Bibliography

Alexov, E. G., & Gunner, M. R. (1997). Incorporating protein conformational flexibility into the calculation of pH-dependent protein properties. *Biophys. J., 74,* 2075–2093.

Alexov, E. G., & Gunner, M. R. (1999). Calculated protein and proton motions coupled to electron transfer: Electron transfer from Q_A^- to Q_B in bacterial photosynthetic reaction centers. *Biochemistry, 38,* 8253–8270.

Allen, J. P., Feher, G., Yeates, T. O., Komiya, H., & Rees, D. C. (1987). Structure of the reation center from *Rhodobacter sphaeroides* R-26: The protein subunits. *Proc. Natl. Acad. Sci. U.S.A., 84,* 6162–6166.

Antosiewicz, J., Briggs, J. M., Elcock, A. H., Gilson, M. K., & McCammon, J. A. (1996). Computing ionization states of proteins with a detailed charge model. *J. Comput. Chem., 17,* 1633–1644.

Antosiewicz, J., McCammon, J. A., & Gilson, M. K. (1994). Prediction of pH-dependent properties of proteins. *J. Mol. Biol., 238,* 415–436.

Apostolakis, J., Muegge, I., Ermler, U., Fritzsch, G., & Knapp, E. W. (1996). Free energy computations on the shift of the special pair redox potential: Mutants of the reaction center of *Rhodobacter sphaeroides*. *J. Am. Chem. Soc., 118,* 3743–3752.

Arata, H., & Parson, W. W. (1981). Delayed fluorescence from *Rhodobacter sphaeroides* reaction centers — enthalpy and free-energy changes accompanying electron-transfer from P-870 to quinones. *Biochim. Biophys. Acta, 638,* 201–209.

Arnoux, B., Gaucher, J.-F., Ducruix, A., & Reiss-Husson, F. (1995). Structure of the photochemical reaction centre of a sphaeroidene-containing purple bacterium *Rhodobacter sphaeroides*. *Acta. Cryst. D, 51,* 368–379.

Baciou, L., Sinning, I., & Sebban, P. (1991). Study of Q_B^- stabilization in herbicide-resistant mutants from the purple bacterium *Rhodopseudomonas viridis. Biochemistry, 30*(37), 9110–9116.

Bartels, C., & Karplus, M. (1997). Multidimensional adaptive umbrella sampling: Applications to main chain and side chain peptide conformations. *J. Comput. Chem., 18,* 1450–1462.

Bartels, C., & Karplus, M. (1998). Probability distributions for complex systems: Adaptive umbrella sampling of the potential energy. *J. Phys. Chem. B, 102,* 865–880.

Bartels, C., Schaefer, M., & Karplus, M. (1998). Adaptive umbrella sampling of the potential energy: Modified updating procedure of the umbrella potential and application to peptide folding. *Theor. Chem. Acc., 101,* 62–66.

Bashford, D. (1997). An object-oriented programming suite for electrostatic effects in biological molecules. In Ishikawa, Y., Oldehoeft, R. R., Reynders, J. V. W., & Tholburn, M. (Eds.), *Scientific Computing in Object-Oriented Parallel Environments*, Vol. 1343 of *Lecture Notes in Computer Science*, pp. 233–240. Springer, Berlin.

Bashford, D., Case, D. A., Dalvit, C., Tennant, L., & Wright, P. E. (1993). Electrostatic calculations of side-chain pK_a values in myoglobin and comparison with NMR data for histidines. *Biochemistry*, *32*, 8045–8056.

Bashford, D., & Gerwert, K. (1992). Electrostatic calculations of the pK_a values of ionizable groups in bacteriorhodopsin. *J. Mol. Biol.*, *224*, 473–486.

Bashford, D., & Karplus, M. (1990). pK_as of ionizable groups in proteins: Atomic detail from a continuum electrostatic model. *Biochemistry*, *29*, 10219–10225.

Bashford, D., & Karplus, M. (1991). Multiple-site titration curves of proteins: An analysis of exact and approximate methods for their calculations. *J. Phys. Chem.*, *95*, 9557–9561.

Bastolla, U., Vendruscolo, M., & Knapp, E. W. (2000). A statistical mechanical method to optimize energy functions for protein folding. *Proc. Natl. Acad. Sci. U.S.A.*, *97*, 3977–3981.

Bates, S. P., van Well, W. J. M., van Santen, R. A., & Smit, B. (1997). Configurational-bias Monte Carlo (CB-MC) calculations of *n*-alkane sorption in zeolites rho and fer. *Molecular Simulation*, *19*, 301–318.

Berg, B. A., & Neuhaus, T. (1992). Multicanonical ensemble: A new approach to simulate first-order phase transitions. *Phys. Rev. Lett*, *68*, 9–12.

Beroza, P., & Fredkin, D. R. (1996). Calculation of amino acid pK_as in a protein from a continuum electrostatic model: Method and sensitivity analysis. *J. Comput. Chem.*, *17*, 1229–1244.

Beroza, P., Fredkin, D. R., Okamura, M. Y., & Feher, G. (1991). Protonation of interacting residues in a protein by a Monte Carlo method: Application to lysozyme and the photosynthetic reaction center. *Proc. Natl. Acad. Sci. U.S.A.*, *88*, 5804–5808.

Beroza, P., Fredkin, D. R., Okamura, M. Y., & Feher, G. (1995). Electrostatic calculation of amino acid titration and electron transfer $Q_A^- Q_B \rightarrow Q_A Q_B^-$ in the reaction center. *Biophys. J.*, *68*, 2233–2250.

Beroza, P., & Case, D. A. (1996). Including side chain flexibility in continuum calculations of protein titration. *J. Phys. Chem.*, *100*, 20156–20163.

Bonvin, A. M. J. J., & van Gunsteren, W. F. (2000). β-hairpin stability and folding: Molecular dynamics studies of the first β-hairpin of tendamistat. *J. Mol. Biol.*, *296*, 255–268.

Born, M. (1920). Volumen und Hydratationswärme der Ionen. *Z. Phys.*, *1*, 45–48.

Braun, W. (1987). Local deformation studies of chain molecules: Differential conditions for changes of dihedral angles. *Biopolymers*, *26*, 1691–1704.

Breneman, C. N., & Wiberg, K. B. (1990). Determining atom-centered monopoles from molecular electrostatic potentials. need for high sampling density in formamide conformational analysis. *J. Comput. Chem.*, *11*(3), 361–373.

Breton, J., Bibikova, M., Oesterhelt, D., & Nabedryk, E. (1999). Conformational heterogenity of the bacteriopheophytin electron acceptor H_A in reaction centers from *Rhodopseudomonas viridis* revealed by Fourier transform infrared spectroscopy and site-directed mutagenesis. *Biochemistry*, *28*, 11541–11552.

