



83. Linear Energy Relationships for the Octahedral Preference of Mg, Ca and Transition Metal Ions  
Pontikis, J. Borden, V. Mart'nek, and J. Florin *In* *Phys. Chem.* **A113**, 3588- 3593 (2009)
82. Phosphatase Inhibition by Vanadyl-Diketone Complexes: Electron Density Effects  
Ziegler, J. Florin, M. A. Ballicora, A. W. Herlinger *In* *Journal of Enzyme Inhibition & Medicinal Chemistry* **24**, 22 - 28 (2009)
81. Protein-Protein Docking and Analysis Reveal That Two Homologous Bacterial Adenylyl Cyclase Toxins Interact with Calmodulin Differently  
Q. Guo, J. E. Jureller, J. T. Warren, E. Solomaha, J. Florin, and W.-J. Tang *J. Biol. Chem.* **283**, 23836- 23845 (2008)
80. Associative Versus Dissociative Mechanisms of Phosphate Monoester Hydrolysis: On the Interpretation of Activation Entropies  
S. C.L. Kamerlin, J. Florin and A. Warshel *In* *ChemPhysChem* **9**, 1767- 1773 (2008)
79. DNA Polymerase Fidelity: Halomethylene-Modified Leaving Groups in Transient Kinetic Assays Indicate Differences at the Chemical Transition State  
A. Sucato, T. G. Upton, B. A. Kashemiroy, J. Osuna, W. A. Beard, S. H. Wilson, J. Florin, A. Warshel, C. E. McKenna and M. F. Goodman, *Biochemistry* **47**, 870-879 (2008)
78. Probing the Two-Metal Ion Mechanism in the Restriction Endonuclease BamHI  
Mones, P. Kulhane, J. Florin, I. Simon and M. Fuxreiter *In* *Biochemistry* **46**, 14514- 14523 (2007).
77. Novel Insights from Atomic-Resolution Crystal Structures of Chemically-Synthesized HIV Protease in Complex with Inhibitors  
E. C. B. Johnson, E. Malito, Y. Shen, B. Pentelute, D. R. Florin, W.-J. Tang, and S. B. H. Kent *In* *Mol. Biol.* **373**, 573-586 (2007)
76. Chelation of Vanadium(V) by Difluoromethylene Bisphosphonate, a Structural Analog of Pyrophosphate  
D. C. Crans, A. A. Holder, T. K. Saha, G. K. S. Prakash, M. Youssif, R. Kultyshev, R. Ismail, M. F. Goodman, J. Borden, and J. Florin *In* *Org. Chem.* **46**, 6723- 6732 (2007)
75. Pol Catalytic Efficiency Mirrors the Asn279-CTP H-bonding Strength  
V. Mart'nek, U. Bren, M. F. Goodman, A. Warshel and J. Florin *In* *FEBS Letters* **581**, 775- 780 (2007)

Chem. B110, 14988D14999 (2006).

67. Computer Simulations of Protein Functions: Searching For the Molecular Origin of the Replication Fidelity of DNA Polymerases. Florin M. F. Goodman and A. Warsh, Proc. Natl. Acad. Sci. USA 102, 6819D6824 (2005).
66. Calcium-Independent Calmodulin Binding and Translocation Catalytic Mechanism of Anthrax Edema Factor. Y. Shen, N. L. Zhukovskaya, Q. Gu, Florin and W-J. Tang, EMBO J. 24, 929-941 (2005).

