

## 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.

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.

Aubert, C., Guidici-Orticoni, M. T., Czjzek, M., Haser, R., Bruschi, M., & Dolla, A. (1998). Structural and kinetic studies of the Y73E-mutant of octaheme cytochrome c<sub>3</sub> (Mr =26000) from *desulfovibrio desulfuricans* Norway. *Biochemistry*, **37**, 2120-2130.

Aubert, C., Mathis, P., Eker, A. P. M., & Brettel, K. (1999a). Intraprotein electron transfer between tyrosine and tryptophan in DNA photolyase from *Anacystis nidulans*. *Proc. Natl. Acad. Sci. U. S. A.*, **96**, 5423-5427.

Aubert, C., Brettel, K., Mathis, P., Eker, A. P. M., & Boussac, A. (1999b). EPR detection of the transient tyrosyl radical in DNA photolyase from *Anacystis nidulans*. *J. Am. Chem. Soc.*, **121**, 8659-8660.

Aubert, C., Vos, M. H., Mathis, P., Eker, A. P. M., & Brettel, K. (2000). Intraprotein radical transfer during photoactivation of DNA photolyase. *Nature*, **405**, 586-590.

Baptista, A. M., Martel, P. J., & Soares, C. M. (1999). Simulation of electron-proton coupling with a Monte Carlo method: Application to cytochrome c<sub>3</sub> using continuum electrostatics. *Biophys. J.*, **76**, 2978-2998.

Barry, B. A., & Babcock, G. T. (1987). Tyrosine radicals are involved in the photosynthetic oxygen-evolving systems. *Proc. Natl. Acad. Sci. U. S. A.*, **84**, 7099-7103.

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<sub>a</sub> values in myoglobin and comparison with NMR data for histidines. *Biochemistry*, **32**, 8045-8056.

Bashford, D., & Gerwert, K. (1992). Electrostatic calculations of the pK<sub>a</sub> values of ionizable groups in bacteriorhodopsin. *J. Mol. Biol.*, **224**, 473-486.

Bashford, D., & Karplus, M. (1990). pK<sub>a</sub>s 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.

Bayly, C. I., Cieplak, P., Cornell, W. D., & Kollman, P. A. (1993). A well-behaved electrostatic potential based method using charge restraints for deriving atomic charges: The RESP model. *J. Phys. Chem.*, **97**, 10269-10280.

Berman, H. M., Westbrook, J., Feng, Z., Gilliland, G., Bhat, T. N., Weissig, H., Shindyalov, I. N., & Bourne, P. E. (2000). The Protein Data Bank. *Nucleic Acids Research*, **28**, 235-242.

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

Beroza, P., & Case, D. A. (1998). Calculations of proton-binding thermodynamics in proteins. *Methods Enzymol.*, **295**, 170-189.

Beroza, P., & Fredkin, D. R. (1996). Calculation of amino acid pK<sub>a</sub>s in a protein from a continuum electrostatic model: Model and sensitivity analysis. *J. Comput. Chem.*, **17**, 1229-1244.

Beroza, P., Fredkin, D. R., Okamura, M. Y., & Feher, G. (1991). Protonation of interesting 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.

Besler, B. H., Merz, K. M., & Kollman, P. A. (1990). Atomic charges derived from semiempirical methods. *J. Comp. Chem.*, **11**, 431-439.

Betz, S. F., & DeGrado, W. F. (1996). Controlling topology and native-like behavior of *de novo*-designed peptides: Design and characterization of antiparallel four-stranded coiled coils. *Biochemistry*, **35**, 6955-6962.

Betz, S. F., Liebman, P. A., & DeGrado, W. F. (1997). De novo design of native proteins: Characterization of proteins intended to fold into antiparallel, rop-like, four-helix bundles. *Biochemistry*, **36**, 2450-2458.

Betz, S. F., Marmorino, J. L., Saunders, A. J., Doyle, D. F., Young, G. B., & Pielak, G. J. (1996). Unusual effects of an engineered disulfide on global and local protein stability. *Biochemistry*, **35**, 7422-7428.

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

Brandt, U. (1996). Bifurcated ubihydroquinone oxidation in cytochrome *bc<sub>1</sub>* complex by proton-gated charge transfer. *FEBS Letters*, **387**, 1-6.

- Brandt, U. (1998). The chemistry and mechanics of ubihydroquinone oxidation at center P (Q<sub>o</sub>) of the cytochrome *bc*<sub>1</sub> complex. *Biochim. Biophys. Acta-Bioenerg.*, **1365**, 261-268.
- Brandt, U., & Trumppower, B. (1994). The proton motive Q cycle in mitochondria. *Crit. Rev. Biochem. Mol. Biol.*, **29**, 165-197.
- Braun, H.-P., Emmermann, M., Kruft, V., & Schmitz, U. K. (1992). The general mitochondrial processing peptidase from potato is an integral part of cytochrome *c* reductase of the respiratory chain. *EMBO J.*, **11**, 3219-3227.
- Braun, H.-P., & Schmitz, U. K. (1995). Are the core proteins of the mitochondrial *bc*<sub>1</sub> complex evolutionary relics of a processing protease. *Trends Biochem. Sci.*, **20**, 171-175.
- Breneman, C. N., & Wiberg, K. B. (1990). Determining atom-centered monopoles from molecular electrostatic potentials. The need for high sampling density in formamide conformational analysis. *J. Comp. Chem.*, **11**, 361-373.
- 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. Comp. Chem.*, **4**, 187-217.
- Bryson, J. W., Betz, S. F., Lu, H. S., Suich, D. J., Zhou, H. X., O'Neil, K. T., & DeGrado, W. F. (1995). Protein design – a hierarchical approach. *Science*, **270**, 935-941.
- Cashmore, A. R., Jarillo, J. A., Xu, Y.-J., & Liu, D. (1999). Cryptochromes: blue light receptors for plants and animals. *Science*, **284**, 760-765.
- Cheung, M. S., Daizadeh, I., Stuchebrukhov, A. A., & Heelis, P.F. (1999) Pathways of electron transfer in Escherichia coli DNA photolyase: Trp(306) to FADH. *Biophysical J.*, **76**, 1241-1249.
- Choma, C. T., Lear, J. D., Nelson, M. J., Dutton, P. L., Robertson, D. E., & DeGrado, W. F. (1994). Design of a heme-binding four-helix bundle. *J. Am. Chem. Soc.*, **116**, 856-865.
- Cometta-Morini, C., Scharnagl, C., & Fischer, S. F. (1993). Proton transfer to ubiquinone Q<sub>B</sub> in the photosynthetic reaction center of *Rps. viridis*: The role of electrostatic interactions. *Int. J. Quantum Chem. Quantum Biol. Symp.*, **20**, 89-106.
- Cornell, W. D., Cieplak, P., Bayly, C. I., & Kollman, P. A. (1993). Application of RESP charges to calculate conformational energies, hydrogen bond energies, and free energies of solvation. *J. Am. Chem. Soc.*, **115**, 9620-9631.
- Crofts, A. R. (1985). in *The Enzymes of Biological Membranes*, Vol. 4 (ed. Martonosi, A. N.) 347-382 (Plenum, New York, 1985).
- Daune, M. (1997). *Molekulare Biophysik*. Vieweg Verlag, Braunschweig.
- DeFelippis, M. R., Murthy, C. P., Broitman, F., Weinraub, D., Faraggi, M., & Klapper, M. H. (1991). Electrochemical properties of tyrosine phenoxy and tryptophan indolyl radicals in peptides and amino acid analogues. *J. Phys. Chem.*, **95**, 3416-3419.

