

**Cristiano R. W. Guimarães**

Pfizer, Inc.  
Global Research and Development  
Eastern Point Road  
Groton, CT 06340  
Phone: (860) 686-2915  
e-mail: cristiano.guimaraes@pfizer.com

**PROFESSIONAL  
EXPERIENCE**

**2007 – present: Pfizer, Inc. (Groton, CT)**  
Principal Scientist  
**2005 – 2007: Amgen, Inc. (South San Francisco, CA)**  
Scientist  
**2001 – 2005: Yale University (New Haven, CT)**  
Postdoctoral Research Associate and Associate Research Scientist  
Research Advisor: Professor William L. Jorgensen

**EDUCATION**

**1998 – 2001: Federal University of Rio de Janeiro (Rio de Janeiro, Brazil)**  
Ph.D. in Organic Chemistry *with distinction* (August 2001)  
Research Advisor: Professor Ricardo Bicca de Alencastro  
**1997 – 1998: Federal University of Rio de Janeiro (Rio de Janeiro, Brazil)**  
M.S. in Organic Chemistry *with distinction* (May 1998)  
Research Advisor: Professor Ricardo Bicca de Alencastro  
**1992 – 1996: Federal University of Rio de Janeiro (Rio de Janeiro, Brazil)**  
B.S. in Chemical Engineering *with distinction*

**PUBLICATIONS**

- Addressing Limitations with the MM-GB/SA Scoring Procedure using the Watermap Method and Free-Energy Perturbation Calculations.*  
**C. R. W. Guimarães**, A. M. Mathiowetz.  
J. Chem. Inf. Model. **50**, 547-559 (2010).
- Thermodynamic Analysis of mRNA Cap Binding by the Human Initiation Factor eIF4E via Free-Energy Perturbations.*  
**C. R. W. Guimarães**, D. J. Kopecky, J. Mihalic, S. Shen, S. Jeffries, S. Thibault, X. Chen, N. Walker, M. Cardozo.  
J. Am. Chem. Soc. **131**, 18139-18146 (2009).
- MM-GB/SA Rescoring of Docking Poses in Structure-Based Lead Optimization.  
**C. R. W. Guimarães**, M. Cardozo.  
J. Chem. Inf. Model. **48**, 958-970 (2008).
- From Docking False-Positive to Active Anti-HIV Agent.*  
G. Barreiro, J. T. Kim, **C. R. W. Guimarães**, C. M. Bailey, R. A. Domaoal, L. Wang, K. S. Anderson, W. L. Jorgensen.  
J. Med. Chem. **50**, 5324-5329 (2007).
- Search for Non-nucleoside Inhibitors of HIV-1 Reverse Transcriptase using Chemical Similarity, Molecular Docking, and MM-GB/SA Scoring.*  
G. Barreiro, **C. R. W. Guimarães**, I. Tubert-Brohman, T. M. Lyons, J. Tirado-Rives, W. L. Jorgensen.  
J. Chem. Inf. Model. **47**, 2416-2428 (2007).
- Human Cytomegalovirus Protease: Why Is the Dimer Required for Catalytic Activity?*  
C. A. F. Oliveira, **C. R. W. Guimarães**, G. Barreiro, R. Bicca de Alencastro.  
J. Chem. Theory Comput. **3**, 278-288 (2007).
- Elucidation of Fatty Acid Amide Hydrolase Inhibition by Potent  $\beta$ -Ketoheterocycle Derivatives from Monte Carlo Simulations.*  
**C. R. W. Guimarães**, D. L. Boger, W. L. Jorgensen.  
J. Am. Chem. Soc. **127**, 17377-17384 (2005).
- Extension of the PDDG/PM3 Semiempirical Molecular Orbital Method to Sulfur, Silicon and Phosphorous.*  
I. Tubert-Brohman, **C. R. W. Guimarães**, W. L. Jorgensen.  
J. Chem. Theory Comput. **1**, 817-823 (2005).
- Effects of Arg90 Neutralization on the Enzyme-Catalyzed Rearrangement of Chorismate to Prephenate.*  
**C. R. W. Guimarães**, M. Udier-Blagović, I. Tubert-Brohman, W. L. Jorgensen.  
J. Chem. Theory Comput. **1**, 617-625 (2005).
- Discovery of a Potent, Selective, and Efficacious Class of Reversible  $\beta$ -Ketoheterocycle Inhibitors of Fatty Acid Amide Hydrolase Effective as Analgesics.*

