# Cristiano R. W. Guimarães

Pfizer, Inc.
Global Research and Development
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**PROFESSIONAL EXPERIENCE**

**2007 – present: Pfizer, Inc. (Cambridge, MA)**

Senior Principal Scientist

- *Chemistry leader in several projects*
- *Design of beyond Rule-of-5 molecules with passive permeability*
- *Application of docking, MM-GB/SA scoring, linear response, and free-energy perturbation theory in structure-based projects*
- *Homology modeling of class B GPCRs*
- *Application of QM methods to investigate conformational equilibria*
- *Use of Docking, shape-based tools, pharmacophore models, and pocket mining in virtual screening of chemical databases*

**2005 – 2007: Amgen, Inc. (South San Francisco, CA)**

Scientist

- *Application of docking, MM-GB/SA scoring, linear response, and free-energy perturbation theory in structure-based projects*
- *Generation of pharmacophore models in ligand-based projects*
- *Homology modeling of GPCRs*
- *HTS analysis*
- *Application of QM methods to investigate reaction mechanisms of the acidic hydrolisis of compounds*

**2001 – 2005: Yale University (New Haven, CT)**

Postdoctoral Research Associate and Associate Research Scientist

Research Advisor: Professor William L. Jorgensen

- *Elucidation of fatty acid amide hydrolase inhibition by potent □-ketoheterocycle derivatives using free-energy perturbation simulations*
- *QM/MM simulations on macrophomate synthase: Diels-Alder versus Michael-Aldol reaction mechanism*
- *QM/MM simulations of the chorismate to prephenate rearrangement in different environments*
- *Development of improved semiempirical methods*
- *Investigation of the induced-fit mechanism and catalytic activity of the human cytomegalovirus protease homodimer via molecular dynamics and QM/MM simulations*
- *Evaluation of the relative octanol/water partition coefficients of thrombin inhibitors via free-energy perturbations*

**EDUCATION**

**1998 – 2001: Federal University of Rio de Janeiro (Rio de Janeiro, Brazil)**
D.Sc. in Organic Chemistry *with distinction* (August 2001)
Research Advisor: Professor Ricardo Bicca de Alencastro
*Thermodynamic analysis of thrombin inhibition by novel benzamidine derivatives via free-energy perturbations.*

**1997 – 1998: Federal University of Rio de Janeiro (Rio de Janeiro, Brazil)**
M.Sc. in Organic Chemistry *with distinction* (May 1998)
Research Advisor: Professor Ricardo Bicca de Alencastro
*Theoretical studies of an Avena sativa phytochrome model and its photochemical cycle using the AM1 and INDO/S methods.*

**1992 – 1996: Federal University of Rio de Janeiro (Rio de Janeiro, Brazil)**
B.S. in Chemical Engineering *with distinction*

**EDITORIAL APPOINTMENTS**

**2002 – present:** Reviewer, Journal of Medicinal Chemistry.
**2003 – present:** Reviewer, Journal of Computational Chemistry.
**2003 – present:** Reviewer, Journal of the American Chemical Society.
**2005 – present:** Reviewer, Journal of Chemical Theory and Computation.
**2005 – present:** Reviewer, Journal of Chemical Information and Modeling.
**2010 – present:** Reviewer, Journal of Molecular Modeling.
**2012 – present:** Reviewer, Expert Opinion on Drug Discovery.

**GRANTS AND HONORS**

**2004 – 2005:** Research Fellowship for Doctors Visiting Catalonia, Spain (declined).
**2001 – 2002:** CNPq (Brazilian Science Foundation) Postdoctoral Fellowship.
**2000 – 2001:** FAPERJ (Research Support Foundation of the Rio de Janeiro State) Prestigious Ph.D. Fellowship.
**1998 – 2000:** CNPq Ph.D. Fellowship.
**1997 – 1998:** CNPq M.Sc. Fellowship.
**2011:** Pfizer Individual Performance Award
**2010:** Pfizer Individual Performance Award
**2008:** Pfizer Individual Performance Award
**2004-2007:** O-1 visa, Aliens with extraordinary ability in the sciences, arts, education, business, or athletics, or extraordinary achievements in the motion picture and television field - Department of State, United States of America.
**2002:** Honorable Mention - Fritz Feigel Award for the best Ph.D. thesis of the Chemistry Institute of the Federal University of Rio de Janeiro.
**2000:** Best Ph.D. Student in Chemistry of the Federal University of Rio de Janeiro.
**2000:** Best Poster Award - Chemistry Division of the XXII Meeting of the Federal University of Rio de Janeiro.
**1999:** Best Poster Award - Medicinal Chemistry Division of the 22$^{nd}$ Annual Meeting of the Brazilian Chemical Society.
**1999:** Best Poster Award - Theoretical Chemistry Division of the 22$^{nd}$ Annual Meeting of the Brazilian Chemical Society.