- Demchuck, E., & Wade, R. C. (1996). Improving the continuum dielectric approach to calculating pK<sub>a</sub>s of ionizable groups in proteins. *J. Phys. Chem.*, **100**, 17373-17387.
- Dixon, W. T., & Murphy, D. (1976). Determination of the acidity constants of some phenol radical cations by means of electron spin resonance. *J. Chem. Soc. Faraday Trans.*, **272**, 1221-1230.
- Dutton, P. L., & Wilson, D. F. (1974). Redox potentiometry in mitochondrial and photosynthetic bioenergetics. *Biochim. Biophys. Acta*, **346**, 165-212.
- Dutton, P. L., Wilson, D. F., & Lee, C. P. (1970). Oxidation-reduction potentials of cytochromes in mitochondria. *Biochemistry*, **9**, 5077-5082.
- Engel, W. D., Schaegger, H., & von Jagow, G. (1980). Ubiquinol-cytochrome *c* reductase (EC 1.10.2.2). Isolation in Triton X-100 by hydroxyapatite and gel chromatography. *Biochim. Biophys. Acta*, **592**, 211-222.
- Fahnenschmidt, M., Rau, H. K., Bittl, R., Haehnel, W., & Lubitz, W. (1999). Characterization of a de novo designed heme protein by EPR and ENDOR spectroscopy. *Chem. Eur. J.*, **5**, 2327-2334.
- Frisch, M. J., Trucks, G. W., Schlegel, H. B., Scuseria, G. E., Robb, M. A., Cheeseman, J. R., Zakrzewski, V. G., Montgomery, J. A., Stratmann, Jr., R. E., Burant, J. C., Dapprich, S., Millam, J. M., Daniels, A. D., Kudin, K. N., Strain, M. C., Farkas, O., Tomasi, J., Barone, V., Cossi, M., Cammi, R., Mennucci, B., Pomelli, C., Adamo, C., Clifford, S., Ochterski, J., Petersson, G. A., Ayala, P. Y., Cui, Q., Morokuma, K., Malick, D. K., Rabuck, A. D., Raghavachari, K., Foresman, J. B., Cioslowski, J., Ortiz, J. V., Stefanov, B. B., Liu, G., Liashenko, A., Piskorz, P., Komaromi, I., Gomperts, R., Martin, R. L., Fox, D. J., Keith, T., Al-Laham, M. A., Peng, C. Y., Nanayakkara, A., Gonzalez, C., Challacombe, M., Gill, P. M. W., Johnson, B., Chen, W., Wong, M. W., Andres, J. L., Gonzalez, C., Head-Gordon, M., Replogle, E. S., & Pople, J. A. (1998). Gaussian 98, Revision A.6. Gaussian, Inc., Pittsburgh PA.
- Gabellini, N., Bowyer, J. R., Hurt, E., Melandri, B. A., & Hauska, G. (1982). A cytochrome *bc*<sub>1</sub> complex with ubiquinol-cytochrome *c*<sub>2</sub> oxidoreductase activity from *Rhodopseudomonas sphaeroides* GA. *Eur. J. Biochem.*, **126**, 105-111.
- Gabellini, N., & Hauska, G. (1983). Characterization of cytochrome *b* in the isolated ubiquinol-cytochrome *c*<sub>2</sub> oxidoreductase from *Rhodopseudomonas sphaeroides* GA. *FEBS Letters*, **153**, 146-150.
- Gallivani, J. P., & Dougherty, D. A. (1999). Cation- $\pi$  interactions in structural biology. *Proc. Natl. Acad. Sci. U. S. A.*, **96**, 9459-9464.
- Ghosh, A., Gonzales, E., & Vangberg, T. (1999). Theoretical Studies of low-spin six-coordinate iron(III) porphyrins relevant to cytochromes b: variable electronic configurations, ligand noninnocence, and macrocycle ruffling. *J. Phys. Chem.*, **103**, 1363-1367.
- Gibas, C. J., & Subramaniam, S. (1996). Explicit solvent models in protein pK<sub>a</sub> calculations. *Biophys. J.*, **71**, 138-147.

Gibney, B. R., Isogai, Y., Rabanal, F., Reddy, K. S., Grosset, A. M., Moser, C. C., & Dutton, P. L. (2000). Self-assembly of heme A and heme B in a designed four-helix bundle: Implications for a cytochrome *c* oxidase maquette. *Biochemistry*, **39**, 11041-11049.

