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*List of Publications*

82. *Phosphatase Inhibition by Vanadyl- $\beta$ -Diketone Complexes: Electron Density Effects*, A. Ziegler, J. Florián, M. A. Ballicora, A. W. Herlinger, *Journal of Enzyme Inhibition & Medicinal Chemistry*, in press, DOI: 10.1080/14756360701841426
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. Florián, and W.-J. Tang, *J. Biol. Chem.* **283**, 23836 - 23845 (2008), doi:10.1074/jbc.M802168200
80. *Associative Versus Dissociative Mechanisms of Phosphate Monoester Hydrolysis: On the Interpretation of Activation Entropies*, S. C. L. Kamerlin, J. Florián and A. Warshel, *ChemPhysChem* **9**, 1767 - 1773 (2008), DOI: 10.1002/cphc.200800356
79. *DNA Polymerase  $\beta$  Fidelity: Halomethylene-Modified Leaving Groups in Transient Kinetic Assays Indicate Differences at the Chemical Transition State*, C. A. Sucato, T. G. Upton, B. A. Kashemirov, J. Osuna, W. A. Beard, S. H. Wilson, J. Florián, A. Warshel, C. E. McKenna, and M. F. Goodman, *Biochemistry* **47**, 870-879 (2008), DOI: 10.1021/bi7014162
78. *Probing the Two-Metal Ion Mechanism in the Restriction Endonuclease BamHI*, L. Mones, P. Kulhánek, J. Florián, I. Simon and M. Fuxreiter, *Biochemistry* **46**, 14514 - 14523 (2007).
77. *Novel Insights from Atomic-Resolution Crystal Structures of Chemically-Synthesized HIV-1 Protease in Complex with Inhibitors*, E. C. B. Johnson, E. Malito, Y. Shen, B. Pentelute, D. Rich, J. Florián, W.-J. Tang, S. B. H. Kent, *J. Mol. Biol.* **373**, 573-586 (2007).
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75. *Pol  $\beta$  Catalytic Efficiency Mirrors the Asn279-dCTP H-bonding Strength*, V. Martínek, U. Bren, M. F. Goodman, A. Warshel and J. Florián, *FEBS Letters* **581**, 775 - 780 (2007).
74. *Do All Pieces Make a Whole? Thiele Cumulants and the Free Energy Decomposition*, M. Bren, J. Florián, J. Mavri, U. Bren, *Theor. Chem. Accounts* **117**, 535 - 540 (2007).
73. *Nitramine Anion Fragmentation: A Mass Spectrometric and Ab Initio Study*, J. Florián, D. K. MacMillan, L. Gao, V. Zhukhovskyy, M. P. Chiarelli, *J. Am. Soc. Mass. Spectr.* **18**, 835 - 841 (2007).
72. *Modifying the  $\beta$ - $\gamma$  Leaving-Group Bridging Oxygen Alters Nucleotide Incorporation Efficiency, Fidelity and Catalytic Mechanism of DNA Polymerase  $\beta$* , Christopher A. Sucato, Thomas G. Upton, Boris A. Kashemirov, Václav Martínek, Yun Xiang, William A. Beard, Vinod K. Batra, Lars C. Pedersen, Samuel H. Wilson, Charles E. McKenna, Jan Florián, Arieh Warshel, and Myron F. Goodman, *Biochemistry* **46**, 461 - 471 (2007).
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