Breton, J., & Nabdryk, E. (1998). Proton uptake upon quinone reduction on bacterial reaction centers: IR signature and possible participation of highly polarizable hydrogen bond network. *Photosynth. Res.*, *55*, 301–307.

Breton, J., Navedryk, E., Mioskowski, C., & Boullais, C. (1996). Protein-quinone interactions in photosynthetic bacterial reaction centers investigated by light-induced FTIR difference spectroscopy. In Michel-Beyerle, M.-E. (Ed.), *The Reaction Center of Photosynthetic Bacteria — Structure and Dynamics*, pp. 381–394. Springer, Berlin.

Brooks, B. R., Bruccoleri, R. E., Olafson, B. D., States, D. J., Swaminathan, S., & Karplus, M. (1983). CHARMM: A program for macromolecular energy, minimization, and dynamics calculation. *J. Comput. Chem.*, *4*, 187–217.

Brzezinski, P., Paddock, M. L., Okamura, M. Y., & Feher, G. (1997). Light-induced electrogenic events associated with proton uptake upon forming Q_B^- in bacterial wild-type and mutant reaction centers. *Biochim. Biophys. Acta*, *1321*, 149–156.

Buono, G. S. D., Figueirisco, F. E., & Levy, R. (1994). Intrinsic pK_as of ionizable residues in proteins: An explicit solvent calculation for lysozyme. *Prot. Struct. Funct. Genet.*, *20*, 85–97.

Chang, C. H., El-Kabbani, O., Riede, D., Norris, J., & Schiffer, M. (1991). Structure of the membrane-bound protein photosynthetic reaction center from *Rhodobacter sphaeroides*. *Biochemistry*, *30*, 5353–5360.

Clementi, C., Vendruscolo, M., Maritan, A., & Domany, E. (1999). Folding Lennard-Jones protein by a contact potential. *Prot. Struct. Funct. Genet.*, *37*, 544–553.

Cometta-Morini, C., Scharnagl, C., & Fischer, S. F. (1993). Proton transfer to ubiquinone Q_B in the photosynthetic reaction center of *Rps. viridis*: The role of electrostatic interactions. *Int. J. Quantum Chem., Quantum Biol. Symp.*, *20*, 89–106.

Constanciel, R., & Contreras, R. (1984). Self-consistent field-theory of solvent effects representation by continuum models — introduction of desolvation contribution. *Theor. Chim. Acta*, *65*, 1–11.

Curado, E. M. F., & Tsallis, C. (1991). Generalized statistical mechanics: Connection with thermodynamics. *J. Phys. A*, *24*, L69–L72.

Daune, M. (1997). *Molekulare Biophysik*. Vieweg Verlag, Braunschweig.

Daura, X., Jaun, B., Seebach, D., van Gunsteren, W. F., & Mark, A. E. (1998). Reversible peptide folding in solution by molecular dynamics simulation. *J. Mol. Biol.*, *280*, 925–932.

Davidson, V. C. (1996). Unraveling the kinetic complexity of interprotein electron transfer reactions. *Biochemistry*, *35*(45), 14035–14039.

Deisenhofer, J., Epp, O., Miki, K., Huber, R., & Michel, H. (1985). Structure of the protein subunits in the photosynthetic reaction center of *Rhodopseudomonas viridis* at 3 Å resolution. *Nature*, *318*, 618–624.

Deisenhofer, J., Epp, O., Sinning, I., & Michel, H. (1995). Crystallographic refinement at 2.3 Å resolution and refined model of the photosynthetic reaction centre from *Rhodopseudomonas viridis*. *J. Mol. Biol.*, *246*, 429–457.

Demchuk, E., & Wade, R. C. (1996). Improving the continuum dielectric approach to calculating pK_as of ionizable groups in proteins. *J. Phys. Chem.*, *100*, 17373–17387.

Dinner, A. R., Lazaridis, T., & Karplus, M. (1999). Understanding β-hairpin formation. *Proc. Natl. Acad. Sci. U.S.A.*, *96*, 9068–9073.

Dodd, L., Boone, T., & Theodorou, D. (1993). A concerted rotation algorithm for atomistic Monte Carlo simulations of polymers and glasses. *Molec. Phys.*, *78*, 961–996.

Duan, Y., & Kollman, P. A. (1998). Pathways to a protein folding intermediate observed in a 1-microsecond simulation in aqueous solution. *Science*, *282*, 740–744.

Ermler, U., Fritzsch, G., Buchanan, S. K., & Michel, H. (1994). Structure of the photosynthetic reaction centre from *Rhodobacter sphaeroides* at 2.6 Å resolution: Cofactors and protein–cofactor interaction. *Structure*, *2*, 925–936.

Escobedo, F. A., & de Pablo, J. J. (1995). Extended continuum configurational bias Monte Carlo methods for simulation of flexible molecules. *J. Chem. Phys.*, *102*(6), 2636–2652.

Frishman, D., & Argos, P. (1995). Knowledge-based secondary structure assignment. *Prot. Struct. Funct. Genet.*, *23*, 566–579.

Fuchsman, W. H., & Appleby, C. A. (1979). CO and O_2 complexes of soybean leghemoglobins: pH effects upon infrared and visible spectra. Comparison with CO and O_2 complexes of myoglobin and hemoglobin. *Biochemistry*, *18*, 1309–1321.

Geyer, C. J. (1991). *Computing Science and Statistics*, pp. 156–163. American Statistical Association, New York.

Gibas, C. J., & Subramaniam, S. (1996). Explicit solvent models in protein pK_a calculations. *Biophys. J.*, *71*, 138–147.

Gilson, M. K., & Honig, B. H. (1991). The inclusion of electrostatic hydration energies in molecular mechanics calculations. *J. Comput.-Aided Mol. Des.*, *5*, 5–20.

Go, N., & Scheraga, H. A. (1970). Ring closure and local conformational deformations of chain molecules. *Macromolecules*, *3*, 178–187.

Grafton, A. K., & Wheeler, R. A. (1999). Amino acid protonation states determine binding sites of the secondary ubiquinone and its anion in the *Rhodobacter sphaeroides* photosynthetic reaction center. *J. Phys. Chem. B*, *103*, 5380–5387.

Graige, M. S., Feher, G., & Okamura, M. Y. (1998). Conformational gating of the electron transfer reaction $Q_A^- Q_B \rightarrow Q_A Q_B^-$ in bacterial reaction centers of *Rhodobacter sphaeroides* determined by driving force assay. *Proc. Natl. Acad. Sci. U.S.A.*, *95*, 11679–11684.