**INVITED LECTURES**

**2012:** *The Many Contributions to Protein-Ligand Binding and Implications in Drug Design.*
Schrodinger Regional User Meeting (Boston, MA)
**2012:** *Use of 3D Properties to Characterize Beyond Rule-of-5 Property Space for Passive Permeation.*
Pfizer Medicinal Chemistry Symposium (Beverly, MA)
**2011:** *MM-GB/SA Scoring versus Free-Energy Perturbation Calculations: Strengths and Pitfalls of Each Approach.*
Montreal Computer-Aided Drug Design Symposium (Montreal, Canada)
**2011:** *Structure-Based Lead Optimization using Approximate and Rigorous Free Energy Methods.*
Free Energy Simulation: From academic research to industrial application (Telluride, CO)
**2011:** *Do Fundão à Pfizer: A Jornada de um Químico Computacional*.
XVII Escola de Verão de Química Farmacêutica (Rio de Janeiro, Brazil)
**2010:** *The Many Contributions to Protein-Ligand Binding and Implications in Drug Design*.
5th Brazilian Symposium on Medicinal Chemistry (Ouro Preto, Brazil)
**2010:** *Addressing Limitations with the MM-GB/SA Scoring Procedure using the WaterMap Method and Free-Energy Perturbation Calculations.*
American Chemical Society 240th National Meeting (Boston, MA)
**2009:** *Physics-Based Scoring in Structure- and Ligand-Based Drug Design.*
Schrodinger Regional User Meeting (Boston, MA)
**2008:** *MM-GB/SA Scoring Made Easy with Knime.*
Schrodinger Regional User Meeting (New York, NY)
**2008:** *Structure-Based Lead Optimization using Approximate and Rigorous Free Energy Methods.*
Schrodinger User Meeting (Portland, OR)
**2007:** *Free-Energy Perturbation Theory and MM-GB/SA Scoring in Structure-Based Drug Design.*
Schrodinger User Meeting (New York, NY)
**2007:** *Free-Energy Perturbation Theory and MM-GB/SA Scoring in Structure-Based Drug Design.*
Structural Bioinformatics Workshop (Campinas, Brazil)
**2007:** *QM/MM Simulations of Enzymatic Reactions.*
Structural Bioinformatics Workshop (Campinas, Brazil)
**2005:** *QM/MM Simulations of Enzymatic Reactions*.
Jorgensen Symposium – 30 Years in the Trenches (New Haven, CT)
**2001:** *Thermodynamic Analysis of Thrombin Inhibition via Free-Energy Perturbation Studies***.**
Pan-American Workshop on Molecular and Material Sciences: Theoretical and Computational Aspects (Gainesville, FL)
**1999:** *Free Energy Calculations: A Challenge in Molecular Modeling.*
College of Pharmacy Seminar Series of the Federal University of Rio de Janeiro (Rio de Janeiro, RJ, Brazil)
**1997:** *Phytochrome Structure: A New Methodological Approach.*
20$^{th}$ Annual Meeting of the Brazilian Chemical Society (Poços de Caldas, MG, Brazil)

**PUBLICATIONS AND PATENTS**

1. *Enantioselective Hydroarylation of Bridged [3.2.1] Heterocycles: An Efficient Entry into the Homoepibatidine Skeleton.*
   R. Brawn, **C. R. W. Guimarães**, K. F. McClure, S. Liras.
   Org Lett. 15, 3424-3427 (2013).

2. *Design and Synthesis of Diazatricyclodecane Agonists of the G-Protein-Coupled Receptor 119.*
   E. Darout, R. P. Robinson, K. F. McClure, **C. R. W. Guimarães** et al.
   J. Med. Chem. 56, 301-319 (2013).

3. *From partial to full agonism: Identification of a novel 2,4,5,6-tetrahydro[3,4-c]pyrazole as a full agonist of the GPR119 receptor.*
   K. Futatsugi, V. Mascitti, **C. R. W. Guimarães** *et al.*
   Bioorg. Med. Chem. Lett. 23, 194-197 (2013).

4. *GPR119 Modulators.*
   **C. R. W. Guimarães**, V. Mascitti, K. F. McClure, M. J. Munchhof, R. P. Robinson.
   PCT Int. Appl. (2013), 23pp. US2013/0072427.