Gilson, M. K. (1993). Multiple-site titration and molecular modelling: Two rapid methods for computing energies and forces for ionizable groups in proteins. *Proteins*, **15**, 266-282.

Gilson, M. K. (1995). Theory of electrostatic interactions in macromolecules. *Curr. Opin. Struct. Biol.*, **5**, 216-223.

Gilson, M. K., & Honig, B. (1986). The dielectric constant of a folded proteins. *Biopolymers*, **25**, 2097-2119.

Gräslund, A., & Sahlin, M. (1996). Electron paramagnetic resonance and nuclear magnetic resonance studies of class I ribonucleotide reductase. *Ann. Rev. Biophys. Biomol. Struct.*, **25**, 259-286.

Gunner, M. R., & Honig, B. (1991). Electrostatic control of midpoint potentials in the cytochrome subunit of the *Rhodopseudomonas viridis* reaction center. *Proc. Natl. Acad. Sci. U. S. A.*, **88**, 9151-9155.

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

Gunner, M. R., Saleh, M. A., Cross, E., ud-Doula, A., & Wise, M. (2000). Backbone dipoles generate positive potentials in all proteins: Origins and implications of the effect. *Biophys. J.*, **78**, 1126-1140.

Hahn, J., Michel-Beyerle, M. E., & Rösch, N. (1998). Conformation of the flavin adenine dinucleotide cofactor FAD in DNA-photolyase: A molecular dynamics study. *J. Mol. Model.*, **4**, 73-82.

Harbury, H. A., Cronin, J. R., Fauger, M. W., Hettinger, T. P., Murphy, A. J., Myer, Y. P., & Vinogradov, S. N. (1965). Complex formation between methionine and a heme peptide from cytochrome *c*. *Proc. Natl. Acad. Sci. U. S. A.*, **54**, 1658-1664.

Harm, W. (1980). Biological effects of ultraviolet radiation. Cambridge University Press, New York.

Harris, D., Loew, G., & Waskell, L. (1998). Structure and spectra of ferrous dioxygen and reduced ferrous dioxygen model cytochrome P450. *J. Am. Chem. Soc.*, **120**, 4308-4318.

Harvey, S. C. (1989). Treatment of electrostatic effects in macromolecular modelling. *Proteins*, **5**, 78-92.

Hatefi, Y. (1978). Preparation and properties of dihydroubiquinone : cytochrome *c* oxidoreductase (complex III). *Methods Enzymol.*, **53**, 35-40.

- Heelis, P. F., Deeble, D. J., Kim, S. T., & Sancar, A. (1992). Splitting of cys-syn cyclobutane thymine-thymine dimers by radiolysis and its relevance to enzymatic photoreaction. *Int. J. Radiat. Biol.* **62**, 137-143.
- Heelis, P. F., Okamura, T., & Sancar, A. (1990). Excited-state properties of *Escherichia coli* DNA photolyase in the picosecond to millisecond time scale. *Biochemistry*, **29**, 5694-5698.
- Hinkle, P. C., Kumar, M. A., Resetar, A., & Harris, D. L. (1991). Mechanistic stoichiometry of mitochondrial oxidative phosphorylation. *Biochemistry*, **30**, 3576-3582.
- Hoganson, C. W., & Babcock, G. T. (1997). A metalloradical mechanism for the generation of oxygen from water in photosynthesis. *Science*, **277**, 1953-1956.
- Holst, M. J., Kozack, R. E., Saied, F., & Subramiam, S. (1994). Treatment of electrostatic effects 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 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.
- Huffman, D. L., Rosenblatt, M. M., & Suslick, K. S. (1998). Synthetic heme-peptide complexes. *J. Am. Chem. Soc.*, **120**, 6183-6184.
- Hurt, E., & Hauska, G. (1981). A cytochrome *f/b<sub>6</sub>* complex of five polypeptides with plastoquinol-plastocyanin-oxidoreductase activity from spinach chloroplasts. *Eur. J. Biochem.*, **117**, 591-599.
- Hurt, E., & Hauska, G. (1982). Identification of the polypeptides in the cytochrome *b<sub>6</sub>/f* complex from spinach chloroplasts with redox-center-carrying subunits. *J. Bioenerg. Biomembr.*, **14**, 405-424.
- Iakovleva, O., Reiner, M., Rau, H., Haehnel, W., & Parak, F. (2001). Mössbauer and EPR study of a cytochrome *b* model. (*in print*).
- Iwata, S., Lee, J. W., Okada, K., Lee, J. K., Iwata, M., Rasmussen, B., Link, T. A., Ramaswamy, S., & Jap, B. K. (1998). Complete structure of the 11-subunit bovine mitochondrial cytochrome *bc<sub>1</sub>* complex. *Science*, **281**, 64-71.
- Izrailev, S., Crofts, A. R., Berry, E. A., & Schulten, K. (1999). Steered molecular dynamics simulation of the Rieske subunit motion in the cytochrome *bc<sub>1</sub>* complex. *Biophys. J.*, **77**, 1753-1768.
- Jewsbury, P., Yamamoto, S., Minato, T., Saito, M., & Kitagawa, T. (1994). The proximal residue largely determines the CO distortion in carbonmonoxy globin proteins. An ab initio study of a heme prosthetic unit. *J. Am. Chem. Soc.* **116**, 11586-11587.
- 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. (1978). A discussion of the solution for the best rotation to relate two sets of vectors. *Acta Cryst. A*, **34**, 827-828.

Kallies, B., & Mitzner, R. (1997). pK<sub>a</sub> values of amines in water from quantum mechanical calculations using a polarized dielectric continuum representation of the solvent. *J. Phys. Chem. B*, **101**, 2959-2967.

Kanai, S., Kikuno, R., Toh, H., Ryo, H., & Todo, T. (1997). Molecular evolution of the photolyase-blue light photoreceptor family. *J. Mol. Evol.*, **45**, 535-548.

