

Literatur

1. Von Dreele, R.B. 2003. Protein crystal structure analysis from high-resolution X-ray powder-diffraction data. *Macromolecular Crystallography* 386:255-267.
2. Huang, Y.P.J., Moseley H.N.B., Baran, M.C., Arrowsmith, C., Powers, R., Tejero, R., Szyperski, T., Montelione, G.T. 2005. An integrated platform for automated analysis of protein NMR structures. *Nucl. Magn. Res. Biol. Macromol.* 394:111.
3. Opella, S.J., F.M. Marassi. 2004. Structure determination of membrane proteins by NMR spectroscopy. *Chem. Rev.* 104:3587-3606.
4. Cornish, V.W., D.R. Benson, C.A. Altenbach, K. Hideg, W.L. Hubbell and P.G. Schutz. 1994. Site-specific incorporation of biophysical probes into proteins. *Proc. Natl. Acad. Sci. USA.* 91:2910-2914.
5. Becker, C., K. Lausecker, M. Balog, T. Kalai, K. Hideg, H.J. Steinhoff, M. Engelhardt. 2005. Incorporation of spin-labelled amino acids into proteins. *Magn. Res. Chem.* 43:S34-S39.
6. Hubbell, W.L., D.S. Cafiso, C. Altenbach. 2000. Identifying conformational changes with site-directed spin labeling. *Nat. Struct. Biol.* 7:735-739.
7. Hubbell, W.L., A. Gross, R. Langen, M.A. Lietzow. 1998. Recent advances in site-directed spin labeling of proteins. *Curr. Opin. Struct. Biol.* 8:649-656.
8. Langen, R., Oh, K.J, Cascio, D., Hubbell, W.L. 2000. Crystal Structures of Spin Labeled T4 Lysozyme Mutants: Implications for the Interpretation of EPR Spectra in Terms of Structure. *Biochemistry* 39:8396-8405.
9. Fanucci, G.E und D.S. Cafiso. 2006. Recent advances and applications of site-directed spin labeling. *Curr. Opin. Struct. Biol.* 16:644-653.
10. Hubbell, W.L., C. Altenbach. 1994. Investigation of structure and dynamics in membrane proteins using site-directed spin labeling. *Curr. Op. Struct. Biol.* 4:566-573.
11. Altenbach, C., K. Yang, D. Farrens, H.G. Khorana und W.L. Hubbell. 1996. Structural features and light-dependent changes in the cytoplasmic interhelical E-F loop region of rhodopsin: a site-directed spin labeling study. *Biochemistry.* 35:12470-12478.
12. Voss, J., M.M. He, W.L. Hubbell und H.R. Kaback. 1996. Site-directed spin labeling demonstrates that transmembrane Domain XII in the lactose permease of Escherichia Coli is an alpha-helix. *Biochemistry.* 35:12915-12918.
13. Hubbell, W.L., H.S: Mchaourab, C. Altenbach und M. Lietzow. 1996. Watching proteins move using site-directed spin labeling. *Structure.* 4: 779-783.
14. Fanucci, G.E., K.A. Cogshall, N. Cadieux, M. Kim, R.J. Kadner und D.S. Cafiso. 2003. Substrate-induced conformational changes of the periplasmic N-terminus of an outer-membrane transporter by site-directed spin labeling. *Biochemistry.* 42:1391-1400.
15. Steinhoff, H.J., R. Mollaaghababa, C. Altenbach, K. Hideg, M. Krebs, H. Khorana, W.L. Hubbel. 1994. Time-resolved detection of structural changes during the photocycle of spin labeled bacteriorhodopsin. *Science.* 266:105-107.

16. Mollaaghababa, R. H.J. Steinhoff, W.L. Hubbell, H.G. Khorana. 2000. Time-resolved site-directed spin-labeling studies of bacteriorhodopsin: Loop-specific conformational changes in M. *Biochemistry* 39: 1120-1127.
17. Farahbakhsh, Z., K. Hideg, W.L. Hubbell. 1993. Photoactivated conformational changes in rhodopsin: a time-resolved spin label study. *Science*. 262:1416-1420.
18. Möbius, K., A. Savitsky, C. Wegener, M. Rato, M. Fuchs, A. Schnegg, A.A. Dubinsky, Y.A. Grishin, I.A. Grigorev, M. Kuhn, D. Duche. 2005. Combining high-field EPR with site-directed spin labeling reveals unique information on proteins in action. *Magn. Res. Chem.* 43:S4-S19.