5. *Identification of Novel Series of Pyrazole and Indole-Urea based DFG-out PYK2 Inhibitors.*
   S. K. Bhattacharya, G. Aspnes, S. Bagley, **C. R. W. Guimarães** *et al.*
   Bioorg. Med. Chem. Lett. 22, 7523-7529 (2012).

6. *An Efficient Synthesis of Bridged Heterocycles from an Ir(I) Bis-Amination/Ring-Closing Metathesis Sequence.*
   R. A. Brawn, C. R. W. Guimarães, K. F. McClure, S. Liras.
   Org Lett. 14, 4802-4805 (2012).

7. *As Múltiplas Contribuições para a Complexação Proteína-Ligante: Consequências em Drug Design.*
   **C. R. W. Guimarães**
   Revista Virtual de Química. 4, 348-364 (2012).

8. *Structure-Guided Design, Synthesis and Evaluation of Guanine-Derived Inhibitors of the eIF4E mRNA-Cap Interaction.*
   X. Chen, D. Kopecky, J. Mihalic, S. Jeffries, X. Min, J. Heath, J. Deignan, L. SuJen, Z. Fu, **C. R. W. Guimarães**, S. Li, S. Johnstone, H. Xu, M. Cardozo, W. Shen, N. Walker, F. Kayser, Z. Wang.
   J. Med. Chem. 55, 3837-3851 (2012).

9. *Exploring Aromatic Chemical Space with NEAT: Novel and Electronically Equivalent Aromatic Template.*
   M. Tu, B. Rai, A. M. Mathiowetz, M. Didiuk, J. A. Pfefferkorn, A. Guzman-Perez, J. Benbow, **C. R. W. Guimarães**, S. Mente, M. M. Hayward, S. Liras.
   J. Chem. Inf. Model. 52, 1114-1123 (2012).

10. *Use of 3D Properties to Characterize Beyond Rule-of-5 Property Space for Passive Permeation.*
    **C. R. W. Guimarães**, A. M. Mathiowetz, M. Shalaeva, G. Goetz, S. Liras.
    J. Chem. Inf. Model. 52, 882-890 (2012).

**11.** *Deconstruction of Activity-Dependent Covalent Modification of Heme in Human Neutrophil Myeloperoxidase by Multistage Mass Spectrometry (MS4).*
K. Geoghegan, A. Varghese, X. Feng, A. Bessire, J. Conboy, R. Ruggeri, K. Ahn, S. Spath, S. Filippov, S. Conrad, P. Carpino, **C. R. W. Guimarães**, F. Vajdos.
Biochemistry 51, 2065-2077 (2012).

**12.** *MM-GB/SA Rescoring of Docking Poses.*
**C. R. W. Guimarães**
In "Methods in Molecular Biology – Computational Drug Discovery and Design", Editor R. Baron, Humana Press, New York, pp. 255-268 (2012).

**13.** *Improving MM-GB/SA Scoring through the Application of the Variable Dielectric Model*.
K. Ravindranathan, J. Tirado-Rives, W. L. Jorgensen, **C. R. W. Guimarães**
J. Chem. Theory Comput. 7, 3859-3865 (2011)**.**

**14.** *A Direct Comparison of the MM-GB/SA Scoring Procedure and Free-Energy Perturbation Calculations using Carbonic Anhydrase as a Test Case: Strengths and Pitfalls of Each Approach.*
**C. R. W. Guimarães**
J. Chem. Theory Comput. 7, 2296-2306 (2011).

**15.** *Understanding the Impact of the P-loop Conformation on Kinase Selectivity.*
**C. R. W. Guimarães**, B. K. Rai, M. J. Munchhof, S. Liu, J. Wang, S. K. Bhattacharya, L. Buckbinder.
J. Chem. Inf. Model. 51, 1199-1204 (2011).

**16.** *Identification of Potent, Noncovalent Fatty Acid Amide Hydrolase (FAAH) Inhibitors.*
D. J. Gustin, Z. Ma, X. Min, Y. Li, C. Hedberg, **C. R. W. Guimarães**, A. C. Porter, M. Lindstrom, D. Lester-Zeiner, G. Xu, T. J. Carlson, S. Xiao, C. Meleza, R. Connors, Z. Wang, F. Kayser.
Bioorg. Med. Chem. Lett. 21, 2492-2496 (2011).