Katz, E., Heleg-Shabtai, V., Willner, I., Rau, H. K., & Haehnel, W. (1998). Rekonstitution eines *de novo* synthetisierten Hämproteins auf eine Oberfläche für bioelektronische Anwendungen. *Angew. Chem.*, **110**, 3443-3447. (*Angew. Chem. Int. Ed.*, **37**, 3253-3256).

Kavanaugh, J. S., Weydert, J. A., Rogers, P. H., & Arnone, A. (1998). High resolution crystal structures of human hemoglobin with mutations at tryptophan 37 $\beta$ : The structural basis for a high affinity T-state. *Biochemistry*, **37**, 4358-4373.

Kilmartin, J. V., & Rossi-Bernardi, L. (1973). Interaction of hemoglobin with hydrogen ions, carbon dioxide, and organic phosphates. *Physiol. Rev.*, **53**, 836-889.

Kim, S. T., Heelis, P. F., Okamura, T., Hirata, Y., Mataga, N., & Sancar, A. (1991). Determination of rates and yields of interchromophore (folate  $\rightarrow$  flavin) energy transfer and intermolecular (folate  $\rightarrow$  DNA) electron transfer in *Escherichia coli* photolyase by time-resolved fluorescence and absorption spectroscopy. *Biochemistry*, **30**, 11262-11270.

Kim, S. T., Li, Y. F., & Sancar, A. (1992). The third chromophore of DNA photolyase: Trp-277 of *Escherichia coli* DNA photolyase repairs thymine dimers by direct electron transfer. *Proc. Natl. Acad. Sci. U. S. A.*, **89**, 900-904.

Kim, S. T., & Sancar, A. (1991). Effect of base, pentose, and phosphodiester backbone structure on binding and repair of pyrimidine dimers by *Escherichia coli* DNA photolyase. *Biochemistry*, **30**, 8623-8630.

Kim, S. T., & Sancar, A. (1993). Photochemistry, photophysics, and mechanism of pyrimidine dimer repair by DNA photolyase. *Photochem. Photobiol.*, **57**, 895-904.

Kim, S. T., Sancar, A., Essenmacher, C., & Babcock, G. T. (1993). Time-resolved EPR studies with DNA photolyase: Excited-state FADH<sup>0</sup> abstracts an electron from Trp-306 to generate FADH<sup>-</sup>, the catalytically active form of the cofactor. *Proc. Natl. Acad. Sci. U. S. A.*, **90**, 8023-8027.

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 dismutase: Effects of ionic strength and amino-acid modification. *Prot. Struct. Funct. Genet.*, **1**, 47-59.

- Kramer, D. M., & Crofts, A. R. (1994a). Reexamination of the properties and function of the *b*-cytochromes of the thylakoid cytochrome *bf* complex. *Biochim. Biophys. Acta-Bioenerg.*, **1184**, 193-201.
- Kramer, D. M., Joliot, A., Joliot, P., & Crofts, A. R. (1994b). Competition among plastoquinol and artificial quinone/quinol couples at the quinol oxidizing site of the cytochrome *bf* complex. *Biochim. Biophys. Acta-Bioenerg.*, **1184**, 251-262.
- Kraulis, P.J. (1991). MOLSCRIPT: A program to produce both detailed and schematic plots of protein structures. *J. Appl. Cryst.*, **24**, 946-950.
- Lancaster, C. R., Michel, H., Honig, B., & Gunner, M. R. (1996). Calculated coupling of electron and proton transfer in the photosynthetic reaction center of *Rhodospseudomonas viridis*. *Biophys. J.*, **70**, 2469-2492.
- Li, J., Fischer, C. L., Chen, J. L., Bashford, D., & Noodleman, L. (1996). Calculation of redox potentials and pK<sub>a</sub> values of hydrated transition metal cations by a combined density functional and continuum dielectric theory. *J. Phys. Chem.*, **96**, 2855-2866.
- Li, Y. F., Heelis, P. F., & Sancar, A. (1991). Active site of DNA photolyase: tryptophan-306 is the intrinsic hydrogen atom donor essential for flavin radical photoreduction and DNA repair in vitro. *Biochemistry*, **30**, 6322-6329.
- Lim, C., Bashford, D., & Karplus, M. (1991). Absolute pK<sub>a</sub> calculations with continuum dielectric methods. *J. Phys. Chem.*, **95**, 5610-5620.
- Link, T. A. (1997). The role of the 'Rieske' iron sulfur protein in the hydroquinone oxidation (Q<sub>p</sub>) site of the cytochrome *bc<sub>1</sub>* complex - The 'proton-gated affinity change' mechanism. *FEBS Letters*, **412**, 257-264.
- Lloyd, E., Hildebrand, D. P., Tu, K. M., & Mauk, A. G. (1995). Conversion of myoglobin into a reversible electron transfer protein that maintains bis-histidine axial ligation. *J. Am. Chem. Soc.*, **117**, 6434-6438.
- MacKerell, Jr., A. D., Bashford, D., Bellot, M., Dunbrack, Jr., R. L., Evanseck, J. D., Field, M. J., Fischer, S., Gao, J., Guo, H., Ha, S., Joseph-McCarthy, D., Kuchnir, L., Kuczera, K., Lau, F. T. K., Mattos, C., Michnick, S., Ngo, T., Nguyen, D. T., Prodhom, B., Reiher, III, W. E., Roux, B., Schlenkrich, M., Smith, J. C., Stote, R., Straub, J., Watanabe, M., Wiórkiewicz-Kuczera, J., Yin, D., & Karplus, M. (1998). All-atom empirical potential for molecular modeling and dynamics studies of proteins. *J. Phys. Chem.*, **102**, 3586-3616.
- Marcus, R. A., & Sutin, N. (1985). Electron transfers in chemistry and biology. *Biochim. Biophys. Acta*, **811**, 265-322.
- Martinez, S. E., Huang, D., Szczepaniak, A., Cramer, W. A., & Smith, J. L. (1994). Crystal structure of chloroplast cytochrome *f* reveals a novel cytochrome fold and unexpected heme ligation. *Structure*, **2**, 95-105.
- Matias, P. M., Morais, J., Coelho, R., Carrondo, M. A., Wilson, K., Dauter, Z., & Sieker, L. (1996). Cytochromes *c3* from *desulfovibrio gigas*: Crystal structure at 1.8Å resolution and evidence for a special calcium-binding site. *Protein Sci.*, **5**, 1342-1354.