Graige, M. S., Paddock, M. L., Bruce, J. M., Feher, G., & Okamura, M. Y. (1996). Mechanism of proton-coupled electron transfer for quinone (Q_B) reduction in reaction centers of *Rb. sphaeroides*. *J. Am. Chem. Soc.*, *118*, 9005–9016.

Gunner, M. R., Nicholls, A., & Honig, B. (1996). Electrostatic potentials in *Rhodopseudomonas viridis* reaction centers: Implication for the driving force and directionality of electron transfers. *J. Phys. Chem.*, *100*, 4277–4291.

Gutowsky, H. S., Chuang, C., Keen, J. D., Klots, T. D., & Emilsson, T. (1985). Microwave rotational spectra, hyperfine interactions, and structure of the hydrogen-fluoride dimers. *J. Chem. Phys.*, *83*, 2070–2077.

Hagler, A. T., Huler, E., & Lifson, S. (1974). Energy function for peptides and proteins. I. Derivation of a consistent force field including the hydrogen bond from amide crystals. *J. Am. Chem. Soc.*, *96*, 5319–5335.

Hansmann, U. H. E. (1997). Parallel tempering algorithm for conformational studies of biological molecules. *Chem. Phys. Lett.*, *281*, 140–150.

Hansmann, U. H. E., Okamoto, Y., & Eisenmenger, F. (1996). Molecular dynamics, Langevin and hybrid Monte Carlo simulations in a multicanonical ensemble. *Chem. Phys. Lett.*, *259*, 321–330.

Hienerwadel, R., Grzybek, S., Fogel, C., Kreutz, W., Okamura, M. Y., Paddock, M. L., Breton, J., Nabedryk, E., & Mäntele, W. (1995). Protonation of Glu L212 following Q_B^- formation in the photosynthetic reaction center of *Rhodobacter sphaeroides*: Evidence from time-resolved infrared spectroscopy. *Biochemistry*, *34*(9), 2832–2843.

Hill, T. L. (1986). *An Introduction to Statistical Thermodynamics.* Dover Publications, New York.

Hoffmann, D., & Knapp, E. W. (1996a). Polypeptide Folding with Off-Lattice Monte Carlo Dynamics: the Method. *Eur. Biophys. J. , 24*, 387–403.

Hoffmann, D., & Knapp, E. W. (1996b). Protein Dynamics with Off-Lattice Monte Carlo Moves. *Phys. Rev. E, 53*, 4221–4224.

Hoffmann, D., & Knapp, E. W. (1997). Folding pathways of a helix–turn–helix model protein. *J. Phys. Chem. B*, *101*, 6734–6740.

Hoffmann, D., Washio, T., Jacob, J., & Gessler, K. (1998). Tackling concrete problems in molecular biophysics using Monte Carlo and related methods: Glycosylation, folding, solvation. In Grassberger, P., Barkema, G. T., & Nadler, W. (Eds.), *Monte Carlo Approach to Biopolymers and Protein Folding*, pp. 153–170. World Scientific, Singapore.

Hoffmann, D. (1996). *Monte Carlo Methoden zur Simulation der Langzeitdynamik von Proteinen*, Vol. 2 of *Wissenschaftliche Schriftenreihe Bioinformatik.* Verlag Dr. Köster, Berlin. Ph. D. thesis, Fachbereich Chemie, Freie Universität Berlin.

Holst, M. J., Kozack, R. E., Saied, F., & Subramiam, S. (1994). Treatment of electrostatic effect in proteins: Multigrid-based newton iterative method for solution of the full nonlinear Poisson-Boltzmann equation.. *Prot. Struct. Funct. Genet.*, *18*, 231–245.

Holst, M. J., & Saied, F. (1995). Numerical solution of the nonlinear Poisson-Boltzmann equation: Developing more robust and efficient methods. *J. Comput. Chem.*, *16*, 337–364.

Honig, B., & Nicholls, A. (1995). Classical electrostatics in biology and chemistry. *Science*, *268*, 1144–1149.

Hubbard, S. J., Eisenmenger, F., & Thornton, J. M. (1994). Modeling studies of the change in conformation required for cleavage of limited proteolytic sites. *Protein Science, 3*, 757–768.

Humphrey, W., Dalke, A., & Schulten, K. (1996). VMD — visual molecular dynamics. *J. Molec. Graphics, 14*, 33–38.

Jewsbury, P., & Kitagawa, T. (1994). The distal residue–CO interaction in carbonmonoxy myoglobins: a molecular dynamics study of the two distal histidine tautomers. *Biophys. J., 67*, 2236–2250.

Johnson, J. B., Lamb, D. C., Frauenfelder, H., Müller, J. D., McMahon, B., Nienhaus, G. U., & Young, R. D. (1996). Ligand binding to heme proteins. VI. Interconversion of taxonomic substates in carbonmonoxymyoglobin. *Biophys. J., 71*, 1563–1573.

Juffer, A. H., Argos, P., & Vogel, H. J. (1997). Calculating acid-dissociation constants of proteins using the boundary element method. *J. Phys. Chem. B, 101*(7664–7673).

Kabsch, W. (1976). A solution for the best rotation to relate two sets of vectors. *Acta Cryst., A 32*, 922–923.

Kabsch, W., & Sander, C. (1983). Dictionary of protein secondary structure: Pattern recognition of hydrogen-bonded and geometrical features. *Biopolymers, 22*, 2577–2637.

Kannt, A., Lancaster, C. R. D., & Michel, H. (1998). The coupling of electron transfer and proton translocation: Electrostatic calculations on *Paracoccus denitrificans* cytochrome *c* oxidase. *Biophys. J., 74*, 708–721.

Karplus, M., & Weaver, D. L. (1994). Protein folding dynamics: The diffusion–collision model and experimental data. *Protein Science, 3*, 650–668.

Kartha, S., Das, R., & Norris, J. R. (1991). Electron transfer in photosynthetic reaction centers. In Sigel, H. (Ed.), *Metal Ions in Biological Systems*, Vol. 27, chap. 10, pp. 323–359.

Kirkwood, J. G. (1934). Theory of solution of molecules containing widely separated charges with special application to zwitterions. *J. Chem. Phys., 2*, 351–361.

Klapper, I., Fine, R., Sharp, K. A., & Honig, B. H. (1986). Focusing of electric fields in the active site of Cu-Zn superoxide dismuatase: Effects of ionic strength and amino-acid modification. *Prot. Struct. Funct. Genet., 1*, 47–59.