**17.** *Activation of the GPR119 Receptor: A Conformation-Based Hypothesis for Understanding Agonist Response.*
K. F. McClure, E. Darout, **C. R. W. Guimarães**, M. P. DeNinno, V. Mascitti, M. J. Munchhof, R. P. Robinson, J. Kohrt, A. R. Harris, D. E. Moore, B. Li, L. Samp, B. A. Lefker, K. Futatsugi, D. Kung, P. D. Bonin, P. Cornelius, R. Wang, E. Salter, S. Hornby, A. S. Kalgutkar, Y. Chen.
J. Med. Chem, 54, 1948-1952 (2011).

**18.** *Design and Evaluation of a 2-(2,3,6-trifluorophenyl)Acetamide Derivative as a Potent Agonist of the GPR119 Receptor.*
V. Mascitti, K. McClure, **C. R. W. Guimarães**, B. Stevens, C. Choi, K. A. Farley, M. Munchhof, R. P. Robinson, K. Futatsugi, S. Lavergne, B. A. Lefker, P. Cornelius, P. D. Bonin, R. Wang, A. Kalgutkar, R. Sharma, Y. Chen.
Bioorg. Med. Chem. Lett. 21, 1306-1309 (2011).

**19.** *Preparation of Ring-Fused Pyrrolidines, Pharmaceutical Compositions Containing Them, and their Use as GPR119 Modulators.*
**C. R. W. Guimarães**, V. Mascitti, K. F. McClure, M. J. Munchhof, R. P. Robinson.
PCT Int. Appl. (2011), 69pp. WO2011036576.

**20.** *Preparation of Pyrimidine Compounds as Therapeutic GPR119 Modulators.*
E. Darout, M. P. Deninno, K. Futatsugi, **C. R. W. Guimarães**, B. A. Lefker, V. Mascitti, K. F. McClure, M. J. Munchhof, R. P. Robinson.
PCT Int. Appl. (2010), 125pp. WO2010128425.

**21.** *Preparation of Pyrimidine Compounds as Therapeutic GPR119 Modulators.*
E. Darout, M. P. Deninno, K. Futatsugi, **C. R. W. Guimarães**, B. A. Lefker, V. Mascitti, K. F. McClure, M. J. Munchhof, R. P. Robinson.
PCT Int. Appl. (2010), 122pp. WO2010128414.

**22.** *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).

**23.** *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).

**24.** *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).

**25.** *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).

**26.** *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).

**27.** *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).

**28.** *Elucidation of Fatty Acid Amide Hydrolase Inhibition by Potent alpha-Ketoheterocycle Derivatives from Monte Carlo Simulations.*
**C. R. W. Guimarães**, D. L. Boger, W. L. Jorgensen.
J. Am. Chem. Soc. 127, 17377-17384 (2005).

**29.** *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).

**30.** *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).

**31.** *Discovery of a Potent, Selective, and Efficacious Class of Reversible alpha-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).

