Desiraju, G. R., *J. Chem. Inf. Model.* **2005**, 45, 725-738.
- [4.31] Gitlin, I.; Carbeck, J. D.; Whitesides, G. M., *Angew. Chem. Int. Ed.* **2006**, 45, 3022-3060.
- [4.32] Desiraju, G. R., *Angew. Chem. Int. Ed.* **1995**, 34, 2311-2327.
- [4.33] Walsh, R. D.; Bradner M. W.; Fleischman, S.; Morales, L. A.; Moulton, B.; Rodríguez-Hornedo, N.; Zaworotko, M. J., *Chem. Commun.* **2003**, 186-187.
- [4.34] Vishweshwar, P.; Nangia, A.; Lynch, V. M., *Cryst. Growth. Des.* **2003**, 3, 783-790.
- [4.35] Ladbury, J. E., *Chem. Biol.* **1996**, 3, 973-980.
- [4.36] Bottoms, C. A.; Smith, P. E.; Tanner, J. J., *Protein Sci.* **2002**, 11, 2125-2137.

CHAPTER 5

- [5.1] Neidle, S., *Nat. Prod. Rep.* **2001**, 18, 291-309.
- [5.2] Lacy, E. R.; Madsen, E. M.; Lee, M.; Wilson, W. D. (2003) Polyamide dimer stacking in the DNA minor groove and recognition of TC mismatched base pairs in DNA. In *Small molecule DNA and RNA binders: From synthesis to nucleic acid complexes*. Demeunynck, M.; Bailly, C.; Wilson, W. D., Eds., WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, pp. 387-413.
- [5.3] Tidwell, R. R.; Boykin, D. W. (2003) Dicationic DNA minor groove binders as antimicrobial agents. In *Small molecule DNA and RNA binders: From synthesis to nucleic acid complexes*. Demeunynck, M.; Bailly, C.; Wilson, W. D., Eds., WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, pp. 414-460.
- [5.4] Wilson, W. D.; Nguyen, B.; Tanious, F. A.; Mathis, A.; Hall, J. E.; Stephens, C. E.; Boykin, D.W., *Curr. Med. Chem. -Anti-Cancer Agent* **2005**, 5, 389-408.
- [5.5] Pindur, U.; Jansen, M.; Lemster, T., *Curr. Med. Chem.* **2005**, 12, 2805-2847.
- [5.6] Dervan, P. B.; Edelson, B. S., *Curr. Opin. Struct. Biol.* **2003**, 13, 284-299.
- [5.7] Berman, H. M.; Westbrook, J.; Feng, Z.; Gilliland, G.; Bhat, T. N.; Weissig, H.; Shindyalov, I. N.; Bourne, P. E., *Nucleic Acid Res.* **2000**, 28, 235-242.
<http://www.rcsb.org/pdb>
- [5.8] Kennard, O., *Pure & Appl. Chem.* **1993**, 65, 1213-1222.
- [5.9] Taberner, L.; Bella, J.; Aleman, C., *Nucleic Acid Res.* **1996**, 24, 3458-3466.
- [5.10] Dervan, P. B., *Bioorg. Med. Chem.* **2001**, 9, 2215-2235.
- [5.11] Moravek, Z.; Neidle, S.; Schneider, B., *Nucleic Acid Res.* **2002**, 30, 1182-1191.
- [5.12] Rohs, R.; Bloch, I.; Sklenar, H.; Shakked, Z., *Nucleic Acid Res.* **2005**, 33, 7048-7057.
- [5.13] Desiraju, G. R.; Steiner, T. (1999) *The weak hydrogen bond in structural chemistry and biology*, Oxford University Press, Oxford.
- [5.14] Sarkhel, S.; Desiraju, G. R., *Proteins* **2004**, 54, 247-259.

References and Notes

- [5.15] Panigrahi, S. K.; Desiraju, G. R., *Proteins* **2007**, ASAP, DOI 10.1002/prot.21253.
- [5.16] Aparna, V.; Rambabu, G.; Panigrahi, S. K.; Sarma, J. A. R. P.; Desiraju, G. R., *J. Chem. Inf. Model.* **2005**, 45, 725-738.
- [5.17] Athri, P.; Wenzler, T.; Ruiz, P.; Brun, R.; Boykin, D. W.; Tidwel, R.; Wilson, W. D., *Bioorg. Med. Chem.* **2006**, 14, 3144-3152.
- [5.18] Seed, J. R.; Boykin, D. W. (2001) Chemotherapy of African trypano-somiasis, In *World Class Parasites, Vol. 1, The African Trypanosomes*. Black, S.; Seed, J. R., Eds., Kluwer Academic Publishers, Boston, pp. 65-78.
- [5.19] Boykin, D. W., *J. Braz. Chem. Soc.* **2002**, 13, 763-771.
- [5.20] Halgren, T., *J. Comput. Chem.* **1996**, 17, 490-519.
- [5.21] MOE Program, Version 2006-08 Chemical Computing Inc, Suite 910-1010 Sherbrooke St. W, Montreal, Quebec, Canada, H3A 2R7.
- [5.22] Tiwari, A. Panigrahi, S. K.; Desiraju, G. R., *HBAT*: A complete package for analysing strong and weak hydrogen bonds in macromolecular crystal structures. (*communicated*)
- [5.23] GOLD 3.0, Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK.
- [5.24] Evans, D. A.; Neidle, S., *J. Med. Chem.* **2006**, 49, 4232-4238.