Kleinfeld, D., Okamura, M. Y., & Feher, G. (1982). The redox free-energy difference between the primary and secondary electron acceptors in reaction centers from *Rhodobacter sphaeroides*. *Biophys. J., 37*, A110.

Kleinfeld, D., Okamura, M. Y., & Feher, G. (1984a). Electron transfer in reaction centers of *Rhodopseudomonas sphaeroides* — I. Determination of the charge recombination pathway of $D^+Q_AQ_B^-$ and free energy and kinetic relations between $Q_A^-Q_B$ and $Q_AQ_B^-$. *Biochim. Biophys. Acta, 766*, 126–140.

Kleinfeld, D., Okamura, M. Y., & Feher, G. (1984b). Electron-transfer kinetics in photosynthetic reaction centers cooled to cryogenic temperatures in the charge-separated state: Evidence for light-induced structural changes. *Biochemistry, 23*, 5780–5786.

Klopman, G. (1967). Solvations: A semi-empirical procedure for including solvation in quantum mechanical calculations of large molecules. *Chem. Phys. Lett., 1*, 200–202.

Knapp, E. W. (1992). Long time dynamics of a polymer with rigid monomer units relating to a protein model: Comparison with the rouse model. *J. Comput. Chem.*, *13*, 793–798.

Knapp, E. W., & Irgens-Defregger, A. (1993). Off-lattice Monte Carlo method with constraints: Long-time dynamics of a protein model without nonbonded interactions. *J. Comput. Chem.*, *14*, 19–29.

Knapp, E., & Irgens-Defregger, A. (1991). Long time dynamics of proteins: An off-lattice Monte Carlo method. In Harms, U. (Ed.), *Supercomputer and Chemistry*, Vol. 2, pp. 83–106. Springer, Berlin.

Koepf, E. K., Petrassi, H. M., Sudol, M., & Kelly, J. W. (1999). WW: An isolated three-stranded antiparallel β-sheet domain that unfolds and refolds reversibly; evidence for a stuctured hydrophobic cluster in urea and GdnHCl and a disordered thermal unfolded state. *Protein Science*, *8*, 841–853.

Koide, S., Huang, X., Link, K., Koide, A., Bu, Z., & Engelman, D. M. (2000). Design of single-layer β-sheets without a hydrophobic core. *Nature*, *403*, 456–460.

Kortemme, T., Ramírez-Alvarado, M., & Serrano, L. (1998). Design of a 20-amino acid, three-stranded β-sheet protein. *Science*, *281*, 253–256.

Kuriyan, J., Wilz, S., Karplus, M., & Petsko, G. A. (1986). X-ray structure and refinement of carbon-monoxy(Fe II)-myoglobin at 1.5 Å resolutions. *J. Mol. Biol.*, *192*, 133–154.

Lancaster, C. R. D., Ermler, U., & Michel, H. (1995). The structures of photosynthetic reaction centers from purple bacteria as revealed by x-ray crystallography. In Blankenship, R. E., Madigan, M. T., & Bauer, C. E. (Eds.), *Anoxygenic Photosynthetic Bacteria*, chap. 23, pp. 503–526. Kluwer Academic Publishers, Dordrecht.

Lancaster, C. R. D., & Michel, H. (1996). New insights into the x-ray structure of the reaction center from *Rhodopseudomonas viridis*. In Michel-Beyerle, M.-E. (Ed.), *The Reaction Center of Photosynthetic Bacteria*, pp. 23–35. Springer, Berlin.

Lancaster, C. R. D., & Michel, H. (1997). The coupling of light-induced electron transfer and proton uptake as derived from crystal structures of reaction centres from *Rhodopseudomonas viridis* modified at the binding site of the secondary quinone, Q_B. *Structure*, *5*, 1339–1359.

Lancaster, C. R. D., & Michel, H. (1999). Refined crystal structures of reaction centres from *Rhodopseudomonas viridis* in complexes with the herbicide atrazine and two chiral atrazine derivatives also lead to a new model of the bound carotenoid. *J. Mol. Biol.*, *286*, 883–898.

Lancaster, C. R. D., Michel, H., Honig, B., & Gunner, M. R. (1996). Calculated coupling of electron and proton transfer in the photosynthetic reaction center of *Rhodopseudomonas viridis*. *Biophys. J.*, *70*, 2469–2492.

Leach, A. R., & Lemon, A. P. (1998). Exploring the conformational space of protein side chains using dead-end elimination and the A* algorithm. *Prot. Struct. Funct. Genet.*, *33*, 227–239.

Li, J., Gilroy, D., Tiede, D. M., & Gunner, M. R. (1998). Kinetic phases in the electron transfer from $P^+Q_A^-Q_B$ to $P^+Q_AQ_B^-$ and the associated processes in *Rhodobacter sphaeroides* R-26 reaction centers. *Biochemistry*, *37*, 2818–2829.

Lide, D. R. (1992). *CRC Handbook of Chemistry and Physics* (73rd edition). CRC Press, Boca Raton.

Ma, B., & Nussinov, R. (1999). Explicit and implicit water simulations of a β-hairpin peptide. *Prot. Struct. Funct. Genet., 37*, 73–87.

Ma, B., & Nussinov, R. (2000). Molecular dynamics simulations of a β-hairpin fragment of protein G: Balance between side-chain and backbone forces. *J. Mol. Biol., 296*, 1091–1104.

MacKerell, A. D., Bashford, D., Bellott, M., Dunbrack Jr., R. L., Field, M. J., Fischer, S., Gao, J., Guo, H., Ha, S., Joseph, D., Kuchnir, L., Kuczera, K., Lau, F. T. K., Mattos, C., Michnik, S., Ngo, T., Nguyen, D. T., Prodhom, B., Roux, B., Schlenkrich, M., Smith, J. C., Stote, R., Straub, J., Wiorkiewicz-Kuczera, J., & Karplus, M. (1992). Self-consistent parameterization of biomolecules for molecular modeling and condensed phase simulation. *FASEB J., 6*, A143.

Mancino, L. J., Dean, D. P., & Blankenship, R. E. (1984). Kinetics and thermodynamics of the $P870^+Q_A^- \rightarrow P870^+Q_B^-$ reaction in isolated reaction centers from the photosynthetic bacterium *Rhodobacter sphaeroides*. *Biochim. Biophys. Acta, 764*, 46–54.

Marcus, R. A. (1956). On the theory of oxidation–reduction reactions involving electron transfer. *J. Chem. Phys., 24*, 966–978.

Marcus, R. A., & Sutin, N. (1985). Electron transfer in chemistry and biology. *Biochim. Biophys. Acta, 811*, 265–322.