**32.** *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).

**33.** *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).

**34.** *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).

**35.** *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).

**36.** *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).

**37.** *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).

**38.** *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).

**39.** *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).

**40.** *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).

**41.** *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).

**42.** *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).

**43.** *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).

**44.** *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).

**45.** *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).

**46.** *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).

**47.** *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).

**48.** *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).

**49.** *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).

**50.** *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).

**51.** *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).

**MEETING ABSTRACTS**

1. *The Many Contributions to Protein-Ligand Binding and Implications in Drug Design.*
   **C. R. W. Guimarães**
   Schrodinger Regional User Meeting, Boston, MA, 2012.
2. *Use of 3D Properties to Characterize Beyond Rule-of-5 Property Space for Passive Permeation.*
   **C. R. W. Guimarães**
   Pfizer Medicinal Chemistry Symposium, Beverly, MA, 2012.
3. *Exploring Aromatic Chemical Space with NEAT: Novel and Electronically Equivalent Aromatic Template.*
   M. Tu, B. Rai, A. M. Mathiowetz, **C. R. W. Guimarães**, S. Mente, M. Didiuk, M. M. Hayward, S. Liras.
   American Chemical Society 242nd National Meeting, Denver, CO, 2011.
4. *Structure-Based Lead Optimization using Approximate and Rigorous Free Energy Methods.*
   **C. R. W. Guimarães**
   Free Energy Simulation: From academic research to industrial application, Telluride, CO, 2011.
5. *MM-GB/SA Scoring versus Free-Energy Perturbation Calculations: Strengths and Pitfalls of Each Approach.*
   **C. R. W. Guimarães**
   Montreal Computer-Aided Drug Design Symposium, Montreal, Canada, 2011.
6. *Do Fundão à Pfizer: A Jornada de um Químico Computacional*
   **C. R. W. Guimarães**
   XVII Escola de Verão de Química Farmacêutica, Rio de Janeiro, Brazil, 2011.
7. *The Many Contributions to Protein-Ligand Binding and Implications in Drug Design.*
   **C. R. W. Guimarães**
   5th Brazilian Symposium on Medicinal Chemistry, Ouro Preto, Brazil, 2010.
8. *Addressing Limitations with the MM-GB/SA Scoring Procedure using the WaterMap Method and Free-Energy Perturbation Calculations.*
   **C. R. W. Guimarães**
   American Chemical Society 240th National Meeting, Boston, MA, 2010.
9. *Discovery of a Novel Series of Potent, Non-Covalent Fatty Acid Amide Hydrolase (FAAH) Inhibitors through Rational Design.*
   D. J. Gustin, Z. Ma, Y. Li, C. Hedberg, X. Min, **C. R. W. Guimarães**, Z. Wang, N. Walker, M. Lindstrom, R. Connors, A. C. Porter, D. Lester-Zeiner, F. Kayser.
   American Chemical Society 240th National Meeting, Boston, MA, 2010.
10. *Identification of a Potent, Noncovalent Series of Fatty Acid Amide Hydrolase (FAAH) Inhibitors.*
    Z. Ma, D. J. Gustin, Y. Li, C. Hedberg, X. Min, **C. R. W. Guimarães**, Z. Wang, M. Lindstrom, A. C. Porter, D. Lester-Zeiner, F. Kayser.
    American Chemical Society 237th National Meeting, Salt Lake City, UT, 2009.
11. *Physics-Based Scoring in Structure- and Ligand-Based Drug Design.*
    **C. R. W. Guimarães**
    **S**chrodinger Regional User Meeting, Boston, MA, 2009.

**12.** *MM-GB/SA Scoring Made Easy with Knime.*
**C. R. W. Guimarães**
Schrodinger Regional User Meeting, New York, NY, 2008.

**13.** *Structure-Based Lead Optimization using Approximate and Rigorous Free Energy Methods*
**C. R. W. Guimarães**
Schrodinger User Meeting, Portland, OR, 2008.

**14.** *Free-Energy Perturbation Theory and MM-GB/SA Scoring in Structure-Based Drug Design.*
**C. R. W. Guimarães**
Schrodinger User Meeting, New York, NY, 2007.

**15.** *Free-Energy Perturbation Theory and MM-GB/SA Scoring in Structure-Based Drug Design.*
**C. R. W. Guimarães**
Structural Bioinformatics Workshop, Campinas, Brazil, 2007.

**16.** *QM/MM Simulations of Enzymatic Reactions.*
**C. R. W. Guimarães**
Structural Bioinformatics Workshop, Campinas, Brazil, 2007.

**17.** *QM/MM Simulations of Enzymatic Reactions.*
**C. R. W. Guimarães**, W. L. Jorgensen.
Jorgensen Symposium – 30 Years in the Trenches, New Haven, CT, 2005.

**18.** *QM/MM Simulations on Macrophomate Synthase: Diels-Alder versus Michael-Aldol Reaction Mechanism.*
**C. R. W. Guimarães**, M. Udier-Blagović, W. L. Jorgensen.
Gordon Research Conference (Computational Chemistry), Plymouth, NH, 2004.

**19.** *Improved Semiempirical Methods: Parameterization of PDDG/PM3 for Sulfur.*
I. Tubert-Brohman, **C. R. W. Guimarães**, W. L. Jorgensen.
American Chemical Society 227th National Meeting, Anaheim, CA, 2004.

**20.** *Advances in QM/MM Simulations for Organic Reactions in Solution.*
W. L. Jorgensen, **C. R. W. Guimarães**, Orlando Acevedo.
American Chemical Society 227th National Meeting, Anaheim, CA, 2004.

**21.** *Improved Semiempirical MO Methods: PDDG/PM3.*
W. L. Jorgensen, I. Tubert-Brohman, **C. R. W. Guimarães**.
American Chemical Society 227th National Meeting, Anaheim, CA, 2004.

**22.** *PDDG/PM3 and PDDG/MNDO: Extension to the Halogens.*
I. Tubert-Brohman, **C. R. W. Guimarães**, M. P. Repasky, W. L. Jorgensen.
American Chemical Society 226th National Meeting, New York, NY, 2003.