CHAPTER 6

- [6.1] Höltje, H.-D.; Folkeis, G. (1997) *Molecular modeling: Basic principles and applications*. VCH, New York.
- [6.2] Leach, A. R. (2001) *Molecular modelling principles and applications*. (2nd edn.) Pearson Education Limited, London.
- [6.3] Young, D. C. (2001) *Computational chemistry a practical guide for applying techniques to real-world problems*. John Wiley & Sons, Inc., New York.

- [6.4] Baker, O. M.; MacKerell Jr., A. D.; Roux, B.; Watanabe, M. (2001) *Computational biochemistry and biophysics*. Marcel Dekker, Inc. New York.
- [6.5] Tsai, C. S. (2002) *An introduction to computational biochemistry*. Wiley-Liss, Inc., New York.
- [6.6] Lewars, E. (2004) *Computational chemistry introduction to the theory and applications of molecular and quantum mechanics*. Kluwer Academic Publishers, Dordrecht.
- [6.7] Mannhold, R.; Kubinyi, H.; Folkers, G., Eds., (2003) *Quantum medicinal chemistry*. Wiley-VCH GmbH & Co. KGaA, Weinheim.
- [6.8] Jensen, F. (1999) *Introduction to computational chemistry*. John Wiley & Sons, New York.
- [6.9] Veszprémi, T.; Fehér, M. (1999) *Quantum chemistry: Fundamentals to applications*. Kluwer, Dordrecht.
- [6.10] Cook, D. B. (1998) *Handbook of computational quantum chemistry*. Oxford, Oxford.
- [6.11] Atkins, P. W.; Friedman, R. S. (1997) *Molecular quantum mechanics*. Oxford, Oxford.
- [6.12] Simons, J.; Nichols, J. (1997) *Quantum mechanics in chemistry*. Oxford, Oxford.
- [6.13] Levine, I. N. (1991) *Quantum chemistry*. Prentice Hall, Englewood Cliffs.
- [6.14] Jug, K.; Neumann, F. (1998) Configuration interaction: Semiempirical calculations. In *Encyclopedia of Computational Chemistry*. Schleyer, P. v. R., Ed., John Wiley & Sons, Chichester, UK, 1, pp. 507-513.
- [6.15] Koch, W.; Holthausen, M. C. (2000) *A chemist's guide to density functional theory*. Wiley-VCH, Weinheim.
- [6.16] Rappé, A. K.; Casewit, C. J. (1997) *Molecular mechanics across chemistry*. University Science Books, Sausalito.
- [6.17] Dobson, J. F.; Vignale, G.; Das, M. P. (1998) *Electronic density functional theory recent progress and new directions*. Plenum, New York.

References and Notes

- [6.18] Schlecht, M. F. (1998) *Molecular modeling on the PC*. Wiley-VCH, New York.
- [6.19] Allinger, N. (1998) Force fields: A brief introduction. In *Encyclopedia of Computational Chemistry*. Schleyer, P. v. R., Ed., John Wiley & Sons, Chichester, UK. Vol 2, pp. 1013-1015.
- [6.20] Jalaie, M.; Lipkowitz, K. B. (2000) Published Force Field Parameters for Molecular Mechanics, Molecular Dynamics, and Monte Carlo Simulations. In *Reviews in computational chemistry*. K. B. Lipkowitz and D. B. Boyd, Eds., Wiley-VCH, New York, 2000, Vol. 14, pp. 441-486.
- [6.21] Gao, J.; Thompson, M. (1998) *Combined quantum and molecular mechanics methods*. American Chemical Society, Washington.
- [6.22] Billing, G. D.; Mikkelsen, K. V. (1997) *Advanced molecular dynamics and chemical kinetics*. John Wiley & Sons, New York.
- [6.23] D. L. Beveridge (1998) Molecular dynamics: DNA. In *Encyclopedia of Computational Chemistry*. Schleyer, P. v. R., Ed., John Wiley & Sons, Chichester, UK, Vol 3, pp. 1620-1628
- [6.24] Balbuena, P. B.; Seminario, J. M. (1999) *Molecular dynamics*. Elsevier, Amsterdam.
- [6.25] Frenkel, D.; Smit, B. (1996) *Understanding molecular simulation*. Academic Press, San Diego.
- [6.26] Jorgensen, W. L. (1998) Monte Carlo simulations for liquids. In *Encyclopedia of Computational Chemistry*. Schleyer, P. v. R., Ed., John Wiley & Sons, Chichester, UK, Vol 3, 1754-1763.
- [6.27] Parrill, A. L.; Reddy, M. R. (1999) Overview of rational drug design. In *Rational drug design: novel methodology and practical applications*. Rami Reddy, M., Parrill, A. L., Eds., American Chemical Society, Washington DC, Vol. 719, pp. 1-11.
- [6.28] E. -L. Allan, *Drug Discovery World* **2002**, 71-75.
- [6.29] Martin, Y. C. (1998) 3D QSAR: Current state, scope and limitations. In *Perspectives in drug discovery and design-3D QSAR in drug design: Recent*