Maróti, P., & Wraight, C. A. (1988). Flash-induced H^+ binding by bacterial photosynthetic reaction centers: Influences of the redox states of the acceptor quinones and primary donor. *Biochim. Biophys. Acta, 934*, 329–347.

Maynard, A. J., Sharman, G. J., & Searle, M. S. (1998). Origin of β-hairpin stability in solution: Structural and thermodynamic analysis of the folding of a model peptide supports hydrophobic stabilization in water. *J. Am. Chem. Soc., 120*, 1996–2007.

McDowell, S. A. C., & Buckingham, A. D. (1991). Isotope effects on the stability of the carbon monoxide–acetylene van der Waals molecule and the hydrogen fluoride dimer. *Chem. Phys. Lett., 182*, 551–555.

McPherson, P. H., Okamura, M. Y., & Feher, G. (1988). Light-induced proton uptake by photosynthetic reaction centers from *Rhodobacter sphaeroides* R-26. I. Protonation of the one-electron states $D^+Q_A^-$, DQ_A^-, $D^+Q_AQ_B^-$ and $DQ_AQ_B^-$. *Biochim. Biophys. Acta, 934*, 348–368.

McPherson, P. H., Okamura, M. Y., & Feher, G. (1993). Light-induced proton uptake by photosynthetic reaction centers from *Rhodobacter sphaeroides* R-26. II. Protonation of the state $DQ_AQ_B^{2-}$. *Biochim. Biophys. Acta, 1144*, 309–324.

McPherson, P. H., Schönfeld, M., Paddock, M. L., Okamura, M. Y., & Feher, G. (1994). Protonation and free energy changes associated with formation of Q_BH_2 in native and Glu-L212→Gln mutant reaction centers from *Rhodobacter sphaeroides*. *Biochemistry, 33*, 1181–1193.

McQuarrie, D. A. (1976). *Statistical Mechanics.* Harper & Row, New York.

Mendes, J., Baptista, A. M., Carrondo, M. A., & Soares, C. M. (1999). Improved modeling of side-chains on proteins with rotamer-based methods: a flexible rotamer model. *Prot. Struct. Funct. Genet., 37,* 530–543.

Miksovska, J., Schiffer, M., Hanson, D. K., & Sebban, P. (1999). Proton uptake by bacterial reaction centers: The protein complex responds in a similar manner to the reduction of either quinone acceptor. *Proc. Natl. Acad. Sci. U.S.A., 96*, 14348–14353.

Miksovska, J., Maróti, P., Tandori, J., Schiffer, M., Hanson, D. K., & Sebban, P. (1996). Distant electrostatic interactions modulate the free energy level of Q_A^- in the photosynthetic reaction center. *Biochemistry, 35*, 15411–15417.

Moore, G. R., & Pettigrew, G. W. (1990). *Cytochromes* c*: Evolutionary, Structural and Physicochemical Aspects.* Springer, Berlin.

Moret, M. A., Pascutti, P. G., Bisch, P. M., & Mundim, K. C. (1998). Stochastic molecular optimization using generalized simulated annealing. *J. Comput. Chem.*, *19*, 647–657.

Morrison, L. E., Schelhorn, J. E., Cotton, T. M., Bering, C. L., & Loach, P. A. (1982). Electrochemical and spectral properties of ubiquinone and synthetic analogs: Relevance to bacterial photosynthesis. In Trumpower, B. L. (Ed.), *Function of Quinones in Energy Conserving Systems*, chap. II.2, pp. 35–58. Academic Press, New York.

Muegge, I., Apostolakis, J., Ermler, U., Fritzsch, G., Lubitz, W., & Knapp, E. W. (1996). Shift of the special pair redox potential: Electrostatic energy computations of the mutants of the reaction center of *Rhodobacter sphaeroides. Biochemistry*, *35*(25), 8359–8370.

Muegge, I., Ermler, U., Fritsch, G., & Knapp, E. W. (1995). Free energy of cofactors at the quinone-Q_A site of the photosynthetic reaction center of *Rhodobacter spheroides* calculated by minimizing the statistical error. *J. Phys. Chem.*, *99*, 89–100.

Muñoz, V., Thompson, P. A., Hofrichter, J., & Eaton, W. A. (1997). Folding dynamics and mechanism of β-hairpin formation. *Nature*, *390*, 196–199.

Nabedryk, E., Breton, J., Hienerwadel, R., Fogel, C., Mäntele, W., Paddock, M. L., & Okamura, M. Y. (1995). Fourier transform infrared difference spectroscopy of secondary quinone acceptor photoreduction in proton transfer mutants of *Rhodobacter sphaeroides. Biochemistry*, *34*, 14722–14732.

Nabedryk, E., Breton, J., Okamura, M. Y., & Paddock, M. L. (1998). Proton uptake by carboxylic acid groups upon photoreduction of the secondary quinone (Q_B) in bacterial reaction centers from *Rhodobacter sphaeroides*: FTIR studies on the effects of replacing Glu H173. *Biochemistry*, *37*, 14457–14462.

Nicholls, A., & Honig, B. (1991). A rapid finite difference algorithm, utilizing successive overrelaxation to solve the Poisson-Boltzmann equation. *J. Comput. Chem.*, *12*, 435–445.

Nozaki, Y., & Tanford, C. (1967). Examination of titration behavior. *Methods Enzymol.*, *11*, 715–734.

Okamura, M. Y., & Feher, G. (1992). Proton transfer in reaction centers from photosynthetic bacteria. *Annu. Rev. Biochem.*, *61*, 861–896.

Osterhout Jr., J. J., Baldwin, R. L., York, E. J., Stewart, J. M., Dyson, J. M., & Wright, P. E. (1989). ^{1}H NMR studies of the solution conformations of an analogue of the C-peptide of ribonuclease A. *Biochemistry, 28*, 7059–7064.

Paddock, M. L., Feher, G., & Okamura, M. Y. (1997). Proton and electron transfer to the secondary quinone (Q_B) in bacterial reaction centers: The effect of changing the electrostatics in the vicinity of (Q_B) by interchanging Asp and Glu at the L212 and L213 sites. *Biochemistry*, *36*, 14238–14249.

Paddock, M. L., McPherson, P. H., Feher, G., & Okamura, M. Y. (1990). Pathway of proton transfer in bacterial reaction centers: Replacement of serine-L223 by alanine inhibits electron and proton tranfers associated with reduction of quinone to dihydroquinone. *Proc. Natl. Acad. Sci. U.S.A.*, *87*, 6803–6807.