**23.** *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.
43rd Sanibel Symposium, St Augustine, FL, 2003.

**24.** *Solvent Effects on the Diastereoselectivity of Michael Additions to Nitro-Olefins from Quantum Mechanical and Molecular Dynamics Calculations.*
T. M. Cardozo, C. A. F. Oliveira, **C. R. W. Guimarães**, J. Jones Jr., R. Bicca de Alencastro.
XXIV Meeting of the Federal University of Rio de Janeiro, Rio de Janeiro, RJ, Brazil, 2002.

**25.** *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.
Workshop on Molecular Modeling in Biophysics: Methods and Applications, Rio de Janeiro, RJ, Brazil, 2002.

**26.** *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.
25th Annual Meeting of the Brazilian Chemical Society, Poços de Caldas, MG, Brazil, 2002.

**27.** *Using Free Energy Perturbations and QM/MM to Obtain Free-Energy Minima and Maxima in Condensed Phase.*
**C. R. W. Guimarães**, M. P. Repasky, J. Chandrasekhar, J. Tirado-Rives, W. L. Jorgensen.
Molecular Simulations in Structural Biology and Drug Discovery. Symposium Honoring Peter A. Kollman, San Francisco, CA, 2002.

**28.** *A Molecular Dynamics and Free-Energy Perturbation Studies of an L-type Calcium Channel Model.*
G. Barreiro, **C. R. W. Guimarães**, R. Bicca de Alencastro.
Molecular Simulations in Structural Biology and Drug Discovery. Symposium Honoring Peter A. Kollman, San Francisco, CA, 2002.

**29.** *Solvent Effects on the Diastereoselectivity of Michael Additions to Nitro-Olefins from Quantum Mechanical and Molecular Dynamics Calculations.*
T. M. Cardozo, **C. R. W. Guimarães**, F. M. da Silva, J. Jones Jr., R. Bicca de Alencastro.
24th Annual Meeting of the Brazilian Chemical Society, Poços de Caldas, MG, Brazil, 2001.

**30.** *Thermodynamic Analysis of Thrombin Inhibition via Free-Energy Perturbation Studies.*
**C. R. W. Guimarães**, R. Bicca de Alencastro.
41st Sanibel Symposium, St Augustine, FL, 2001.

**31.** *A Molecular Dynamics Study of an L-type Calcium Channel Model.*
G. Barreiro, **C. R. W. Guimarães**, R. Bicca de Alencastro.
41st Sanibel Symposium, St Augustine, FL, 2001.

**32.** *Thermodynamic Analysis of Thrombin Inhibition via Free-Energy Perturbation Studies.*
**C. R. W. Guimarães**, R. Bicca de Alencastro.
2001 Pan-American Workshop on Molecular and Material Sciences: Theoretical and Computational Aspects, Gainesville, FL, 2001.

**33.** *A Molecular Dynamics Study of an L-type Calcium Channel Model.*
G. Barreiro, **C. R. W. Guimarães**, R. Bicca de Alencastro.
2001 Pan-American Workshop on Molecular and Material Sciences: Theoretical and Computational Aspects, Gainesville, FL, 2001.

**34.** *Solvent Effects on the Diastereoselectivity of Michael Additions to Nitro-Olefins from Quantum Mechanical and Molecular Dynamics Calculations.*
T. M. Cardozo, **C. R. W. Guimarães**, F. M. da Silva, J. Jones Jr., R. Bicca de Alencastro.

XXII Meeting of the Federal University of Rio de Janeiro, Rio de Janeiro, RJ, Brazil, 2000.

**35.** *Molecular Dynamics of Liquid 1-octanol: Evaluation of Relative Octanol/Water Partition Coefficients of Thrombin Inhibitors via Free-Energy Perturbations.*
C. A. F. de Oliveira, **C. R. W. Guimarães**, R. Bicca de Alencastro.
XXII Meeting of the Federal University of Rio de Janeiro, Rio de Janeiro, RJ, Brazil, 2000.

**36.** *Reduction of Dioxindols to Triptofols: A Semiempirical Study.*
R. Amorim, **C. R. W. Guimarães,** R. B. da Silva, S. J. Garden, A. C. Pinto, R. Bicca de Alencastro.
XXII Meeting of the Federal University of Rio de Janeiro, Rio de Janeiro, RJ, Brazil, 2000.

**37.** *Development of a Molecular Dynamics Program for the Simulation of Atomic and Molecular Systems.*
C. A. F. de Oliveira, **C. R. W. Guimarães**, R. Bicca de Alencastro.
XXII Meeting of the Federal University of Rio de Janeiro, Rio de Janeiro, RJ, Brazil, 2000.