- advances*. Kubinyi, H.; Folkers, G.; Martin, Y. C., Eds., Kluwer Academic Publishers, London, Vol. 12/13/14, pp. 3-23.
- [6.30] Abraham, D. J. (2003) *Burger's medicinal chemistry and drug discovery*. (Sixth edn.). John Wiley & Sons Inc., New Jersey, Vol. 1.
- [6.31] Weber, I. T.; Harrison, R. W. (1998) Molecular mechanics calculations on protein-ligand complexes. In *Perspectives in drug discovery and design-3D QSAR in drug design: ligand-protein interactions and molecular similarity*. Kubinyi, H.; Folkers, G.; Martin, Y. C., Eds., Kluwer Academic Publishers, London, Vol. 2, pp. 115-127.
- [6.32] Muegge, I.; Rarey, M. (2001) Small molecule docking and scoring. In *Reviews in computational chemistry*. Lipkowitz, K. B.; Boyd, D. B., Eds., John Wiley & Sons Inc., New York, Vol 17, pp. 1-46.
- [6.33] Gohlke, H.; Klebe, G., *Angew. Chem. Int. Ed.* **2002**, 41, 2644-2676.
- [6.34] Grzybowski, B. A.; Ishchenko, A. V.; Shimada, J.; Shakhnovich, E. I., *Acc. Chem. Res.* **2002**, 35, 261-269.
- [6.35] Kitchen, D. B.; Decornez, H.; Furr, J. R.; Bajorath, J., *Nat. Rev. Drug Discov.* **2004**, 3, 935-949.
- [6.36] Feher, M., *Drug Discov. Today* **2006**, 11, 421-428.
- [6.37] Babine, R. E; Abdel-Meguid, S. S., Eds., (2004) *Protein crystallography in drug design*. Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim.
- [6.38] Zartler, E. R.; Shapiro, M. J., *Curr. Opin. Chem. Biol.* **2005**, 9, 366-370.
- [6.39] Schneider, G.; Fechner, U. *Nat. Rev. Drug Discov.* **2005**, 4, 649-663.
- [6.40] Sirois, S.; Wei, D. -Q.; Du, Q.; Chou, K. -C., *J. Chem. Inf. Model.* **2004**, 44, 1111-1122.
- [6.41] Lyne, P. D.; Kenny, P. W.; Cosgrove, D. A.; Deng, C.; Zabludoff, S.; Wendoloski, J. J.; Ashwell, S., *J. Med. Chem.* **2004**, 47, 1962-1968.
- [6.42] Lengauer, T.; Lemmen, C.; Rarey, M.; Zimmermann, M., *Drug Discov. Today.* **2004**, 9, 27-34.
- [6.43] Willet, P., *Drug Discov. Today* **2006**, 11, 1046-1053.
- [6.44] Klebe, G., *Drug Discov. Today* **2006**, 11, 580-594.

References and Notes

- [6.45] Ekins, S.; Swaan, P. W. (2004) Development of computational models for enzymes, transporters, channels, and receptors relevant to ADME/Tox. In *Reviews in computational chemistry*. Lipkowitz, K. B.; Larter, R.; Cundari, T. R.; Boyd, D. B., Eds., John Wiley & Sons Inc., Hoboken, New Jersey. Vol 20, pp. 333-376.
- [6.46] Tetko, I. V.; Bruneau, P.; Mewes, H. W.; Rohrer, D. C.; Poda, G. I., *Drug Discov. Today* **2006**, 11, 700-707.
- [6.47] Gasteiger, J.; Engel, T. (2003) *Chemoinformatics*. Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim.
- [6.48] Gasteiger, J. (2003) *Hand book of chemoinformatics*. Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim.
- [6.49] Bajorath, J. (2004) *Chemoinformatics: Concepts, methods and tools for drug discovery*. Methods in Molecular Biology. Vol. 275. Humana Press, New Jersey.
- [6.50] (a) Engel, T., *J. Chem. Inf. Model.* **2006**, 46, 2267-2277. (b) Chen, W. L., *J. Chem. Inf. Model.* **2006**, 46, 2230-2255. (c) Gasteiger, J., *J. Med. Chem.* **2006**, 50, 6429-6434.
- [6.51] Wermuth, C. G.; Ganellin, C. R.; Lindberg, P.; Mitscher, L. A., *Annu. Rep. Med. Chem.* **1998**, 33, 385-395.
- [6.52] Güner, O. F. (2000) *Pharmacophore: perception, development and use in drug design*. International university line: CA.
- [6.53] Langer, T.; Hoffman, R. D. (2006) *Pharmacophore and pharmacophore searches*. WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.
- [6.54] Boyle, R. (1685) *Of the reconcileableness of specific medicines to the corpuscular philosophy*. Samuel Smith, London, pp. 72-75.
- [6.55] Fränkel, S. (1901) *Die Arzneimittel-Synthese auf Grundlage der Beziehungen zwischen chemischem Aufbau und Wirkung*. Julius Springer, Berlin, pp. 13-41.
- [6.56] Langley, J. N., *J. Physiol.* **1878**, 1, 339-369.
- [6.57] Langley, J. N., *J. Physiol.* **1905**, 33, 374-413.
- [6.58] Ehrlich, P.; Morgenroth, J., *Berl. Klin. Wochenschr.* **1900**, 37, 453-457.