Paddock, M. L., Rongey, S. H., Feher, G., & Okamura, M. Y. (1989). Pathway of proton transfer in bacterial reaction centers: Replacement of glutamic acid 212 in the L subunit by glutamine inhibits quinone (secondary acceptor) turnover. *Proc. Natl. Acad. Sci. U.S.A.*, *86*, 6602–6606.

Pak, Y., & Wang, S. (1999). Folding of a 16-residue helical peptide using molecular dynamics simulation with Tsallis effective potential. *J. Chem. Phys.*, *111*, 4359–4361.

Palmer, K. A., & Scheraga, H. A. (1991). Standard-geometry chains fitted to x-ray derived structures: Validation of the rigid-geometry approximation. I. Chain closure through a limited search of "loop" conformations. *J. Comput. Chem.*, *12*(4), 505–526.

Pande, V. S., & Rokhsar, D. S. (1999). Molecular dynamics simulations of unfolding and refolding of a β-hairpin fragment of protein G. *Proc. Natl. Acad. Sci. U.S.A.*, *96*, 9062–9067.

Pham, T.-N., Koide, A., & Koide, S. (1998). A stable single-layer β-sheet without a hydrophobic core. *Nature Structural Biology*, *5*, 115–119.

Press, W., Teukolsky, S., Vetterling, W., & Flannery, B. (1992). *Numerical Recipes in C* (2^{nd} edition). Cambridge University Press.

Prince, R. C., Dutton, P. L., & Bruce, J. M. (1983). Menaquinones and plastoquinones in aprotic solvents. *FEBS Lett.*, *160*, 273–276.

Rabenstein, B. (1997). Protonierungs- und Redoxzustände der Chinone im bakteriellen photosynthetischen Reaktionszentrum von *Rhodopseudomonas viridis*. Master's thesis, Fachbereich Chemie, Freie Universität Berlin.

Rabenstein, B. (1999). Karlsberg online manual. http://lie.chemie.fu-berlin/karlsberg/.

Rabenstein, B., Hoffmann, D., & Knapp, E. W. (1999). Simulation of oligopeptide folding or how do residues talk. In *Biological Physics - Third International Symposium*, Vol. 487 of *AIP Conference Proceedings*, pp. 54–68. American Institute of Physics, Melville, New York.

Rabenstein, B., & Knapp, E. W. (2000a). Calculated pH-dependent population of CO-myoglobin conformers. *Biophys. J.*, in press.

Rabenstein, B., & Knapp, E. W. (2000b). Problems evaluating energetics of electron transfer from Q_A^- to Q_B: the light-exposed and dark-adapted bacterial reaction center. In *ACS proceedings*, p. submitted. ACS.

Rabenstein, B., Ullmann, G. M., & Knapp, E. W. (1998a). Calculation of protonation patterns in proteins with structural relaxation and molecular ensembles — application to the photosynthetic reaction center. *Eur. Biophys. J.*, *27*, 626–637.

Rabenstein, B., Ullmann, G. M., & Knapp, E. W. (1998b). Energetics of electron transfer and protonation reactions of the quinones in the photosynthetic reaction center of *Rhodopseudomonas viridis*. *Biochemistry*, *37*, 2488–2495.

Rabenstein, B., Ullmann, G. M., & Knapp, E. W. (2000). Electron transfer between the quinones in the photosynthetic reaction center and its coupling to conformational changes. *Biochemistry, 39*, 10487–10496.

Ramachandran, G., Ramakrishnan, C., & Sasisekharan, V. (1963). Stereochemistry of polypeptide chain configurations. *J. Mol. Biol., 7*, 95–99.

Ramírez-Alvarado, M., Blanco, F. J., & Serrano, L. (1996). *De novo* design and structural analysis of a model β-hairpin system. *Nature Structural Biology, 3*, 604–612.

Ray, G. B., Li, X.-Y., Ibers, J. A., Sessler, J. L., & Spiro, T. G. (1994). How far can proteins bend the FeCO unit? Distal polar effects in heme proteins and models. *J. Am. Chem. Soc., 116*, 162–176.

Ripoll, D. R., Vorobjev, Y. N., Liwo, A., Vila, J. A., & Scheraga, H. A. (1996). Coupling between folding and ionization equilibria: Effects of pH on the conformational preferences of polypeptides. *J. Mol. Biol., 264*, 770–783.

Robson, B., & Garnier, J. (1988). *Introduction to Proteins and Protein Engineering*, pp. 86 f. Elsevier, Amsterdam.

Roccatano, D., Amadei, A., di Nola, A., & Berendsen, H. J. C. (1999). A molecular dynamics study of the 41–56 β-hairpin from B1 domain of protein G. *Protein Science, 8*, 2130–2143.

Sampogna, R. V., & Honig, B. (1994). Environmental effects on the protonation states of active site residues in bacteriorhodopsin. *Biophys. J., 66*, 1341–1352.

Sandberg, L., & Edholm, O. (1999). A fast and simple method to calculate protonation states in proteins. *Prot. Struct. Funct. Genet., 36*, 474–483.

Sartori, F. (1997). *Entwicklung einer Energiefunktion für die Dynamik von Polypeptiden im Raume der Torsionswinkel*. Ph.D. thesis, Fachbereich Chemie, Freie Universität Berlin.

Sartori, F., Melchers, B., Böttcher, H., & Knapp, E. W. (1998). An energy function for dynamics simulations of polypeptides in torsion angle space. *J. Chem. Phys., 108*, 8264–8276.

Sayle, R., & Bissell, A. (1992). RasMol: A program for fast realistic rendering of molecular structures with shadows. In *Proceedings of the 10th Eurographics UK '92 Conference*. University of Edinburgh.

Scarsi, M., Apostolakis, J., & Caflisch, A. (1997). Continuum electrostatic energies of macromolecules in aqueous solution. *J. Phys. Chem. A, 101*, 8098–8106.

Schaefer, M., Bartels, C., & Karplus, M. (1998). Solution conformations and thermodynamics of structured peptides: Molecular dynamics simulation with an implicit solvation model. *J. Mol. Biol., 284*, 835–848.

Schaefer, M., & Froemmel, C. (1990). A precise analytical method for calculating the electrostatic energy of macromolecules in aqueous solution. *J. Mol. Biol., 216*, 1045–1066.

Schaefer, M., & Karplus, M. (1996). A comprehensive analytical treatment of continuum electrostatics. *J. Phys. Chem., 100*, 1578–1599.

Schaefer, M., Sommer, M., & Karplus, M. (1997). pH-dependence of protein stability: Absolute electrostatic free energy differences between conformations. *J. Phys. Chem. B, 101*, 1663–1683.

Sebban, P., Maróti, P., & Hanson, D. K. (1995). Electron and proton transfer to the quinones in the bacterial photosynthetic reaction centers: Insight from combined approaches of molecular genetics and biophysics. *Biochimie, 77,* 677–694.