19. Jacobsen, K., S. Oga, W.L. Hubbell and T. Risse. 2005. Determination of the Orientation of T4 Lysozyme Vectorially Bound to a Planar-Supported Lipid Bilayer Using Site-Directed Spin Labeling. *Biophysical J.* 88:4351-4365.
20. Altenbach, C., W. Froncisz, R. Hemker, H. Mchaourab, W.L. Hubbell. 2005. Accessibility of nitroxide side chains: absolute Heisenberg exchange rates from power saturation EPR. *Biophys. J.* 89:2103-2112.
21. Farahbakhsh, Z., C. Altenbach, W.L. Hubbell. 1992. Spin labeled cysteins as sensors for protein-lipid interaction and conformation in rhodopsin. *Photochem. Photobiol.* 56:1019-1033.
22. Nielson, R.D., K. Che, M.H. Gelb, B.H. Robinson. 2005. A ruler for determining the position of proteins in membranes. *J. Am. Chem. Soc.* 127:6430-6442.
23. Altenbach, C. D. Greenhalgh, H.G. Khorana und W.L. Hubbell. 1994. A collision gradient method to determine the immersion depth of nitroxides in lipid bilayers: application to spin labeled mutants of bacteriorhodopsin. *Proc. Natl. Acad. Sci.* 91: 1667-1671.
24. Rabenstein, M.D., Y.K. Shin. 1995. Determination of the distance between two spin labels attached to a macromolecule. *Proc. Natl. Acad. Sci. USA* 92: 8239-8243.
25. Zhou, Z., S.C. DeSensi, R.A. Stein, S. Brandon, M. Dixit, E.J. McArdle, E.M. Warren, H.K. Kroh, L. Song, C.E. Cobb et al. 2005. Solution structure of the cytoplasmic domain of erythrocyte membrane band 3 determined by site directed spin labeling. *Biochemistry* 44:15115-15128.
26. Altenbach, C., K.J. Oh, R.J. Trabanino, K. Hideg, W.L. Hubbell. 2001. Estimation of inter-residue distances in spin labeled proteins at physiological temperatures: experimental strategies and practical limitations. *Biochemistry*. 40:15471-15482.
27. Steinhoff, H.J., N. Radzwill, W. Thevis, V. Lenz, D. Brandenburg, A. Antson, G. Dodson, A. Wollmer. 1997. Determination of Interspin Distances between Spin Labels Attached to Insulin: Comparison of Electron Paramagnetic Resonance Data with the X-Ray Structure. *Biophys. J.* 73:3287-3298.
28. Borbat, P.P., H. Mchaourab, H.J. Freed. 2002. Protein structure determination using long-distance constraints from double-quantum coherence ESR: study of T4 lysozyme. *J. Am. Chem. Soc.* 124:5304-5314.
29. Borovykh, I.V., S. Ceola, P. Gajula, P. Gast, H.J. Steinhoff, M. Huber. 2006. Distance between a native cofactor and a spin label in the reaction centre of Rhodobacter sphaeroides by a two-frequency pulsed electron paramagnetic resonance method and molecular dynamics simulations. *J. Mag. Res.* 180:178-185.
30. Jeschke, G. 2002. Distance measurements in the nanometer range by pulse EPR. *ChemPhysChem* 3:927-932.
31. Budil, D.E., S. Lee, S. Saxena and H.J. Freed. 1996. Nonlinear-Least-Squares Analysis of slow-motion EPR spectra in one and two Dimensions using a Modified Levenberg-Marquart algorithm. *J. Magn. Reson. A.* 120:155-189

32. Budil, D.E., K.L. Sale, K.A. Khairy and P.G. Fajer. 2006. Calculating Slow-Motional Electron Paramagnetic Resonance Spectra from Molecular Dynamics Using a Diffusion Operator Approach. *J. Phys. Chem. A*. 110:3703-3713.
33. Robinson, B.H., L.J. Slutsky and F.P. Auteri. 1992. Direct simulation of continuous wave electron paramagnetic resonance spectra from Brownian dynamics trajectories. *J. Chem. Phys.* 96:2609-2616.
34. Steinhoff, H.J. and W.L. Hubbell. 1996. Calculation of electron paramagnetic resonance spectra from Brownian dynamics trajectories: application to nitroxide side chains in proteins. *Biophys. J.* 71:2201-2212.
35. Steinhoff, H.J., M. Müller, C. Beier, M. Pfeiffer. 2000. Molecular dynamics simulation and EPR spectroscopy of nitroxide side chains in bacteriorhodopsin. *J. Mol. Liq.* 84:17-27.