- [6.59] Maehle, A. H.; Prull, C. R.; Halliwell, R. F., *Nat. Rev. Drug Discov.* **2002**, 1, 637-641.
- [6.60] Albert, A. (1979) *Selective Toxicity. The physicochemical basis of therapy.* Chapman and Hall, London, p. 23.
- [6.61] Fischer, E., *Ber. Dtsch. Chem. Ges.* **1894**, 27, 2985-2993.
- [6.62] Woods, D. D., *Br. J. Exp. Pathol.* **1940**, 21, 74-90.
- [6.63] Woods, D. D.; Fildes, P., *Chem. Ind.* **1940**, 59, 133-134.
- [6.64] Dodds, E. C.; Lawson, W., *Proc. R. Soc. London, Ser. B* **1938**, 125, 122-132.
- [6.65] Schueler, F. W., *Science* **1946**, 103, 221-223.
- [6.66] Easson, L. H.; Stedman, E., *Biochem. J.* **1933**, 27, 1257-1266.
- [6.67] Beckett, A. H. (1959) Stereochemical factors in biological activity. In *Fortschritte der Arzneimittel Forschung.* Birkhäuser Verlag, Basel, pp. 455-530.
- [6.68] Farmer, P. S.; Ariëns, E. J., *Trends Pharmacol. Sci.* **1982**, 3, 362-365.
- [6.69] Barlow, R. B. (1964) *Introduction to chemical pharmacology.* (2nd edn.) Methuen, London.
- [6.70] Belleau, B. (1963) An analysis of drug-receptor interactions. In *Modern concepts in the relationship between structure and pharmacological activity.* Brunings, K. J., Ed., Pergamon Press, Oxford, pp. 75-99.
- [6.71] Pullmann, B.; Coubeils, J. L.; Courrière, P.; Gervois, J. P., *J. Med. Chem.* **1972**, 15, 17-23.
- [6.72] Wermuth, C. G.; Schwartz, J.; Leclerc, G.; Garnier, J. P.; Rouot, B., *Chim. Thér.* **1973**, 1, 115-116.
- [6.73] Gund, P. (1977) Three-dimensional pharmacophoric pattern searching. In *Progress in Molecular and Subcellular Biology.* Han, F. E., Ed., Berlin, Springer-Verlag, Vol. 5, pp. 117-143.
- [6.74] Gund, P., *Ann. Reports Med. Chem.* **1979**, 14, 299-308.
- [6.75] Humblet, C.; Marshall, F. R., *Ann. Reports Med. Chem.* **1980**, 15, 267-276.
- [6.76] Gund, P.; Wipke, W. T.; Langridge, R., Computer searching of a molecular structure file for pharmacophoric patterns. In *Proc Intl Conf on Computers in*

References and Notes

- Chem Res and Educa, Ljubljana, July 12-17, **1973**, Amsterdam, Elsevier, **1974**, 3:5/33-39.
- [6.77] Crippen G. M., *J. Comp. Phys.* **1977**, 24, 96-107.
- [6.78] Marshall, G. R. (**1993**) Binding-site modeling of unknown receptors. In *3D QSAR in Drug Design, Theory Methods and Applications*. Kubinyi, H., Ed., ESCOM, Leiden, pp. 80-116.
- [6.79] Wermuth, C. G., Langer, T. (**1993**) Pharmacophore identification. In *3D QSAR in Drug Design. Theory Methods and Applications*. Kubinyi, H., Ed., ESCOM, Leiden, pp. 117-136.

CHAPTER 7

- [7.1] Klebe, G., *Drug Discov. Today* **2006**, 11, 580-594.
- [7.2] Schneider, G.; Böhm, H., -J., *Drug Discov. Today* **2002**, 7, 64-70.
- [7.3] Rauh, D.; Klebe, G.; Stubbs, M. T., *J. Mol. Biol.* **2004**, 335, 1325-1341.
- [7.4] Wilson, E. K., *C&EN*. **2004**, 82, 46-47.
- [7.5] Cavasotto, C. N.; Abagyan, R. A., *J. Mol. Biol.* **2004**, 337, 209-225.
- [7.6] The well-known Lipinski's rule of five may be regarded as a rudimentary form of first generation VS. Lipinski, C. A.; Lombardo, F.; Dominy, B. W.; Feeney, P. J., *Adv. Drug Deliv. Rev.* **1997**, 23, 3-25.
- [7.7] Sirois, S.; Wei, D. -Q.; Du, Q.; Chou, K. -C., *J. Chem. Inf. Model.* **2004**, 44, 1111-1122.
- [7.8] Keserü, G. M., *J. Comput. Aided Mol. Des.* **2001**, 15, 649-657.
- [7.9] Rollinger, J. M.; Hornick, A.; Langer, T.; Stuppner, H.; Prast, H., *J. Med. Chem.* **2004**, 47, 6248-6254.
- [7.10] Rastelli, G.; Pacchioni, S.; Sirawaraporn, W.; Sirawaraporn, R.; Parenti, M. D.; Ferrari, A. M., *J. Med. Chem.* **2003**, 46, 2834-2845.
- [7.11] Muegge, I.; Enyedy, I. J., *Curr. Med. Chem.* **2004**, 11, 693-707.
- [7.12] Grüneberg, S.; Stubbs, M. T.; Klebe, G., *J. Med. Chem.* **2002**, 45, 3588-3602.