Sham, Y. Y., Chu, Z. T., & Warshel, A. (1997). Consistent calculation of pK_a's of ionizable residues in proteins: Semi-microscopic and microscopic approaches. *J. Phys. Chem. B, 101,* 4458–4472.

Sharp, K. A., & Honig, B. (1990). Electrostatic interactions in macromolecules. *Ann. Rev. Biophys. Biophys. Chem., 19,* 301–332.

Shire, S. J., Hanania, G. I. H., & Gurd, F. R. N. (1975). Electrostatic effects in myoglobin. application of the modified Tanford-Kirkwood theory to myoglobins from horse, california grey whale, harbor seal, and claifornia sea lion. *Biochemistry, 14,* 1352–1358.

Shopes, R. J., & Wraight, C. A. (1985). The acceptor quinone complex of *Rhodopseudomonas viridis* reaction centers. *Biochim. Biophys. Acta, 806,* 348–356.

Simonson, T., & Brooks, C. L. (1996). Charge separation and the dielectric constant of proteins: Insights from molecular dynamics. *J. Am. Chem. Soc., 118,* 8452–8458.

Simonson, T., & Perahia, D. (1995a). Internal and interfacial dielectric properties of cytochrome c from molecular dynamics in aqueous solution. *Proc. Natl. Acad. Sci. U.S.A., 92,* 1082–1086.

Simonson, T., & Perahia, D. (1995b). Microscopic dielectric properties of cytochrome c from molecular dynamics simulation in aqueous solution. *J. Am. Chem. Soc., 117,* 7987–8000.

Simonson, T., Perahia, D., & Bricogne, G. (1992). Intramolecular dielectric screening in proteins. *J. Mol. Biol., 218,* 859–886.

Sitkoff, D., Sharp, K. A., & Honig, B. (1994). Accurate calculation of hydration free energies using macroscopic solvent models. *J. Phys. Chem., 98,* 1978–1988.

Sklenar, H., Lavery, R., & Pullman, B. (1986). The flexibility of the nucleic acids: (I) "SIR", a novel approach to the variation of polymer geometry in constrained systems. *J. Biomol. Struct. Dynam., 3,* 967–987.

Sklenar, H., Eisenhaber, F., Poncin, M., & Lavery, R. (1990). Including solvent and counterion effects in the force fields of macromolecular mechanics: The field integrated electrostatic approach (FIESTA). In Beveridge, D. L., & Lavery, R. (Eds.), *Theoretical Biochemistry & Molecular Biophysics,* pp. 317–335. Adenine Press, New York.

Springer, B. A., Sliger, S. G., Olson, J. S., & Phillips Jr., G. N. (1994). Mechanisms of ligand recognition in myoglobin. *Chem. Rev., 94,* 699–714.

Still, W. C., Tempczyk, A., Hawley, R. C., & Hendrickson, T. (1990). Semianalytical treatment of solvation for molecular mechnics and dynamics. *J. Am. Chem. Soc., 112,* 6127–6129.

Stowell, M. H. B., McPhillips, T. M., Rees, D. C., Soltis, S. M., Abresch, E., & Feher, E. (1997). Light-induced structural changes in photosynthetic reaction center: Implications for mechanism of electron-proton transfer. *Science, 276,* 812–816.

Street, A. G., & Mayo, S. L. (1999). Intrinsic β-sheet propensities result from van der Waals interactions between side chains and the local backbone. *Proc. Natl. Acad. Sci. U.S.A., 96,* 9074–9076.

Stroop, R. (1993). Molekulardynamik-Simulation großer Protein-Wasser-Systeme: Das Reaktionszentrum der bakteriellen Photosynthese. Master's thesis, Fachbereich Chemie, Freie Universität Berlin.

Swallow, A. J. (1982). Physical chemistry of semiquinones. In Trumpower, B. L. (Ed.), *Function of Quinones in Energy Conserving Systems*, chap. II.3, pp. 59–72. Academic Press, New York.

Takahashi, E., & Wraight, C. A. (1992). Proton and electron transfer in the acceptor quinone complex of *Rhodobacter sphaeroides* reaction centers: Characterization of site-directed mutants of the two ionizable residues, Glu^{L212} and Asp^{L213}, in the Q_B binding site. *Biochemistry, 31*, 855–866.

Takano, M., Yamato, T., Higo, J., Suyama, A., & Nagayama, K. (1999). Molecular dynamics of a 15-residue poly(L-alanine) in water: Helix formation and energetics. *J. Am. Chem. Soc., 121*, 605–612.

Tandori, J., Sebban, P., Michel, H., & Baciou, L. (1999). In *Rhodobacter sphaeroides* reaction centers, mutation of proline L209 to aromatic residues in the vicinity of a water channel alters the dynamic coupling between electron and proton transfer processes. *Biochemistry, 38*, 13179–13187.

Tanford, C., & Kirkwood, J. G. (1957). Theory of protein titration curves. *J. Am. Chem. Soc., 79*, 5333–5347.

Tanokura, M. (1983). ^{1}H-NMR study on the tautomerism of the imidazole ring of histidine residues. I. Microscopic p*K* values and molar ratios of tautomers in histidine-contacting peptides. *Biochim. Biophys. Acta, 742*, 576–585.

Tiede, D. M., Vázquez, J., Córdova, J., & Marone, P. A. (1996). Time-resolved electrochromism associated with the formation of quinone anions in the *Rhodobacter sphaeroides* R26 reaction center. *Biochemistry, 35*(33), 10763–10775.

Tsallis, C., & Stariolo, D. A. (1996). Generalized simulated annealing. *Physica A, 233*, 395–406.

Ullmann, G. M. (1995). Analyse und Auswahl von Konformationen der Aminosäureseitenketten zur Simulation der Langzeitdynamik von Proteinen mit einer Monte-Carlo-Methode. Master's thesis, Universität Witten/Herdecke and Freie Universität Berlin.

Ullmann, G. M. (2000). The coupling of protonation and reduction in proteins with multiple redox centers. theory, computational method, and application to cytochrome c3. *J. Phys. Chem. B, 104*, 6293–6301.

Ullmann, G. M., Hauswald, M., Jensen, A., & Knapp, E. W. (2000). Superposition of ferredoxin and flavodoxin using their electrostatic potentials. Implications for their interactions with photosystem I and ferredoxin:NADP reductase. *Prot. Struct. Funct. Genet., 38*, 301–309.