36. Beier, C. and H.J. Steinhoff. 2006. A Structure-Based Simulation Approach for Electron Paramagnetic Resonance Spectra Using Molecular and Stochastic Dynamics Simulations. *Biophysical J.* 91:2647-2664.
37. Stoica, I. 2004. Using Molecular Dynamics To Simulate Electron Spin Resonance Spectra of T4 Lysozyme. *J. Phys. Chem. B*. 108: 1771-1782.
38. Arnold, G.E., R.L. Ornstein. 1997. Protein Hinge Bending as Seen in Molecular Dynamics Simulations of Native and M6I Mutant T4 Lysozymes. *Biopolymers*. 41: 533-544.
39. Goto, N.K., N.R. Skrynnikov, F.W. Dahlquist, L.E. Kay. 2001. What is the Average Conformation of Bacteriophage T4 Lysozyme in Solution? A Domain Orientation Study Using Dipolar Couplings Measured by Solution NMR. *J. Mol. Biol.* 308:745-764.
40. Arnold, G.E., J.I. Manchester, B.D. Townsend, R.L. Ornstein. 1994. Investigation of Domain Motions in Bacteriophage T4 Lysozyme. *J. Biomolec. Struc. Dyn.* 12:457-474.
41. Arnold, G.E., R.L. Ornstein. 1992. A molecular dynamics simulation of bacteriophage T4 Lysozyme. *Protein Engineering*. 5:703-714.
42. de Groot, B.L., S. Hayward, D.M.F. van Aalten, A. Amadei, H.J.C. Berendsen. 1998. Domain Motions in Bacteriophage T4 Lysozyme: A Comparison Between Molecular Dynamics and Crystallographic Data. *Proteins* 31:116-127.
43. Heinz, D.W., Baase, W.A., Dahlquist, F.W., Matthews, B.W. 1993. How amino-acid insertions are allowed in an alpha-helix of T4 lysozyme. *Nature*. 361:561-564.
44. Mayer-Kuckuk, T. 1985. Atomphysik. *Teubner Studienbücher, Stuttgart*.
45. Gordy, W. 1980. Theory and Applications of Electron Spin Resonance. *Wiley and Sons, New York*.
46. Weltner, W. 1989. Magnetic Atoms and Molecules. *Dover Publications, New York*.
47. Atherton, N.M. 1973. Electron Spin Resonance: Theory and Applications. *Wiley and Sons, New York*.
48. Atkins, P.W., R. S. Friedman. 1997. Molecular Quantum Mechanics. *Oxford University Press*.
49. Landau, L., E.M. Lifschitz. 1979. Quantenmechanik. *Akademie-Verlag, Berlin*.
50. Libertini, L.J., O.H. Griffith. 1970. Orientation Dependence of the Electron Spin Resonance Spectrum of Di-t-butyl Nitroxide. *J. Chem. Phys.* 53:1359-1367.
51. Slichter, C.P. 1990. Principles of Magnetic Resonance 1. Series in Solid-State Sciences. *Springer-Verlag, Berlin Heidelberg*.
52. Berendsen, H.J.C., D. van der Spoel, R. van Drunen. 1995. GROMACS: A message-passing parallel molecular dynamics implementation. *Comp. Phys. Comm.* 91:43-56.
53. Lindahl, E., B. Hess, D. van der Spoel. 2001. Gromacs 3.0: A package for molecular simulation and trajectory analysis. *J. Mol. Mod.* 7:306-317.

54. Van der Spoel, D., E. Lindahl, B. Hess, A.R. van Buren, E. Apol, P.J. Meulenhoff, D.P. Tieleman, A.L.T.M. Sijbers, K.A. Feenstra, R. van Drunen and H.J.C. Berendsen. 2004. Gromacs User Manual version 3.2. www.gromacs.org.
55. Cornell, W.D., P. Cieplak, C.I. Bayly, I.R. Gould, K. Merz, D.M. Ferguson, D.C. Spellmeyer, T. Fox, J.W. Caldwell, P.A. Kollman. 1995. A Second Generation Force Field for the Simulation of Proteins, Nucleic Acids and Organic Molecules. *J. Am. Chem. Soc.* 117:5179-5197.
56. Brooks, B.R., R.E. Bruccoleri, B.D. Olafson, D.J. States, S. Swaminathan, M. Karplus. 1982. CHARMM: A Program for Macromolecular Energy, Minimization, and Dynamics Calculations. *J. Comp. Chem.* 4:187-217.