- [7.13] Vieth, M.; Brooks, H. B.; Hamdouchi, C.; Mcmillen, W.; Sawyer, J. S.; Yingling, J. M.; Zhang, F., *Cell. Mol. Biol. Lett.* **2003**, 8, 566-567.
- [7.14] Hert, J.; Willett, P.; Wilton, D. J.; Acklin, P.; Azzaoui, K.; Jacoby, E.; Schuffenhauer, A., *J. Chem. Inf. Model.* **2006**, 46, 462-470.
- [7.15] Lengauer, T.; Lemmen, C.; Rarey, M.; Zimmermann, M., *Drug Discov. Today* **2004**, 1, 27-34.
- [7.16] Mustata, G. I.; Brigo, A.; Briggs, J. M., *Bioorg. Med. Chem. Lett.* **2004**, 14, 1447-1454.
- [7.17] Aronov, A. M.; Murko, M. A., *J. Med. Chem.* **2004**, 47, 5616-5619.
- [7.18] Parenti, M. D.; Pacchioni, S.; Ferrari, A. M.; Rastelli, G., *J. Med. Chem.* **2004**, 47, 4258-4267.
- [7.19] Renner, S.; Schneider, G., *J. Med. Chem.* **2004**, 47, 4653-4664.
- [7.20] Li, M. Y.; Tsaib, K. C.; Xia, L., *Bioorg. Med. Chem. Lett.* **2005**, 15, 657-664.
- [7.21] Krovat, E. M.; Fruhwirth, K. H.; Langer, T., *J. Chem. Inf. Model.* **2005**, 45, 146-159.
- [7.22] Vema, A.; Panigrahi, S. K.; Rambabu, G.; Gopalakrishnan, B.; Sarma, J. A. R. P.; Desiraju, G. R., *Bioorg. Med. Chem.* **2003**, 11, 4643-4653.
- [7.23] Hou, T.; Zhu, L.; Chen, L.; Xu, X., *J. Chem. Inf. Model.* **2003**, 43, 273-287.
- [7.24] Szántai-Kis, C.; Kövesdi, I.; Eros, D.; Bánhegyi, P.; Ullrich, A.; Kéri, G.; Orfi, L., *Curr. Med. Chem.* **2006**, 13, 277-287.
- [7.25] Aparna, V.; Rambabu, G.; Panigrahi, S. K.; Sarma, J. A. R. P.; Desiraju, G. R., *J. Chem. Inf. Model.* **2005**, 45, 725-738.
- [7.26] Dar, A. C.; Wybenga-Groot, L. E.; Sicheri, F. (2005) The eukaryotic protein kinase domain. In *Modular Protein Domains*, Cesareni, G.; Gimona, M.; Sudol, M.; Yaffe, M., Eds., Wiley-VCH Verlag GmbH & Co. KGaA, pp. 181-209.
- [7.27] Yang, J.; Yu, Y.; Duerksen-Hughes, P. J., *Mutat. Res.* **2003**, 543, 31-58.
- [7.28] Blume-Jensen, P.; Hunter, T., *Nature* **2001**, 411, 355-365.