**38.** *A Molecular Dynamics Study on the Structure of Liquid 1-Octanol and Its Water Saturated Solution.*
C. A. F. de Oliveira, **C. R. W. Guimarães**, R. Bicca de Alencastro.
XXVI Congress of Theoretical Chemists of Latin Expression, Caxambu, MG, Brazil, 2000.

**39.** *Evaluating Relative Affinities and Relative Octanol/Water Partition Coefficients of Thrombin Inhibitors via Free-Energy Perturbations.*
**C. R. W. Guimarães**, C. A. F. de Oliveira, R. Bicca de Alencastro.
Computational Biophysics, Nice, France, 2000.

**40.** *Reduction of Dioxindols to Triptofols: A Semiempirical Study.*
R. Amorim, **C. R. W. Guimarães,** R. B. da Silva, S. J. Garden, A. C. Pinto, R. Bicca de Alencastro.
23rd Annual Meeting of the Brazilian Chemical Society, Poços de Caldas, MG, Brazil, 2000.

**41.** *Molecular Dynamics of the Liquid State of 1-Octanol.*
C. A. F. de Oliveira, **C. R. W. Guimarães**, R. Bicca de Alencastro.
23rd Annual Meeting of the Brazilian Chemical Society, Poços de Caldas, MG, Brazil, 2000.

**42.** *Evaluating Relative Affinities of Thrombin Inhibitors via Free-Energy Perturbations.*
**C. R. W. Guimarães**, R. Bicca de Alencastro.
23rd Annual Meeting of the Brazilian Chemical Society, Poços de Caldas, MG, Brazil, 2000.

**43.** *A Molecular Dynamics Study on the Structure of Liquid 1-Octanol.*
C. A. F. de Oliveira, **C. R. W. Guimarães**, R. Bicca de Alencastro.
40th Sanibel Symposium, St Augustine, FL, 2000.

**44.** *Evaluating Relative Affinities of Thrombin Inhibitors Using the Free-Energy Perturbation Technique.*
**C. R. W. Guimarães,** C. A. M. Fraga, E. J. Barreiro, R. Bicca de Alencastro.
40th Sanibel Symposium, St Augustine, FL, 2000.

**45.** *Evaluating Relative Affinities of Thrombin Inhibitors Using Molecular Dynamics Techniques.*
**C. R. W. Guimarães,** C. A. M. Fraga, E. J. Barreiro, R. Bicca de Alencastro.
X Brazilian Symposium of Theoretical Chemistry, Caxambu, MG, Brazil, 1999.

**46.** *Evaluating Relative Octanol/Water Partition Coefficients of Thrombin Inhibitors via Free-Energy Perturbations.*
C. A. F. de Oliveira, **C. R. W. Guimarães**, R. Bicca de Alencastro.
X Brazilian Symposium of Theoretical Chemistry, Caxambu, MG, Brazil, 1999.

**47.** *Evaluating Relative Octanol/Water Partition Coefficients of Thrombin Inhibitors via Free-Energy Perturbations.*
C. A. F. de Oliveira, **C. R. W. Guimarães**, R. Bicca de Alencastro.
XXI Meeting of the Federal University of Rio de Janeiro, Rio de Janeiro, RJ, Brazil, 1999.

**48.** *Evaluating Relative Affinities of Thrombin Inhibitors Using Molecular Dynamics Techniques.*
**C. R. W. Guimarães,** C. A. M. Fraga, E. J. Barreiro, R. Bicca de Alencastro.
22nd Annual Meeting of the Brazilian Chemical Society, Poços de Caldas, MG, Brazil, 1999.

**49.** *Evaluating Relative Octanol/Water Partition Coefficients of Thrombin Inhibitors via Free-Energy Perturbations.*
C. A. F. de Oliveira, **C. R. W. Guimarães**, R. Bicca de Alencastro.
22nd Annual Meeting of the Brazilian Chemical Society, Poços de Caldas, MG, Brazil, 1999.

**50.** *Theoretical Investigation of the Diastereoselectivity Observed During the Formation of Acyl-hydrazone Derivatives.*
**C. R. W. Guimarães,** C. A. M. Fraga, E. J. Barreiro, R. Bicca de Alencastro.
22nd Annual Meeting of the Brazilian Chemical Society, Poços de Caldas, MG, Brazil, 1999.

