

**Jan Florián**

Department of Chemistry and Biochemistry, Loyola University Chicago, Chicago, IL 60660

Phone: (773) 508-3785, E-mail: jfloria@luc.edu, <http://www.researcherid.com/rid/E-1554-2012>

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**List of Publications**

98. *Flexible Docking-Based MD/SMD Calculations of Protein–Protein Contacts in a Complex of Cytochrome P450 1A2 with Cytochrome b5*, P. Jeřábek, J. Florián, M. Stiborová and V. Martínek, **Biochemistry** 53, 6695–6705 (2014).
97. *Quantum Mechanical Analysis of Nonenzymatic Nucleotidyl Transfer Reactions: Kinetic and Thermodynamic Effects of  $\beta$ – $\gamma$  Bridging Groups of dNTP Substrates*, Z. Zhang, J. Eloge and J. Florián, **Biochemistry** 53, 4180 - 4191 (2014).
96. *Metal Ion Complexes of N,N'-Bis(2-Pyridylmethyl)-1,3-Diaminopropane-N,N'-Diacetic Acid, H<sub>2</sub>bppd*, D. Kissel, J. Florián, C. McLauchlan and A. Herlinger, **Inorg. Chem.** 53, 3414 – 3416 (2014).
95. *Spectroscopic Evidence of Work Function Alterations Due to Photoswitchable Monolayers on Gold Surfaces*, M. A. Bartucci, J. Florián and J. W. Ciszek, **J. Phys. Chem. C** 117, 19471 - 19476 (2013).
94. *Empirical Valence Bond Simulations of the Chemical Mechanism of ATP to cAMP Conversion by Anthrax Edema Factor*, L. Mones, W.-J. Tang and J. Florián, **Biochemistry** 52, 2672 – 2682 (2013).
93. *Catalytic Effects of Mutations of Distant Protein Residues in Human DNA Polymerase  $\beta$ : Theory and Experiment*, Martin Klvaňa, Drew L. Murphy, Petr Jeřábek, Myron F. Goodman, Arieh Warshel, Joann B. Sweasy and J. Florián, **Biochemistry** 51, 8829 – 8843 (2012).
92. *Intramolecular Base Stacking of Dinucleoside Monophosphate Anions in Aqueous Solution*, S. Jafilan, L. Klein, C. Hyun, and J. Florián, **J. Phys. Chem. B** 116, 3613 - 3618 (2012).
91. *Prechemistry Barriers and Checkpoints Do Not Contribute to Fidelity and Catalysis As Long As They Are Not Rate Limiting*, B. R. Prasad, S. C. L. Kamerlin, J. Florián and A. Warshel, **Theor. Chem. Acc.** 131, 1288 (2012).
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89. *CH– $\pi$  Interactions Do Not Contribute to Hydrogen Transfer Catalysis by Glycerol Dehydratase*, Y. Liu, A. A. Gallo, W. Xu, R. Bajpai and J. Florián, **J. Phys. Chem. A** 115, 11162 - 11166 (2011).
88. *Quantum Tunnelling in Enzyme-Catalysed Reactions (Book Review)* J. Florián, **J. Am. Chem. Soc.** 132, 6866 (2010).
87. *Enantioselectivity of Haloalkane Dehalogenases and Its Modulation by Surface Loop Engineering*, Z. Prokop, Y. Sato, J. Březovský, T. Mozga, R. Chaloupková, T. Koudeláková, P. Jeřábek, V. Stepánková, R. Natsume, J. G.E. van Leeuwen, D. B. Janssen, J. Florián, Y. Nagata, T. Senda and J. Damborsky, **Ang. Chem. Int. Ed.** 49, 6111 - 6115 (2010).
86. *QM/MM (ONIOM) Study of Glycerol Binding and Hydrogen Abstraction by the Coenzyme B12-Independent Dehydratase*, Y. Liu, W. Xu, A. A. Gallo, J. Florián, Y.-S. Liu, S. Mora, **J. Phys. Chem. B** 114, 5497 - 5502 (2010).
85. *On Defining the Hydrogen-Ion Concentration*, C. E. Moore, B. Jaselskis and J. Florián, **J. Chem. Educ.** 87, 922 - 923 (2010).
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83. *Linear Energy Relationships for the Octahedral Preference of Mg, Ca and Transition Metal Ions*, G. Pontikis, J. Borden, V. Martínek, and J. Florián, **J. Phys. Chem. A** 113, 3588 - 3593 (2009).
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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).
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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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