References and Notes

- [7.29] Stamos, J.; Sliwkowski, M. X.; Eigenbrot, C., *J. Biol. Chem.* **2002**, 277, 46265-46272.
- [7.30] Yarden, Y.; Ullrich, A., *Ann. Rev. Biochem.* **1988**, 57, 443-478.
- [7.31] Ullrich, A.; Schlessinger, J., *Cell* **1990**, 61, 203-212.
- [7.32] Pedersen, M. W.; Poulsen, H. S., *Sci. Med.* **2002**, 8, 206-217.
- [7.33] Traxler, P.; Bold, G.; Buchdunger, E.; Caravatti, G.; Furet, P.; Manley, P.; O'Reilly, T.; Wood, J.; Zimmermann, J., *Med. Res. Rev.* **2001**, 21, 499-512.
- [7.34] Atkins, J. H.; Gershell, L. J., *Nature Rev. Can.* **2002**, 1, 491-492.
- [7.35] Cohen, P., *Nature Rev. Drug Discov.* **2002**, 1, 309-315.
- [7.36] Dancey, J.; Sausville, E. A., *Nature Rev. Drug Discov.* **2003**, 2, 296-313.
- [7.37] Hubbard, S. R., *Curr. Opin. Struct. Biol.* **2002**, 12, 735-741.
- [7.38] Levitzki, A., *Acc. Chem. Res.* **2003**, 36, 462-469.
- [7.39] Traxler, P.; Furet, P., *Pharmacol. Ther.* **1999**, 82, 195-206.
- [7.40] Morin, M. J., *Oncogene*, **2000**, 19, 6574-6583.
- [7.41] Sarma, J. A. R. P., A kinase inhibitor database consisting of 136 678 compounds with chemical, biological, pharmacological and toxicological data was curated from journals and patents. GVK BIOSCIENCES Private Limited, August, **2004**.
- [7.42] Wissner, A.; Brawner Floyd, M. B.; Rabindran, S. K.; Nilakantan, R.; Greenberger, L. M.; Shen, R.; Wang, Y. F.; Tsou, H. R., *Bioorg. Med. Chem. Lett.* **2002**, 12, 2893-2897.
- [7.43] Traxler, P.; Bold, G.; Frei, J.; Lang, M.; Lydon, N.; Mett, H.; Buchdunger, E.; Meyer, T.; Mueller, M.; Furet, P., *J. Med. Chem.* **1997**, 40, 3601-3616.
- [7.44] *Catalyst, Accelrys* : San Diego, CA, **1997**.
- [7.45] Xue, L.; Stahura, F. L.; Bajorath, J., *J. Chem. Inf. Model.* **2004**, 44, 2032-2039.
- [7.46] Agrafiotis, D. K.; Myslik, J. C.; Salemme, F. R., *Molecular Diversity*, **1999**, 4, 1-22.
- [7.47] Güner, O. F., Ed., **(2000)** *Pharmacophore: perception, development and use in drug design*. International university line: CA.

- [7.48] Smellie, A.; Teig, S. L.; Towbin, P., *J. Comput. Chem.* **1995**, 16, 171-187.
- [7.49] Berman, H. M.; Westbrook, J.; Feng, Z.; Gilliland, G.; Bhat, T. N.; Weissig, H.; Shindyalov, I. N.; Bourne, P. E., *Nucleic Acid Res.* **2000**, 28, 235-242.
<http://www.rcsb.org/pdb>
- [7.50] Wood, E. R.; Truesdale, A. T.; McDonald, O. B.; Yuan, D.; Hassell, A.; Dickerson, S. H.; Ellis, B.; Pennisi, C.; Horne, E.; Lackey, K.; Alligood, K. J.; Rusnak, D. W.; Gilmer, T. M.; Shewchuk, L., *Cancer Res.* **2004**, 64, 6652-6659.
- [7.51] MOE Program, Version 2006-08 Chemical Computing Inc, Suite 910-1010 Sherbrooke St. W, Montreal, Quebec, Canada, H3A 2R7.
- [7.52] Halgren, T., *J. Comput. Chem.* **1996**, 17, 490-519.
- [7.53] Wolber, G.; Langer, T., *J. Chem. Inf. Model.* **2005**, 45, 160-169.
- [7.54] GOLD 3.0, Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK.
- [7.55] Kirchmair, J.; Laggner, C.; Wolber, G.; Langer, T., *J. Chem. Inf. Model.*, **2005**, 45, 422-430.
- [7.56] Kirchmair, J.; Wolber, G.; Laggner, C.; Langer, T., *J. Chem. Inf. Model.* **2006**, 46, 1848-1861.

CHAPTER 8

- [8.1] Cummings, J. L., *N. Engl. J. Med.* **2004**, 351, 56-67.
- [8.2] Robichaud, A. J., *Curr. Top. Med. Chem.* **2006**, 6, 553-568.
- [8.3] Brimijoin, S., *Prog. Neurobiol.* **1983**, 21, 291-322.
- [8.4] Barnard, E. A. (1974) *The Peripheral Nervous System*. Plenum Press, New York.
- [8.5] Giacobini, E., *Neurochem. Res.* **2000**, 25, 1185-1190.
- [8.6] Giacobini, E., *Jpn. J. Pharmacol.* **1997**, 74, 225-241.
- [8.7] Carreiras, M. C.; Marco, J. L., *Curr. Pharm. Des.* **2004**, 10, 3167-3175.