57. MacKerell, A.D., D. Bashford, M. Bellott, R.L. Dunbrack, J.D. Evanseck, M.J. Field, S. Fischer, J. Gao, H. Guo, S. Ha et al., M. Karplus. 1998. All-Atom Empirical Potential for Molecular Modeling and Dynamics Studies of Proteins. *J. Phys. Chem. B.* 102:3586-3616.
58. Hockney, R.W., S. Goel, J. Eastwood. 1974. Quiet highresolution computer models of a plasma. *J. Com. Phys.* 14:148-158.
59. Berendsen, H.J.C. 1991. Transport properties computed by linear response through weak coupling to a bath. *Computer Simulations in Material Science.* 139-155.
60. Wolynes, P.G. and J.M. Deutch. 1977. Dynamical orientation correlations in solution. *J. Chem. Phys.* 67:733-741.
61. Van Gunsteren, W.F. and H.J.C. Berendsen. 1982. Algorithms for brownian dynamics. *Molecular Physics.* 45:637-647
62. Branca, A.C., D.M. Heyes. 1998. Algorithms for Brownian Dynamics Simulations. *Phys. Rev. E.* 58:2611-2615.
63. Budil, D.E., S. Lee, S. Saxena and H.J. Freed. 1996. Nonlinear-Least-Squares Analysis of slow-motion EPR spectra in one and two Dimensions using a Modified Levenberg-Marquart algorithm. *J. Magn. Reson. A.* 120:155-189.
64. Berliner, L.J., J. Reuben. 1989. Spin Labeling: Theory and Applications. Biological Magnetic Resonance 8. *Plenum Press, New York.*
65. Mchaourab, H.S., M.A. Lietzow, K. Hideg and W. Hubbell. 1996. Motion of Spin-Labeled Side Chains in T4 Lysozyme. Correlation with Protein Structure and Dynamics. *Biochemistry.* 35: 7692-7704.
66. Columbus, L., T. Kalai, J. Jeko, K. Hideg and W.L. Hubbell. 2001. Molecular Motion of Spin Labeled Side Chains in α -Helices: Analysis by Variation of Side Chain Structure. *Biochemistry.* 40:3828-3846.
67. Mchaourab, H.S., T. Kalai, K. Hideg and W. Hubbell. 1999. Motion of Spin-Labeled Side Chains in T4 Lysozyme: Effect of Side Chain Structure. *Biochemistry.* 38: 2947-2955.
68. Columbus, L. and W.L. Hubbell. 2004 Mapping Backbone Dynamics in Solution with Site-Directed Spin Labeling: GCN4-58 bZip Free and Bound to DNA. *Biochemistry* 43:7273-7287.
69. Columbus, L. and W.L. Hubbell. 2002, A new spin on protein dynamics. *TRENDS in Biochemical Sciences* 27:288-295.
70. Isas, J.M., R. Langen, H.T. Haigler, W.L. Hubbel. 2002. Structure and dynamics of a helical hairpin and loop region in Annexin 12:A site-directed spin labeling study. *Biochemistry.* 41:1464-1476.
71. Bell, J.A., K.P.Wilson, X.J. Zhang, H.R. Faber, H. Nicolson, B.W. Matthews. 1991. Comparison of the crystal Structure of Bacteriophage T4 lysozyme at low, medium, and high ionic strength. *Proteins* 10:10-21.
72. Kuroki, R. et al. 1993. A covalent enzyme-substrate intermediate with saccharide distortion in a mutant T4 Lysozyme. *Science.* 262: 2030-2033.

73. Timofeev, V.P. and V.I. Tsetlin. 1983. Analysis of mobility of protein side-chains by spin-label technique. *Biophys. Struct. Mech.* 10:93-108.
74. InsightII, Version 2005, Molecular Modeling System, Accelrys 2005, San Diego.
75. Herbst, A. Theoretische Simulationen zur Dynamik spin-markierter Proteine. 2003. *Diplomarbeit, FU Berlin.*
76. Gaussian 98, M.J. Frisch, G.W. Trucks, H.B. Schlegel, G.E. Scuseria, M.A. Robb, J.R. Cheeseman, V.G. Zakrzewski, J.A. Montgomery et al. 1998. Gaussian, Inc., Pittsburgh PA.
77. Boyd, D. 1972. Conformational dependence of the electronic energy levels in disulfides. *J. Am. Chem. Soc.* 94:8799-8804.