Ullmann, G. M., Hauswald, M., Jensen, A., Kostić, N. M., & Knapp, E. W. (1997). Comparison of the physiologically-equivalent proteins cytochrome c_6 and plastocyanin on the basis of their electrostatic potentials. Tryptophane 63 in cytochrome c_6 may be isofunctional with tyrosine 83 in plastocyanin. *Biochemistry, 36*, 16187–16196.

Ullmann, G. M., & Knapp, E. W. (1999). Electrostatic models for computing protonation and redox equilibria in proteins. *Eur. Biophys. J. , 28*, 533–551.

Ullmann, G. M., Knapp, E. W., & Kostić, N. M. (1997). Computational simulation and analysis of the dynamic association between plastocyanin and cytochrome *f*. Consequences for the electron-transfer reaction. *J. Am. Chem. Soc.*, *119*, 42–52.

Ullmann, G. M., & Kostić, N. M. (1995). Electron-tunneling paths in various electrostatic complexes between cytochrome c and plastocyanin. Anisotropy of the copper-ligand interactions and dependence of the iron-copper electronic coupling on the metalloprotein orientation. *J. Am. Chem. Soc.*, *117*, 4766–4774.

Ullmann, G. M., Muegge, I., & Knapp, E.-W. (1996). Shifts of the special pair redox potential of mutants of *Rhodobacter sphaeroides* calculated with Delphi and Charmm energy functions. In Michel-Beyerle, E. M. (Ed.), *The Reaction Centers of Photosynthetic Bacteria. Structure and Dynamics*, pp. 143–155. Springer, Berlin.

Vagedes, P., Rabenstein, B., Åqvist, J., Marelius, J., & Knapp, E. W. (2000). The deacylation step of acetylcholinesterase: Computer simulation studies. *J. Am. Chem. Soc.*, in press.

van Gunsteren, W., & Karplus, M. (1981). Effects of constraints, solvent and crystal enviroment on protein dynamics. *Nature*, *293*, 677–678.

Vendruscolo, M., Najmanovich, R., & Domany, E. (2000). Can a pairwise contact potential stabilize native protein folds against decoys obtained by threading?. *Prot. Struct. Funct. Genet.*, *38*, 134–148.

Vila, J. A., Ripoll, D. R., Vorobjev, Y. N., & Scheraga, H. A. (1998). Computation of the structure-dependent pK_a shifts in a polypentapeptide of the poly[f_V(IPGVG),f_E(IPGEG)] family. *J. Phys. Chem. B*, *102*, 3065–3067.

Wang, H., & Sung, S.-S. (2000). Molecular dynamics simulations of three-strand β-sheet folding. *J. Am. Chem. Soc.*, *122*, 1999–2009.

Wang, H., Warady, J., Ng, L., & Sung, S.-S. (1999). Molecular dynamics simulations of β-hairpin folding. *Prot. Struct. Funct. Genet.*, *37*, 325–333.

Warshel, A., Russell, S. T., & Churg, A. K. (1984). Macroscopic models for studies of electrostatic interactions in proteins: Limitations and applicability. *Proc. Natl. Acad. Sci. U.S.A.*, *81*, 4785–4789.

Warshel, A., & Åqvist, J. (1991). Electrostatic energy and macromolecular function. *Ann. Rev. Biophys. Biophys. Chem.*, *20*, 267–298.

Warshel, A., Papazyan, A., & Muegge, I. (1997). Microscopic and semimacroscopic redox calculations: What can and cannot be learned from continuum models. *JBIC*, *2*, 143–152.

Warshel, A., & Russel, S. T. (1984). Calculations of electrostatic interaction in biological systems and in solution. *Q. Rev. Biophys.*, *17*, 283–422.

Warwicker, J., & Watson, H. C. (1982). Calculation of the electric potential in the active site cleft due to α-helix dipoles. *J. Mol. Biol.*, *157*, 671–679.

Wavefunction, Inc., Irvine, CA (1995). Spartan version 4.0..

Wilbur, D. J., & Allerhand, A. (1976). Titration behavior of individual tyrosine residues of myoglobins from sperm whale, horse, and red kangaroo: Application of natural abundance carbon 13 nuclear magnetic resonance spectroscopy. *J. Biol. Chem.*, *251*, 5187–5194.

Williams, R. W., Chang, A., Juretić, D., & Loughran, S. (1987). Secondary structure predictions and medium range interactions. *Biochim. Biophys. Acta*, *916*, 200–204.

Wlodek, S. T., Antosiewicz, J., & McCammon, J. A. (1997). Prediction of titration properties of structures of a protein derived from molecular dynamics trajectory. *Protein Science*, *6*, 373–382.

Wraight, C. A. (1979). Electron acceptors of bacterial photosynthetic reaction centers. 2. H^+ binding coupled to secondary electron transfer in the quinone acceptor complex. *Biochim. Biophys. Acta*, *548*, 309–327.

Wraight, C. A., & Stein, R. R. (1980). Redox equilibrium in the acceptor quinone complex of isolated reaction centers and the mode of action of o-phenanthroline. *FEBS Lett.*, *113*, 73–77.

Wu, M. G., & Deem, M. W. (1999). Analytical rebridging Monte Carlo: Application to *cis/trans* isomerization in proline-containing, cyclic peptides. *J. Chem. Phys.*, *111*, 6625–6632.

Yang, A.-S., Gunner, M. R., Sompogna, R., & Honig, B. (1993). On the calculation of pK_as in proteins. *Prot. Struct. Funct. Genet.*, *15*, 252–265.

Yang, A.-S., & Honig, B. (1994). Structural origins of pH and ionic strength effects on protein stability. *J. Mol. Biol.*, *237*, 602–614.

Yang, F., & Phillips Jr., G. N. (1996). Crystal structure of CO-, deoxy- and met-myoglobins at various pH values. *J. Mol. Biol.*, *256*, 762–774.

You, T., & Bashford, D. B. (1995). Conformation and hydrogen ion titration of proteins: A continuum electrostatic model with conformational flexibility. *Biophys. J.*, *69*, 1721–1733.

Zauhar, R. Y., & Varnek, A. (1996). A fast and space-efficient boundary element method for computing electrostatic and hydration effects in large molecules. *J. Comput. Chem.*, *17*, 864–877.

Zhou, J. S., & Kostić, N. M. (1993). Gating of photoinduced electron transfer from zinc cytochrome *c* and tin cytochrome *c* to plastocyanin. effects of solution viscosity on rearrangements of the metalloprotein complex. *J. Am. Chem. Soc.*, *115*, 10796–10804.

Zwanzig, R., Szabo, A., & Bagchi, B. (1992). Levinthal's paradox. *Proc. Natl. Acad. Sci. U.S.A.*, *89*, 20–22.