References and Notes

- [8.8] (a) Lushington, G. H.; Guo, J. X.; Hurley, M. M., *Curr. Top. Med. Chem.* **2006**, *6*, 57-73. (b) Hurley, M. M.; Balboa, A.; Lushington, G. H.; Guo, J., *Chem. Biol. Interact.* **2005**, 157-158, 321-325. (c) Wlodek, S. T.; Shen, T.; McCammon, J. A., *Biopolymers* **2000**, *53*, 265-271. (d) Barril, X.; Orozco, M.; Luque, F. J., *J. Med. Chem.* **1999**, *42*, 5110-5119. (e) Antosiewicz, J.; Wlodek, S. T.; McCammon, J. A., *Biopolymers* **1996**, *39*, 85-94. (f) Antosiewicz, J.; Gilson, M. K.; Lee, I. H.; McCammon, J. A., *Biophys. J.* **1995**, *68*, 62-68.
- [8.9] (a) Niu, C.; Xu, Y.; Xu, Y.; Luo, X.; Duan, W.; Silman, I.; Sussman, J. L.; Zhu, W.; Chen, K.; Shen, J.; Jiang, H., *J. Phys. Chem. B. Condens. Matter Mater. Surf. Interfaces Biophys.* **2005**, *109*, 23730-23738. (b) Senapati, S.; Bui, J. M.; McCammon, J. A., *J. Med. Chem.* **2005**, *48*, 8155-8162. (c) Kousba, A. A.; Sultatos, L. G.; Poet, T. S.; Timchalk, C., *Toxicol. Sci.* **2004**, *80*, 239-248. (d) Boyd, A. E.; Dunlop, C. S.; Wong, L.; Radic, Z.; Taylor, P.; Johnson, D. A., *J. Biol. Chem.* **2004**, *279*, 26612-26618. (e) Xu, Y.; Shen, J.; Luo, X.; Silman, I.; Sussman, J. L.; Chen, K.; Jiang, H., *J. Am. Chem. Soc.* **2003**, *125*, 11340-11349. (f) Bui, J. M.; Henchman, R. H.; McCammon, J. A., *Biophys. J.* **2003**, *85*, 2267-2272. (g) Kua, J.; Zhang, Y.; McCammon, J. A., *J. Am. Chem. Soc.* **2002**, *124*, 8260-8267. (h) Shen, T.; Tai, K.; Henchman, R. H.; McCammon, J. A., *Acc. Chem. Res.* **2002**, *35*, 332-340. (i) Shen, T. Y.; Tai, K.; McCammon, J. A., *Phys. Rev. E Stat. Nonlin. Soft Matter Phys.* **2001**, *63*, 041902. (j) Van Belle, D.; De Maria, L.; Iurcu, G.; Wodak, S. J., *J. Mol. Biol.* **2000**, *298*, 705-726. (k) Axelsen, P. H.; Harel, M.; Silman, I.; Sussman, J. L., *Protein Sci.* **1994**, *3*, 188-197.
- [8.10] (a) El Yazal, J.; Rao, S. N.; Mehl, A.; Slikker, W., Jr., *Toxicol. Sci.* **2001**, *63*, 223-232. (b) Mager, P. P.; Weber, A., *Drug Des. Discov.* **2003**, *18*, 127-150. (c) Zaheer-ul-Haq; Wellenzohn, B.; Tonmunpheap, S.; Khalid, A.; Choudhary, M. I.; Rode, B. M., *Bioorg. Med. Chem. Lett.* **2003**, *13*, 4375-4380. (d) Kurunczi, L.; Olah, M.; Oprea, T. I.; Bologa, C.; Simon, Z., *J. Chem. Inf. Model.* **2002**, *42*, 841-846. (e) Sippl, W.; Contreras, J. M.; Parrot, I.; Rival, Y. M.; Wermuth, C. G., *J. Comput. Aided Mol. Des.* **2001**, *15*, 395-410.

- (f) Spassova, D. P.; Singh, A. K., *SAR QSAR Environ. Res.* **2001**, 11, 453-471.
- (g) Kaur, J.; Zhang, M. Q., *Curr. Med. Chem.* **2000**, 7, 273-294. (h) Hasegawa, K.; Kimura, T.; Funatsu, K., *J. Chem. Inf. Model.* **1999**, 39, 112-120. (i) Recanatini, M.; Cavalli, A.; Hansch, C., *Chem. Biol. Interact.* **1997**, 105, 199-228. (j) Tong, W.; Collantes, E. R.; Chen, Y.; Welsh, W. J., *J. Med. Chem.* **1996**, 39, 380-387.
- [8.11] (a) Bernard, P.; Kireev, D. B.; Chretien, J. R.; Fortier, P. L.; Coppet, L., *J. Comput. Aided Mol. Des.* **1999**, 13, 355-371. (b) Inoue, A.; Kawai, T.; Wakita, M.; Iimura, Y.; Sugimoto, H.; Kawakami, Y., *J. Med. Chem.* **1996**, 39, 4460-4470. (c) Zaheer-Ul-Haq, Z. U.; Wellenzohn, B.; Liedl, K. R.; Rode, B. M., *J. Med. Chem.* **2003**, 46, 5087-5090. (d) Alisaraie, L.; Haller, L. A.; Fels, G., *J. Chem. Inf. Model.* **2006**, 46, 1174-1187. (e) da Silva, C. H.; Campo, V. L.; Carvalho, I.; Taft, C. A., *J. Mol. Graph. Model.* **2006**, 25, 169-175. (f) Xie, Q.; Tang, Y.; Li, W.; Wang, X. H.; Qiu, Z. B., *J. Mol. Model.* **2006**, 12, 390-397. (g) Alisaraie, L.; Fels, G., *J. Mol. Model.* **2006**, 12, 348-354. (h) Graves, A. P.; Brenk, R.; Shoichet, B. K., *J. Med. Chem.* **2005**, 48, 3714-3728. (i) Guo, J.; Hurley, M. M.; Wright, J. B.; Lushington, G. H., *J. Med. Chem.* **2004**, 47, 5492-5500. (j) Pilger, C.; Bartolucci, C.; Lamba, D.; Tropsha, A.; Fels, G., *J. Mol. Graph. Model.* **2001**, 19, 374-378.
- [8.12] (a) Rollinger, J. M.; Hornick, A.; Langer, T.; Stuppner, H.; Prast, H., *J. Med. Chem.* **2004**, 47, 6248-6254. (b) Dickerson, T. J.; Beuscher, A. E. 4th; Rogers, C. J.; Hixon, M. S.; Yamamoto, N.; Xu, Y.; Olson, A. J.; Janda, K. D., *Biochemistry* **2005**, 44, 14845-14853. (c) Mizutani, M. Y.; Itai, A., *J. Med. Chem.* **2004**, 47, 4818-4828.
- [8.13] MOE Program, version 2006-08 Chemical Computing Inc, Suite 910-1010 Sherbrooke St. W, Montreal, Quebec, Canada, H3A 2R7.
- [8.14] Alisi, M. A.; Brufani, M.; Filocamo, L.; Gostoli, G.; Licandro, E.; Cesta, M. C.; Lappa, S.; Marchesini, D.; Pagella, P., *Bioorg. Med. Chem. Lett.* **1995**, 5, 2077-2080.