**51.** *Theoretical Studies on the Reduction of Disubstituted 3-methyleneoxindoles by the NADH Model Hantzsch Ester.*
C. A. F. de Oliveira, **C. R. W. Guimarães**, M. B. Correa, S. J. Garden, A. C. Pinto, R. Bicca de Alencastro.
XX Meeting of the Federal University of Rio de Janeiro, Rio de Janeiro, RJ, Brazil, 1998.

**52.** *Phytochrome Structure 2. The Case of Chromopeptides.*
**C. R. W. Guimarães**, J. D. da Motta Neto, R. Bicca de Alencastro.
14th International IUPAC Conference on Physical Organic Chemistry, Florianópolis, SC, Brazil, 1998.

**53.** *Theoretical Studies on the Reduction of Disubstituted 3-methyleneoxindoles by the NADH Model Hantzsch Ester.*
C. A. F. de Oliveira, **C. R. W. Guimarães**, M. B. Correa, S. J. Garden, A. C. Pinto, R. Bicca de Alencastro.
21st Annual Meeting of the Brazilian Chemical Society, Poços de Caldas, MG, Brazil, 1998.

**54.** *Phytochrome Structure: A New Methodological Approach***.**
**C. R. W. Guimarães**, J. D. da Motta Neto, R. Bicca de Alencastro.
21st Annual Meeting of the Brazilian Chemical Society, Poços de Caldas, MG, Brazil, 1998.

**55.** *Phytochrome Structure: A New Methodological Approach.*
**C. R. W. Guimarães**, J. D. da Motta Neto, R. Bicca de Alencastro.
38th Sanibel Symposium, St Augustine, FL, 1998.

**56.** *Phytochrome Structure: A New Methodological Approach.*
**C. R. W. Guimarães**, J. D. da Motta Neto, R. Bicca de Alencastro.
IX Brazilian Symposium of Theoretical Chemistry, Caxambu, MG, Brazil, 1997.

**57.** *Modeling Interactions of the Phytochrome Chromophore with some Aminoacids.*
**C. R. W. Guimarães**, J. D. da Motta Neto, R. Bicca de Alencastro.
20th Annual Meeting of the Brazilian Chemical Society, Poços de Caldas, MG, Brazil, 1997.

**58.** *A Semiempirical Study of a Phytochrome Model.*
**C. R. W. Guimarães**, J. D. da Motta Neto, R. Bicca de Alencastro.
37th Sanibel Symposium, St Augustine, FL, 1997.

**59.** *A Semiempirical Study of the Isomerization Process on a Phytochrome Model.*
**C. R. W. Guimarães**, R. Bicca de Alencastro.
XVIII Meeting of the Federal University of Rio de Janeiro, Rio de Janeiro, RJ, Brazil, 1996.

**60.** *A Conformational Study of the Phytochrome Chromophore Using the AM1 Method.*
**C. R. W. Guimarães**, G. C. da Silva, R. Bicca de Alencastro.
19th Annual Meeting of the Brazilian Chemical Society, Poços de Caldas, MG, Brazil, 1996.

**61.** *Theoretical Analysis of the Binding Process between Farnesil-cysteine Analogs and the Methyl-transferase Enzyme.*
**C. R. W. Guimarães**, R. Bicca de Alencastro.
VIII Brazilian Symposium of Theoretical Chemistry, Caxambu, MG, Brazil, 1995.

**62.** *Theoretical Analysis of the Binding Process between Farnesil-cysteine Analogs and the Methyl-transferase Enzyme.*
**C. R. W. Guimarães**, R. Bicca de Alencastro.
XVII Meeting of the Federal University of Rio de Janeiro, Rio de Janeiro, RJ, Brazil, 1995.

**63.** *Theoretical Analysis of the Binding Process between Farnesil-cysteine Analogs and the Methyl-transferase Enzyme.*
**C. R. W. Guimarães**, C. R. Peruso, R. Bicca de Alencastro.
18th Annual Meeting of the Brazilian Chemical Society, Caxambu, MG, Brazil, 1995.

**64.** *A Comparative Study between the AM1 Semiempirical Method and the MM2 Force Field on the Equilibrium of Photochromic Substances.*
**C. R. W. Guimarães**, R. Bicca de Alencastro.
XVI Meeting of the Federal University of Rio de Janeiro, Rio de Janeiro, RJ, Brazil, 1994.

**65.** *Molecular Mechanics Calculations on Photochromic Substances.*
**C. R. W. Guimarães**, R. Bicca de Alencastro.
17th Annual Meeting of the Brazilian Chemical Society, Caxambu, MG, Brazil, 1994.