- D. L. Boger, H. Miyauchi, W. Du, C. Hardouin, R. A. Fecik, H. Cheng, I. Hwang, M. P. Hedrick, D. Leung, O. Acevedo, **C. R. W. Guimarães**, W. L. Jorgensen, B. F. Cravatt.  
J. Med. Chem. 48, 1849-1856 (2005).
11. *A Molecular Dynamics Study on Liquid 1-Octanol. Part 3. Evaluating Relative Octanol/Water Partition Coefficients of Thrombin Inhibitors via Free-Energy Perturbations.*  
C. A. F. Oliveira, **C. R. W. Guimarães**, H. Mello, A. Echevarria, R. Bicca de Alencastro.  
Int. J. Quantum Chem. 102, 542-553 (2005).
  12. *Macrophomate Synthase: QM/MM Simulations Address the Diels-Alder versus Michael-Aldol Reaction Mechanism.*  
**C. R. W. Guimarães**, M. Udier-Blagović, W. L. Jorgensen.  
J. Am. Chem. Soc. 127, 3577-3588 (2005).
  13. *On the Application of Simple Explicit Water Models to the Simulations of Biomolecules.*  
**C. R. W. Guimarães**, G. Barreiro, C. A. F. Oliveira, R. Bicca de Alencastro.  
Braz. J. Phys. 34, 126-136 (2004).
  14. *Extension of the PDDG/PM3 and PDDG/MNDO Semiempirical Molecular Orbital Methods to the Halogens.*  
I. Tubert-Brohman, **C. R. W. Guimarães**, M. P. Repasky, W. L. Jorgensen.  
J. Comput. Chem. 25, 138-150 (2004).
  15. *Synthetic and Theoretical Studies on the Reduction of Electron Withdrawing Group Conjugated Olefins Using the Hantzsch 1,4-dihydropyridine Ester.*  
S. J. Garden, **C. R. W. Guimarães**, C. A. F. Oliveira, M. B. Correa, A. C. Pinto, R. Bicca de Alencastro.  
J. Org. Chem. 68, 8815-8822 (2003).
  16. *Investigation of the Induced-Fit Mechanism and Catalytic Activity of the Human Cytomegalovirus Protease Homodimer via Molecular Dynamics Simulations.*  
C. A. F. Oliveira, **C. R. W. Guimarães**, G. Barreiro, R. Bicca de Alencastro.  
Proteins 52, 483-491 (2003).
  17. *Contributions of Conformational Compression and Preferential Transition State Stabilization to the Rate Enhancement by Chorismate Mutase.*  
**C. R. W. Guimarães**, M. P. Repasky, J. Chandrasekhar, J. Tirado-Rives, W. L. Jorgensen.  
J. Am. Chem. Soc. 125, 6892-6899 (2003).
  18. *Investigation of Solvent Effects for the Claisen Rearrangement of Chorismate to Prephenate: Mechanistic Interpretation via Near Attack Conformations.*  
M. P. Repasky, **C. R. W. Guimarães**, J. Chandrasekhar, J. Tirado-Rives, W. L. Jorgensen.  
J. Am. Chem. Soc. 125, 6663-6672 (2003).
  19. *Potential of Mean Force Calculations on an L-Type Calcium Channel Model.*  
G. Barreiro, **C. R. W. Guimarães**, R. Bicca de Alencastro.  
Protein Eng. 16, 209-215 (2003).
  20. *Thrombin Inhibition by Novel Benzamidine Derivatives: A Free-Energy Perturbation Study.*  
**C. R. W. Guimarães**, R. Bicca de Alencastro.  
J. Med. Chem. 45, 4995-5004 (2002).
  21. *Metodologias em Modelagem Molecular de Biomoléculas.*  
R. Bicca de Alencastro, M.G. Albuquerque, O. A. Santos Filho, **C. R. W. Guimarães**, G. Barreiro, N. C. Romeiro, R. C. A. Martins, C. A. F. Oliveira.  
In "A Arte de Vencer Desafios: Um Tributo a Claudio Costa Neto", Editor M. A. Chaer do Nascimento, Rio de Janeiro, pp. 29-41 (2002).
  22. *Metodologias em Modelagem Molecular de Biomoléculas.*  
R. Bicca de Alencastro, M.G. Albuquerque, O. A. Santos Filho, **C. R. W. Guimarães**, G. Barreiro, N. C. Romeiro, R. C. A. Martins, and C. A. F. Oliveira.  
In: Santos, Hélio F.; Coura, Pablo Z.; Dantas, Sócrates O.; Barone, Paulo M. V. B. (Org.). Escola Brasileira de Estrutura Eletrônica. São Paulo, pp. 191-201 (2002).
  23. *A Molecular Dynamics Study on Liquid 1-Octanol. Part 2. The Water-Saturated 1-Octanol Solution.*  
C. A. F. de Oliveira, **C. R. W. Guimarães**, R. Bicca de Alencastro.  
Int. J. Quantum Chem. 90, 786-791 (2002).
  24. *A Molecular Dynamics Study of an L-Type Calcium Channel Model.*  
G. Barreiro, **C. R. W. Guimarães**, R. Bicca de Alencastro.  
Protein Eng. 15, 109-122 (2002).
  25. *Thermodynamic Analysis of Thrombin Inhibition by benzamidine and p-methylbenzamidine via Free-Energy Perturbations: Inspection of Intraperturbed-Group Contributions Using the Finite Difference Thermodynamic Integration (FDTI) Method.*  
**C. R. W. Guimarães**, R. Bicca de Alencastro.  
J. Phys. Chem. B 106, 466-476 (2002).
  26. *Evaluating the Relative Free Energy of Hydration of New Thrombin Inhibitor Candidates Using the Finite Difference*