References and Notes

- [8.15] Obata, R.; Sunazuka, T.; Ootoguro, K.; Tomoda, H.; Harigaya, Y.; Omura, S., *Bioorg. Med. Chem. Lett.* **2000**, 10, 1315-1316.
- [8.16] Clark, J. K.; Cowley, P.; Muir, A. W.; Palin, R.; Pow, E.; Prosser, A. B.; Taylor, R.; Zhang, M. Q., *Bioorg. Med. Chem. Lett.* **2002**, 12, 2565-2568.
- [8.17] Palin, R.; Clark, J. K.; Cowley, P.; Muir, A. W.; Pow, E.; Prosser, A. B.; Taylor, R.; Zhang, M. Q., *Bioorg. Med. Chem. Lett.* **2002**, 12, 2569-2572.
- [8.18] Rampa, A.; Bisi, A.; Belluti, F.; Gobbi, S.; Valenti, P.; Andrisano, V.; Cavrini, V.; Cavalli, A.; Recanatini, M., *Bioorg. Med. Chem.* **2000**, 8, 497-506.
- [8.19] Martinez, A.; Lanot, C.; Perez, C.; Castro, A.; Lopez-Serrano, P.; Conde, S., *Bioorg. Med. Chem.* **2000**, 8, 731-738.
- [8.20] Tabarrini, O.; Cecchetti, V.; Temperini, A.; Filipponi, E.; Lamperti, M. G.; Fravolini, A., *Bioorg. Med. Chem.* **2001**, 9, 2921-2928.
- [8.21] Bedford, C. D.; Harris, R. N., 3rd; Howd, R. A.; Miller, A.; Nolen, H. W., 3rd; Kenley, R. A., *J. Med. Chem.* **1984**, 27, 1431-1438.
- [8.22] Bedford, C. D.; Harris, R. N., 3rd; Howd, R. A.; Goff, D. A.; Koolpe, G. A.; Petesch, M.; Miller, A.; Nolen, H. W., 3rd; Musallam, H. A.; Pick, R. O., *J. Med. Chem.* **1989**, 32, 493-503.
- [8.23] Recanatini, M.; Cavalli, A.; Belluti, F.; Piazzini, L.; Rampa, A.; Bisi, A.; Gobbi, S.; Valenti, P.; Andrisano, V.; Bartolini, M.; Cavrini, V., *J. Med. Chem.* **2000**, 43, 2007-2018.
- [8.24] Halgren, T., *J. Comput. Chem.* **1996**, 17, 490-519.
- [8.25] *Catalyst* version 4.7, Accelrys: Burlington, MA.
- [8.26] GOLD 3.0, Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK.
- [8.27] Kryger, G.; Harel, M.; Giles, K.; Toker, L.; Velan, B.; Lazar, A.; Kronman, C.; Barak, D.; Ariel, N.; Shafferman, A.; Silman, I.; Sussman, J. L., *Acta Crystallogra. Sect. D* **2000**, 56, 1385-1394.
- [8.28] Berman, H. M.; Westbrook, J.; Feng, Z.; Gilliland, G.; Bhat, T. N.; Weissig, H.; Shindyalov, I. N.; Bourne, P. E., *Nucleic Acid Res.* **2000**, 28, 235-242.
<http://www.rcsb.org/pdb>

- [8.29] Irwin, J. J.; Shoichet, B. K., *J. Chem. Inf. Model.* **2005**, 45, 177-182.
- [8.30] Sussman, J. L.; Harel, M.; Frolow, F.; Oefner, C.; Goldman, A.; Toker, L.; Silman, I., *Science* **1991**, 253, 872-879.
- [8.31] Kirchmair, J.; Laggner, C.; Wolber, G.; Langer, T., *J. Chem. Inf. Model.* **2005**, 45, 422-430.
- [8.32] Kirchmair, J.; Wolber, G.; Laggner, C.; Langer, T., *J. Chem. Inf. Model.*, **2006**, 46, 1848-1861.