- McQuarrie, D. A. (1976). *Statistical mechanics*. Publishers, Harper & Row, New York.
- Menyhard, D. K., & Keseru, G. M. (1998). Stereoelectronic control on the coordination of substrates to globin proteins. The role of proximal His93 on the NO release from myoglobin. *J. Am. Chem. Soc.*, **120**, 7991-7992.
- Metropolis, N., Rosenbluth, A. W., Rosenbluth, M. N., & Teller, A. H. (1953). Equation of state calculation by fast computing machines. *J. Phys. Chem.*, **21**, 1087-1092.
- Mitchell, P. (1961). Coupling of phosphorylation to electron transfer by a chemiosmotic type of mechanism. *Nature*, **191**, 144-148.
- Mitchell, P. (1976). Possible molecular mechanisms of the protonmotive function of cytochrome systems. *J. Theor. Biol.*, **62**, 327-367.
- Momot K. I., & Walker F. A. (1997). Investigations of rotation of axial ligands in six-coordinate low-spin iron(III) tetraphenylporphyrinates: Measurement of rate constants from saturation transfer experiments and comparison to molecular mechanic calculations. *J. Phys. Chem.*, **101**, 2787-2795.
- Mouesca, J. M., Chen, J. L., Noodleman, L., Bashford, D., & Case, D. A. (1994). Density functional/Poisson-Boltzmann calculations of redox potentials for iron-sulfur clusters. *J. Am. Chem. Soc.*, **116**, 11898-11914.
- Muegge, I., Apostolakis, J., Ermler, U., Fritsch, 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**, 8359-8370.
- Munro, O. Q., Marques, H. M., Debrunner, P. G., Mohanrao, K., & Scheidt, W. R. (1995). Structural and molecular mechanics studies on highly ruffled low-spin (porphyrinato)iron(III) complexes. *J. Am. Chem. Soc.*, **117**, 935-954.
- Munro, O. Q., Serth-Guzzo, J. A., Turkovska-Tyrk, I., Mohanrao, K., Shokhireva, T. Kh., Walker, F. A., Debrunner, P. G., & Scheidt, W. R. (1999). Two crystalline forms of low-spin [Fe(TMP)(5-MeHIm)<sub>2</sub>]ClO<sub>4</sub>. Relative parallel and perpendicular axial ligand orientations. *J. Am. Chem. Soc.*, **121**, 11144-11155.
- Mutter, M., Altmann, E., Altmann, K. H., Hersperger, R., Koziej, P., Nebel, K., Tuchscherer, G., Vuilleumier, S., Gremlich, H. U., & Müller, K. (1988). Non-native architectures in protein design and mimicry. *Helv. Chim. Acta*, **71**, 835-847.
- Nakamura, H. (1996). Roles of electrostatic interaction in proteins. *Quart. Rev. Biophys.*, **29**, 1-90.
- Nakamura, M., Ikeue T., Neya, N., Fanasaki, N., & Nakamura, N. (1996). Fixation of the 2-methylimidazole ligand and anomalous pyrrole chemical shifts in bis-(2-methylimidazole)(meso-tetraalkylporphyrinato)iron(III) chloride caused by the non-planar porphyrin ring. *Inorg. Chem.*, **35**, 3731-3732.
- Nelson, B. D., & Gellerfors, P. (1974). The redox properties of the cytochromes of purified complex III. *Biochim. Biophys. Acta*, **357**, 358-364.

Nelson, B. D., & Gellerfors, P. (1975). Alkali-induced reduction of *b*-cytochromes in purified complex III from beef heart-mitochondria. *Biochim. Biophys. Acta*, **396**, 202-209.

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

Oberoi, H., & Allewell, N. M. (1993). Multigrid solution of the nonlinear Poisson-Boltzmann equation of titration curves. *Biophys. J.*, **65**, 48-55.

Page, C. C., Moser, C. C., Chen, X. X., & Dutton, P. L. (1999). Natural engineering principles of electron tunnelling in biological oxidation-reduction. *Nature*, **402**, 47-52.

Papa, S., Guerrieri, F., & Izzo, G. (1979). Redox Bohr-effects in the cytochrome system of mitochondria. *FEBS Letters*, **105**, 213-216.

Park, H. W., Kim, S. T., Sancar, A., & Deisenhofer, J. (1995). Crystal-structure of DNA photolyase from *Escherichia coli*. *Science*, **268**, 1866-1872.

Payne, G., Heelis, P. F., Rohrs, B. R., & Sancar, A. (1987). The active form of *Escherichia coli* DNA photolyase contains a fully reduced flavin and not a flavin radical, both in vivo and in vitro. *Biochemistry*, **26**, 7121-7127.

Perutz, M. F. (1978). Electrostatic effects in proteins. *Science*, **201**, 1187-1191.

Polam, J. R., Shokhireva, T. Kh., Raffi, K., Simons, U., & Walker, F. A. (1997). Rates of axial ligand rotation in diamagnetic d<sup>6</sup> Co(III) and Fe(II) porphyrinates. *Inorg. Chim. Acta*, **263**, 109-117.

Pond, A. E., Roach, M. P., Sono, M., Rux, A. H., Franzen, S., Hu, R., Thomas, M. R., Wilks, A., Dou, Y., Ikeda-Saito, M., de Montellano, P. R. O., Woodruff, W. H., Boxer, S. G., & Dawson, J. H. (1999). Assignment of the heme axial ligand(s) for the ferric myoglobin (H93G) and heme oxygenase (H25A) cavity mutants as oxygen donors using magnetic circular dichroism. *Biochemistry*, **38**, 7601-7608.