65. Structure and Torsional Flexibility of the Linkage between Guanine and Fluorene Residues in the Deoxyguanosine-Aminofluorene and Deoxyguanosine-Acetylaminofluorene Carcinogenic Adducts  
J. Floriņ and J. Borden, *Theor. Chem. Accounts* **13**, 28-34 (2005).
64. Structural and Kinetic Analyses of the Interaction of Anthrax Adenylyl Cyclase Toxin with Reaction Products, cAMP and Pyrophosphate.  
Guo, Y. Shen, N. L. Zhukovskaya, Floriņ and W.-J. Tang, *J. Biol. Chem.* **279**, 29427-29435 (2004).
63. Empirical Valence Bond and Related Approaches  
Warshel and J. Floriņ in: *Encyclopedia of Computational Chemistry*, P. v. R. Schleyer, W. L. Jorgensen, H.F. Schaefer III, P. R. Schreiner, W. Thiel, R. Glen (eds.), DOI: 10.1002/0470845015.cu0002, John Wiley & Sons, Ltd. (2004).
62. Computer Simulation of the Chemical Catalysis of DNA Polymerases: Discriminating Between Alternative Nucleotide Insertion Mechanisms for T7 DNA Polymerase  
Floriņ M. F. Goodman and A. Warshel, *J. Am. Chem. Soc.* **125**, 8163-8177 (2003).
61. Computer Simulation Studies of the Fidelity of DNA Polymerase  
Floriņ M. F. Goodman and A. Warshel, *Biopolymers* **68**, 286-299 (2003)
60. Theoretical Investigation of the Binding Free Energies and Key Substrate Recognition Components of the Replication Fidelity of Human DNA Polymerase  
J. Floriņ M. F. Goodman and A. Warshel, *J. Phys. Chem. B* **106**, 5739-5753 (2002).
59. Molecular Dynamics Free Energy Simulations of the Binding Contribution to the Fidelity of T7 DNA Polymerase  
J. Floriņ A. Warshel and M. F. Goodman, *Phys. Chem. B* **106**, 5754-5760 (2002).
58. Comment on Molecular Mechanics for Chemical Reactions  
Floriņ J. Phys. Chem. **A106**, 5046-5047 (2002).
57. Ab initio Evaluation of the Potential Surface for General Base/Acid Catalyzed Thiolytic Hydrolysis of Formamide and Hydrolysis of Methyl Thiolfornate: A Reference Solution Reaction for Studies of Cysteine Proteases  
M. Strajbl, J. Floriņ and A. Warshel, *J. Phys. Chem. B* **105**, 4471-4480 (2001).

50. Ab initio/LD Studies of Chemical Reactions in Aqueous Solution: The Reference Energy Surfaces for the Acylation Reactions Occuring in Serine and Cysteine Proteases, J. Florin and A. Warshel,

Theophanides, Eds., Kluwer, Dordrecht, 1997, pp. 77.

33. Coupled Cluster and Density Functional Calculations of the Molecular Structure, Infrared Spectra, Raman Spectra, and Harmonic Force Constants for Methanol. Floriņ J. Leszczynski, B. G. Johnson and L. Goodman. *Mol. Phys.* **91**, 439- 447 (1997).
32. Molecular Structure, Vibrational Spectra and Quantum Mechanical Force Fields of Modified Oligonucleotide Linkages: 1. Methyl Methoxymethyl Phosphonate. Strajbl, V. Baumruk, J. Floriņ, L. Bednřrovř, I. Rosenberg and J. Stepřek. *Mol. Struct.* **415**, 161- 177 (1997)
31. Activation of Alcohols and Ketones by Surface Hydroxyls of Strong Solid Acids. Subekovř, J. Kotrla, J. Floriņ, T. Bolom, J. Fraissard, L. Heeribout, C. Doremieux. *Studies in Surface Science and Catalysis* **101**, 761- 770 (1996).
30. Nonplanar DNA Base Pairs. Sponer, J. Floriņ, P. Hobza and J. Leszczynski. *Biomol. Struct. Dyn.* **13**, 827- 833 (1996).
29. Ab Initio Investigation of Molecular Structure of Methyl Methoxymethyl Phosphonate, a Promising Nuclease Resistant Alternative of Phosphodiester Linkage. Strajbl and J. Floriņ. *J. Biomol. Struct. Dyn.* **13**,