*Thermodynamic Integration (FDTI) Method.*

**C. R. W. Guimarães**, R. Bicca de Alencastro.

Int. J. Quantum Chem.: Quantum Biol. Symp. 85, 713-726 (2001).

**27.** *A Molecular Dynamics Study on Liquid 1-Octanol.*

C. A. F. de Oliveira, **C. R. W. Guimarães**, R. Bicca de Alencastro.

Int. J. Quantum Chem.: Quantum Biol. Symp. 80, 999-1006 (2000).

**28.** *A New Nicotinic Acetylcholine Minireceptor Model: A Theoretical Thermodynamic Analysis of Simultaneous Cation- $\pi$  and Hydrogen Bond Interactions.*

G. Barreiro, **C. R. W. Guimarães**, R. Bicca de Alencastro, E. J. Barreiro.

Journal of Molecular Structure (Theochem), 532, 11-22 (2000).

**29.** *Phytochrome Structure 2. The Case of Chromopeptides.*

**C. R. W. Guimarães**, J. D. da Motta Neto, R. Bicca de Alencastro.

Atualidades de Físico-Química Orgânica, 11, 405-424 (1998).

**30.** *Phytochrome Structure: A New Methodological Approach.*

**C. R. W. Guimarães**, J. D. da Motta Neto, R. Bicca de Alencastro.

Int. J. Quantum Chem.: Quantum Biol. Symp. 70, 1145-1157 (1998).