78. Jiao, D., M. Barfield, J.E. Combariza and V.J. Hruby. 1992. Ab initio molecular-orbital studies of the rotational barriers and the S-33 and C-13 chemical shieldings for dimethyl disulfide. *J. Am. Chem. Soc.* 114:3639-3643.
79. Fraser, R.R., G Boussard, J.K. Saunders, J.B. Lambert and C.E. Mixan. 1971. Barriers to rotation about sulfur-sulfur bond in acyclic disulfides. *J. Am. Chem. Soc.* 93: 3822-3823.
80. Murzyn, K., T. Rog, W. Blichatsky, M. Dutka, J. Pyka, S. Szytula, W. Froncisz. 2006. Influence of the Disulfide Bond Configuration on the Dynamics of the Spin Label Attached to Cytochrome c. *Proteins.* 62:1088-1100.
81. Improta, R., A. di Matteo, V. Barone. 2000. Effektive modeling of intrinsic and environmental effects on the structure and electron paramagnetic resonance parameters of nitroxides by an integrated quantum mechanical/molecular mechanics/polarizable continuum model approach. *Theor. Chem. Acc.* 104:273-279.
82. Pfeiffer, M., T. Rink, K. Gerwert, D. Oesterhelt, H.J. Steinhoff. 1999. Site-directed spin-labeling reveals the orientation of the amino acid side chains in the E-F loop of bacteriorhodopsin. *J. Mol. Biol.* 287:163-171.
83. Jorgensen, F.S., J.P. Snyder. 1979. Disulfide conformational analysis-the nature of the S-S rotation barrier. *Tetrahedron* 35:1399-1407.
84. Fleissner, M.R., D. Cascio, M.R. Sawaya, K. Hideg, W.L. Hubbell. Crystal structure data of T4 Lysozyme at 300K, unpublished results.
85. Katti, S.K., D.M. LeMaster. 1990. Crystal structure of Thioredoxin from Escherichia Coli at 1.68 Å Resolution. *J. Mol. Biol.* 212:167-184.
86. Rosenfeld, R.E.J., R. Parthasarathy. 1975. Structure and conformation of amino acids containing sulfur. *Acta Crystallogr., Sect. B* 31:462-468.
87. Risse, T., W.L. Hubbell, J.M. Isas, H.T. Haigler. 2003. Structure and dynamics of Annexin 12 bound to a planar lipid bilayer. *Phys. Rev. Lett.* 91.
88. Jacobsen, K., W.L. Hubbell, O.P. Ernst, T. Risse. 2006. Partielle Entfaltung von T4-Lysozym auf einer Quarzoberfläche: Analyse der Strukturänderungen adsorbierter Proteine durch ESR-Spektroskopie. *Angew. Chem.* 118:3959-3963.
89. Berendsen, H.J.C., J.P.M. Postma, W.F. van Gunsteren, J. Hermans. 1981. Intramolecular Forces. *Reidel, Dordrecht p.* 331.
90. Discover. May 1994. *Biosym Technologies, San Diego, CA*
91. Protein Data Bank, Kristallstrukturen von T4 Lysozym (1ZWN, 1ZUR, 1ZYT, 102L, 103L, 109L, 111L, 112L, 114L, 115L, 118L, 122L, 127L, 139L)
92. Palmer, A.G., III. 2004. NMR Characterization of the Dynamics of Biomacromolecules. *Chem. Rev.* 104:3623-3640.
93. Palmer, A.G., III., F. Massi. 2006. Characterization of the Dynamics of Biomacromolecules using Rotating-Frame Spin Relaxation NMR Spectroscopy. *Chem. Rev.* 106:1700-1719.
94. Massi, F., Palmer A.G. 2003. Temperature Dependence of NMR Order Parameters and Protein Dynamics. *J. Am. Chem. Soc.* 125:11158-11159.

95. Protein Data Bank, Kristallstrukturen von T4 Lysozym mit Spinsonde (2CUU (131R1), 1ZYT (82R1)).
96. Cafiso, D.S. 2002. Peptide-membrane interactions determined using site-directed spin labeling. *Current Topics in Membranes*. 52:3-29
97. Hubbell, W.L., personal communication.
98. Zeeman, P. 1897. *Phil. Mag.* 43:226.
99. Dee, K.C., D.A. Puleo, R. Bizios. 2002. Protein-surface interactions. *Tissue-Biomaterials Interactions* 45-49.
100. Latour, R.A. 2005. Biomaterials: Protein-Surface Interactions. *Encyclopedia of Biomaterials and Biomedical Engineering*. 1-15.
101. W.H. Press, Numerical Recipes in Fortran 77, Second Edition (1992)