Popović, D. M., & Knapp, E. W. (2001). Computation of the redox potentials in the serie of artificial mutant heme proteins. (in preparation)

Popović, D. M., Zarić, S. D., Rabenstein, B., & Knapp E. W. (2001a). Artificial cytochrome *b*: Computer modeling and evaluation of redox potentials. *J. Am. Chem. Soc.*, **123**, 6040-6053.

Popović, D. M., Zmirić, A., Zarić, S. D., & Knapp E. W. (2001b). Energetics of radical transfer in DNA photolyase. (in press in *J. Am. Chem. Soc.*)

Potter, M. J., Gilson, M. K., & McCammon, J. A. (1994). Small molecule pK<sub>a</sub> prediction with continuum electrostatics calculations. *J. Am. Chem. Soc.*, **116**, 10298-10299.

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

Rabenstein, B., & Knapp, E. W. (2001). Calculated pH-dependent population of CO-myoglobin cofomers. *Biophysical J.*, **80**, 1141-1150.

- 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 *Rhodospseudomonas 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.
- Rau, H. K., DeJonge, N., & Haehnel, W. (1998). Modular synthesis of *de novo*-designed metalloproteins for light-induced electron transfer. *Proc. Natl. Acad. Sci. U. S. A.*, **95**, 11526-11531.
- Rau, H. K., DeJonge, N., & Haehnel, W. (2000). Combinatorial synthesis of four-helix bundle hemoproteins for tuning of cofactor properties. *Angew. Chem. Int. Ed.*, **39**, 250-253.
- Rau, H. K., & Haehnel, W. (1998). Design, synthesis, and properties of a novel cytochrome *b* model. *J. Am. Chem. Soc.*, **120**, 468-476.
- Reichard, P., & Ehrenberg, A. (1983). Ribonucleotide reductase – A radical enzyme. *Science*, **221**, 514-519.
- Richardson, W. H., Peng, C., Bashford, D., Noodleman, L., & Case, D. A. (1997). Incorporating solvation effects into density functional theory: Calculation of absolute acidities. *Int. J. Quant. Chem.*, **61**, 207-217.
- 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.
- Robertson, D. E., Ding, H., Chelminski, P. R., Slaughter, C., Hsu, J., Moomaw, C., Tokito, M., Daldal, F., & Dutton, P. L. (1993). Hydrobiquinone-cytochrome *c*<sub>2</sub> oxidoreductase from *Rhodobacter capsulatus*: Definition of a minimal, functional isolated preparation. *Biochemistry*, **32**, 1310-13
- Robertson, D. E., Farid, R. S., Moser, C.C., Urbauer, J-L., Mulholland, S. E., Pidikiti, R., Lear, J. D., Wand, A.J., DeGrado, W. F., & Dutton, P. L. (1994). Design and Synthesis of multi-heme proteins. *Nature*, **368**, 425-432.
- Rovira, C., & Parrinello, M. (1999). Factors influencing ligand-binding properties of heme models: a first principle study of picket-fence and protoheme complexes. *Chem. Eur. J.*, **5**, 250-262.
- Ryckaert, J., Ciccotti, G., & Berendsen, H. (1977). Numerical integration of the Cartesian equations of motion of a system with constraints. *J. Comp. Phys.*, **23**, 327-341.

Safo, M. K., Nasset, M. J. M., Walker, F. A., Debrunner, P. G., & Scheidt, W. R. (1997). Models of the cytochromes. Axial ligand orientation and complex stability in iron(II) porphyrinates: the case of the non-interacting  $d\pi$  orbitals. *J. Am. Chem. Soc.*, **119**, 9438-9448.

Safo, M. K., Walker, F. A., Raitsimring A. M., Walters, W. P., Dolata D. P., Debrunner, P. G., & Scheidt, W. R. (1994). Axial ligand orientation in iron(III) porphyrinates: Effect of axial  $\pi$ -acceptors. Characterization of the low-spin complex  $[\text{Fe}(\text{TPP})(4\text{-CNPY})_2]\text{ClO}_4$ . *J. Am. Chem. Soc.*, **116**, 7760-7770.

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

Sancar, A. (1994). Structure and function of DNA photolyase. *Biochemistry*, **33**, 2-9.

Sancar, A. (1996). No "end of history" for photolyase. *Science*, **272**, 48-49.

Sancar, A., & Sancar, G. B. (1988). DNA repair enzymes. *Ann. Rev. Biochem.*, **57**, 29-67.

Sancar, G. B., Smith, F. W., & Sancar, A. (1985). Binding of *Escherichia coli* DNA photolyase to UV-irradiated DNA. *Biochemistry*, **24**, 1849-1855.

Schaegger, H., Brandt, U., Gencic, S., & von Jagow, G. (1995). Ubiquinol-cytochrome-*c* reductase from human and bovine mitochondria. *Methods Enzymol.*, **260**, 82-96.

Schaegger, H., Link, T. A., Engel, W. D., & von Jagow, G. (1986). Isolation of the eleven protein subunits of the  $bc_1$  complex from beef heart. *Methods Enzymol.*, **126**, 224-237.

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, R. E., Moser, C. C., Rabanal, F., & Dutton, P. L. (1998). Design, synthesis, and characterization of a photoactivatable flavocytochrome molecular maquette. *Proc. Natl. Acad. Sci. U. S. A.*, **95**, 10465-10470.

Shelnutt, J. A., Franko, R., Ma, J. G., Lu, Y., & Ferreira, G. C. (2000). Porphyrin interactions with wild-type and mutant mouse ferrochelatase. *Biochemistry*, **39**, 2517-2529.

Shelnutt, J. A., Song, X. Z., Jenzen, W., Jaquinod, L., Khoury, R. G., Medforth, C. J., Jia, S. L., Ma, J. G., & Smith, K. M. (1998). Substituent-induced perturbation symmetries and distortions of meso-tert-butylporphyrins. *Inorg. Chem.*, **37**, 2117-2128.

