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List of Publications

98. Flexible Docking-Based MD/SMD Calculations of ProteinEP Tm /F4.0 1 Tf [ J24 8D91 Q q 0.24 0 0 0.24

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83. Linear Energy Relationships for the Octahedral Preference of Mg, Ca and Transition Metal Ions  
Pontikis, J. Borden, V. Mart'nek, and J. Florin *Phys. Chem.* **113**, 3588- 3593 (2009)
82. Phosphatase Inhibition by Vanadyl-Diketone Complexes: Electron Density Effects  
Ziegler, J. Florin, M. A. Ballicora, A. W. Herlinger *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 *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. Kulhaneck, J. Florin, I. Simon and M. Fuxreiter *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, *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 *Org. Chem.* **46**, 6723- 6732 (2007)
75. Pol I Catalytic Efficiency Mirrors the Asn279-CTP Hbonding Strength  
V. Mart'nek, U. Bren, M. F. Goodman, A. Warshel and J. Florin *FEBS Letters* **581**, 775- 780 (2007)
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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. Warshel, 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  
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61. Computer Simulation Studies of the Fidelity of DNA Polymerase  
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57. Ab initio Evaluation of the Potential Surface for General Base/Acid Catalyzed Thiolytic of Formamide and Hydrolysis of Methyl Thiolfornate: A Reference Solution Reaction for Studies of Cysteine Proteases  
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