Shokhirev, N. V., Shokhireva, T. Kh., Polam, J. R., Watson, C. T., Raffii, K., Simons, U., & Walker, F. A. (1997). 2D NMR investigations of the rotation of axial ligands in six-coordinate low-spin iron(III) and cobalt(III) tetraphenylporphyrinates having 2,6-disubstituted phenyl rings: quantitation of rate constants from  $^1\text{H}$  EXSY cross-peak intensities. *J. Phys. Chem.*, **101**, 2778-2786.

Shokhirev, N. V., & Walker, F. A. (1998). Co- and counterrotation of magnetic axes and axial ligands in low-spin ferriheme systems. *J. Am. Chem. Soc.*, **120**, 981-990.

Siegbahn, P. E. M., Blomberg, M. R. A., & Crabtree, R. H. (1997). Hydrogen transfer in the presence of amino acid radicals. *Theor. Chem. Acc.*, **97**, 289-300.

Sigel, H. D., & Sigel, A. (1994). *Metalloenzymes involving amino acid residue and related radicals*, Metals Ions in Biological Systems (Dekker, New York), Vol. 30.

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.

Sjoberg, B.M. (1994). The ribonucleotide reductase jigsaw puzzle – A large piece falls into place. *Structure*, **2**, 793-796.

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

Smerdon, S.J., Krzywda, S., & Wilkinson, A. J. (1993). Serine<sup>92</sup> (F7) contributes to the control of heme reactivity and stability in myoglobin. *Biochemistry*, **32**, 5132-5138.

Soares, C. M., Martel, P. J., & Carrondo, M. A. (1997). Theoretical studies on the redox-Bohr effect in cytochrome *c*<sub>3</sub> from *Desulfovibrio vulgaris* Hildenborough. *JBIC*, **2**, 714-727.

Solar, S., Getoff, G., Surdhar, P. S., Armstrong, D. A., & Singh, A. (1991). Oxidation of tryptophan and N-methylindole by N<sub>3</sub><sup>•</sup>, Br<sub>2</sub><sup>•-</sup>, and (SCN)<sub>2</sub><sup>•-</sup> radicals in light- and heavy-water solutions: A pulse radiolysis study. *J. Phys. Chem.*, **95**, 3636-3643.

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

Stryer, L. (1988). *Biochemistry*. III edition. Freeman W. H. and Company, New York.

Stubbe, J., & van der Donk, W. A. (1998). Protein radicals in enzyme catalysis. *Chemical Reviews*, **98**, 705-762.

Tamada, T., Kitadokoro, K., Higuchi, Y., Inaka, K., Yasui, A., de Ruiter, P. E., Eker, A. P. M., & Miki, K. (1997). Crystal structure of DNA photolyase from *Anacystis nidulans*. *Nature Struct. Biol.*, **4**, 887-891.

Tanford, C. (1962). The interpretation of hydrogen ion titration curves of proteins. *Adv. Prot. Chem.*, **17**, 69-165.

Tanford, C., & Roxby, R. (1972). Interpretation of protein titration curves. Application to lysozyme. *Biochemistry*, **11**, 2192-2198.

Tommos, C., Skalicky, J. J., Pilloud, D. L., Wand, A. J., & Dutton, P. L. (1999). *De novo* proteins as models of radical enzymes. *Biochemistry*, **38**, 9495-9507.

Uhlen, U., & Eklund, H. (1994). Structure of ribonucleotide reductase protein R1. *Nature*, **370**, 533-539.

Ullmann, M. G. (1998). Simulation and analysis of docking and molecular dynamics of electron-transfer protein complexes. PhD Thesis, Freie Universität Berlin.

Ullmann, M. G. (2000). The coupling of protonation and reduction in proteins with multiple centers: theory, computational method, and application to cytochrome  $c_3$ . *J. Phys. Chem. B*, **104**, 6293-6301.

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., 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.

Urban, P. F., & Klingenberg, M. (1969). On the redox potentials of ubiquinone and cytochrome  $b$  in the respiratory chain. *Eur. J. Biochem.*, **9**, 519-525.

Vagedes, P., Rabenstein, B., Aqvist, J., Marelius, J., & Knapp, E.W. (2000). The deacylation step of acetylcholinesterase: Computer simulation studies. *J. Am. Chem. Soc.*, **122**, 12254-12262.

Vangberg, T., & Ghosh, A. (1999). A first-principle quantum chemical analysis of the factors controlling ruffling deformations of porphyrins: insights from the molecular structures and potential energy surfaces of silicon, phosphorus, germanium, and arsenic porphyrins and of a peroxidase compound I model. *J. Am. Chem. Soc.*, **121**, 12154-12160.

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

Voet, D., & Voet, J. G. (1995). *Biochemistry*. II edition. John Wiley & Sons, Inc., New York.

Voigt, P., Popović, D. M., & Knapp, E. W. (2001). Calculation of redox potentials of the hemes in the bacterial photosynthetic reaction center. (in preparation)

Von Jagow, G., Engle, W. D., Schaeffer, H., Machleidt, W., & Machleidt, I. (1981). *Vectorial reactions in electron and ion transport in mitochondria and bacteria* (Palmieri, F., Quagliariello, E., Siliprandi, N. and Slater, E. C., eds.). Elsevier/North-Holland: Amsterdam; pp. 149-161.

Von Jagow, G., Schaeffer, H., Engle, W. D., Machleidt, W., & Machleidt, I. (1978). Beef heart complex III: Isolation and characterization of cytochrome *b*. *FEBS Letters*, **91**, 121-125.

Von Jagow, G., & Sebald, W. (1978). *b*-type cytochromes. *Ann. Rev. Biochem.*, **49**, 281-314.

Walker, F. A. (1999). Magnetic spectroscopic (EPR, ESEEM, Mössbauer, MCD and NMR) studies of low-spin ferriheme centers and their corresponding heme proteins. *Coord. Chem. Rev.*, **185-186**, 471-534.

Walker, F. A., Huynh, B. H., Schedt, W. R., & Osvath, S. R. (1986). Models of the cytochromes *b*. Effect of axial ligand plane orientation on the EPR and Mössbauer spectra of low-spin ferrihemes. *J. Am. Chem. Soc.*, **108**, 5288-5297.

Walker F. A., Nasri, H., Turowska-Tyrk, I., Mohanrao, K., Watson, C. T., Shokhirev N. V., Debrunner, P. G., & Scheidt, W. R. (1996).  $\pi$ -acid ligands in iron(III) porphyrinates. Characterization of low-spin bis(tert-butylisocyanide) (porphyrinato) iron(III) complexes having  $(d_{xz}, d_{yz})^4(d_{xy})^1$  ground state. *J. Am. Chem. Soc.*, **118**, 12109-12118.

Wallace, C. J. A., & Clark-Lewis, I. (1992). Functional role of heme ligation in cytochrome *c*. *J. Biol. Chem.*, **267**, 3852-3861.

Walsh, S. T. R., Cheng, H., Bryson, J. W., Roder, H., & DeGrado, W. F. (1999). Solution structure and dynamics of a de novo designed three-helix bundle. *Proc. Natl. Acad. Sci. U. S. A.*, **96**, 5486-5491.

Wang, J., Mauro, J. M., Edwards, S. L., Oatley, S. J., Fishel, L. A., Ashford, V. A., Xuong, N. H., & Kraut, J. (1990). X-ray structures of recombinant yeast cytochrome *c* peroxidase and three heme-cleft mutants prepared by site-directed mutagenesis. *Biochemistry*, **29**, 7160-7169.

Wardman, P. (1989). Reduction potentials of one-electron couples involving free radicals in aqueous solution. *Phys. Chem. Ref. Data*, **18**, 1637-1657; list of tables 1658-1755.

Warshel, A. (1981). Electrostatic basis of structure-function correlation in proteins. *Acc. Chem. Res.*, **14**, 284-290.

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

Warshel, A., & Papazyan, A. (1998). Electrostatic effects in macromolecules: Fundamental concepts and practical modeling. *Curr. Op. Struct. Biol.*, **8**, 211-217.

Warshel, A., Papazyan, A., & Muegge, I. (1997). Microscopic and semimicroscopic 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. *Quart. Rev. Biophys.*, **17**, 283-422.

Warshel, A., Russel, 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.

- Warwicker, J., & Watson, H. C. (1982). Calculation of the electrostatic potential in the active site cleft due to  $\alpha$ -helix dipoles. *J. Mol. Biol.*, **157**, 671-679.
- Weiss, H., & Kolb, H. J. (1979). Isolation of mitochondrial succinate:ubiquinone reductase, cytochrome *c* reductase and cytochrome *c* oxidase from *Neurospora crassa* using nonionic detergent. *Eur. J. Biochem.*, **99**, 139-149.
- Wikström, M. K. F. (1973). The different cytochrome *b* components in the respiratory chain of animal mitochondria and their role in electron transport and energy conservation. *Biochim. Biophys. Acta*, **301**, 155-193.
- Wikström, M. K., & Berden, J. A. (1972). Oxidoreduction of cytochrome *b* in the presence of antimycin. *Biochim. Biophys. Acta*, **283**, 403-420.
- Willner, I., Heleg-Shabtai, V., Blonder, R., Katz, E.; Tao, G., Brückmann, A. F., & Heller, A. (1996). Electrical wiring of glucose oxidase by reconstitution of FAD-modified monolayers assembled onto Au-electrodes. *J. Am. Chem. Soc.*, **118**, 10321-10322.
- Willner, I., Heleg-Shabtai, V., Katz, E., Rau, H. K., & Haehnel, W. (1999). Integration of a reconstituted de novo synthesized hemoprotein and native metalloproteins with electrode supports for bioelectronic and bioelectrocatalytic applications. *J. Am. Chem. Soc.*, **121**, 6455-6468.
- Wilson, G. S. (1983). Electrochemical studies of porphyrin redox reactions as cytochrome models. *Bioelectrochem. Bioenerg.*, **1**, 172-179.
- Winkelmann, D., Popović, D. M., & Knapp E. W. (2001). *Anacystis Nidulans* DNA photolyase: Energetics of radical transfer during the charge separation. (in preparation)
- Wyman, J. (1964). Linked functions and reciprocal effects in hemoglobin: A second look. *Adv. Prot. Chem.*, **19**, 223-286.
- Wyman, J. (1968). Regulation in macromolecules as illustrated by haemoglobin. *Quart. Rev. Biophys.*, **1**, 35-81.
- Xia, D., Yu, C., Kim, H., Xia, J., Kachurin, A. M., Zhang, L., Yu, L., & Deisenhofer, J. (1997). Crystal structure of the cytochrome *bc<sub>1</sub>* complex from bovine heart mitochondria. *Science*, **277**, 60-66.
- Yang, A.-S., Gunner, M. R., Sompogna, R., & Honig, B. (1993). On the calculation of pK<sub>a</sub>s in proteins. *Prot. Struct. Funct. Genet.*, **15**, 252-265.
- Yasui, A. & Eker., A. P. M. (1998). in *DNA Damage and Repair, Vol. 2: DNA Repair in Higher Eukaryotes* (eds Nickoloff, J. A. & Hoekstra, M. F.) pp. 9-32 (Humana, Totowa).
- 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.
- Zarić, S. D., Popović, D. M., & Knapp, E. W. (2000). Metal ligand aromatic cation- $\pi$  interactions in metalloproteins: Ligands coordinated to metal interact with aromatic residues. *Chem. Eur. J.*, **6**, 3935-3942.



Zarić, S. D., Popović, D. M., & Knapp, E. W. (2001). Factors determining the orientation of axially coordinated imidazoles in heme proteins. *Biochemistry*, **40**, 7914-7928.

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.

Zhang, Z., Huang, L., Shulmeister, V. M., Chi, Y.-I., Kim, K. K., Hung, L.-W., Crofts, A. R., Berry, A., & Kim, S.-H. (1998). Electron transfer by domain movement in cytochrome *bc<sub>1</sub>*. *Nature*, **392**, 677-684.