

## **César Augusto F. de Oliveira**

McCammon Research Group  
Department of Chemistry and Biochemistry  
University of California, San Diego  
9500 Gilman Drive, La Jolla, CA 92093-0365  
Phone: 858-357-1759  
e-mail: cesar@mccammon.ucsd.edu

### **PROFESSIONAL EXPERIENCE**

#### **2011 – Present: Research Specialist**

Howard Hughes Medical Institute  
University of California, San Diego  
Research Advisor: Professor J. Andrew Mccammon

#### **2005 – 2011: Postdoctoral Research Associate**

Howard Hughes Medical Institute  
University of California, San Diego  
Research Advisor: Professor J. Andrew Mccammon

Development and Application of:

- Accelerated Molecular Dynamics Simulation.
- Free Energy methods.
- Drug Design/Discovery methodologies.

### **EDUCATION**

#### **2001 – 2005: PhD in Chemistry**

Federal University of Rio de Janeiro (Rio de Janeiro, Brazil)  
Research Advisor: Professor Ricardo Bicca de Alencastro.

*Thesis: "Catalytic Activity of the Serine Protease of Human Cytomegalovirus: A Theoretical Study."*

- Investigation of the Induced-Fit Mechanism and Catalytic Activity of the Human Cytomegalovirus Protease Homodimer via Molecular Dynamics Simulations.
- Human Cytomegalovirus Protease: Why is the Dimer Required for Catalytic Activity?

#### **1996 – 2001: B.S. in Chemical Engineering**

Federal University of Rio de Janeiro (Rio de Janeiro, Brazil).

*Undergraduate Research :*

- Evaluation of the Relative Octanol/Water Partition Coefficients of Thrombin Inhibitors via Free-Energy Perturbations.
- Molecular Dynamics Study on Liquid 1-Octanol and Its Water-Saturated Solution.
- Theoretical Study of the Reduction of Electron Withdrawing Group Conjugated Olefins by the Hantzsch 1,4-dihydropyridine Ester.

## TEACHING

**2001 – 2005: Federal University of Rio de Janeiro (Rio de Janeiro, Brazil).**

Teaching assistant (2003): Organic Chemistry II - undergraduate.

**2005 – Present: University of California, San Diego.**

Authored and delivered lecture on: “Special Topics on Emerging Technologies in Multiscale Modeling”.

National Biomedical Computation Resource Summer Institute,  
San Diego Super Computer Center (2010 and 2011)

Mentored undergraduate and graduate students. Supervised and directed daily research activities and co-authored resulting articles.

- Jacob Durrant (Graduate student):
  - a) *Design of MMP2 inhibitors: Including Receptor Flexibility and Induced fit-Effects into Drug Design.*
  - b) *POVME: An Algorithm for Measuring Binding-Pocket Volume.*
  - c) *Inclusion of Receptor Flexibility in Docking Analyses of Metalloproteinases types 2 and 3 Reveals that Pyrone-Based Molecules Work as Conformation Selective Inhibitors.*
  - d) *Design of MMP2 inhibitors: Including Receptor Flexibility and Induced fit-Effects into Drug Design.*
- William Sinko (Graduate Student)
  - a) *Applying Molecular Dynamics Simulations to Identify Rarely Sampled Ligand-bound Conformational States of Undecaprenyl Pyrophosphate Synthase, an Antibacterial Target.*
  - b) *Guide to Virtual Screening: Application to the Akt Phosphatase PHLPP.*
- Michelle Zhou (Undergraduate Student)
  - a) *Large-Scale Conformational Changes of Trypanosoma cruzi Proline Racemase Predicted by Accelerated Molecular Dynamics Simulation.*

## GRANTS AND HONORS

Proposals for computational resources that have resulted in allocations awarded to the McCammon group.

- Special-purpose Machine for Molecular Dynamics (ANTON) at Pittsburg Supercomputing Center
- Ranger at Texas Advanced Computing Center.

**2004 – 2005:** FAPERJ (Research Support Foundation of the Rio de Janeiro State) Prestigious Ph.D. Fellowship.

**2001 – 2004:** CNPq (Brazilian Science Foundation) Ph.D. Fellowship.

**1998 – 2001:** CNPq Undergraduate Fellowship.

**2004:** Best Ph.D. Student in Chemistry of the Federal University of Rio de Janeiro.

**2000:** Honorable Mention - XXVI Meeting of the Federal University of Rio de Janeiro.

**2004:** Best Poster Award - Chemistry Division of the XXVI Meeting of the Federal University of Rio de Janeiro.

**2003:** Honorable Mention - Chemistry Division of the XXV Meeting of the Federal University of Rio de Janeiro.

**2000:** Honorable Mention - XXII Meeting 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.

**INVITED  
LECTURES**

**2010:** *Studying the Cross-Reaction Between Trypanosoma Cruzi Antibodies and Human Beta-1 Adrenergic Receptor.*

Pharmacology Research Discussions, University of California, San Diego.

**2008:** *Design of Matrix Metalloproteinase inhibitors.*

Pharmacology Research Discussions, University of California, San Diego.

**2004:** *Computer Simulation of Biological Systems: Principles and Applications.*

Seminar Series of the Department of Organic Chemistry of the Federal University of Rio de Janeiro, Rio de Janeiro, RJ, Brazil.

**2000:** *Molecular Dynamics of Liquid 1-Octanol: Evaluation of Relative Octanol/Water Partition Coefficients of Thrombin Inhibitors via Free-Energy Perturbations.*

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

**2000:** *Molecular Dynamics of the 1-Octanol Liquid State.*

23<sup>th</sup> Annual Meeting of the Brazilian Chemical Society, Poços de Caldas, MG, Brazil.

**1998:** *Theoretical Calculations on the Reduction of Isatin Derivatives.*

XX Meeting of the Federal University of Rio de Janeiro - Chemistry Division, Rio de Janeiro, RJ, Brazil.

**JOURNAL  
MANUSCRIPT  
REVIEW**

Journal of American Chemical Society

Journal of Chemical Theory and Computation

Journal of Chemical Physics

Journal of Computer Aided-Molecular Design

Journal of Molecular Graphics and Modelling

Bioorganic & Medicinal Chemistry Letters

Journal of Biomolecular Structure and Dynamics

**PUBLICATIONS**

1. *TIR1/AFBs and Aux/IAAs constitute a combinatorial co-receptor system to perceive auxin with differential sensitivities.*  
L. I. A. Calderón Villalobos, S. Lee, **C. A. F. Oliveira**, A. Ivetac, W. Brandt, L. Armitage, L. B. Sheard, X. Tan, G. Parry, H. Mao, J. A. Mccammon, N. Zheng, R. Napier, S. Kepinski, M. Estelle. Nat. Struct. Biol. (submitted)
2. *Benzoic Acids Target Both cis- and trans-prenyl Transferases: A Crystallographic Investigation.*  
Y. Zhang, Y. Liu, W. Zhu, R. Cao, J. No, F. Lin, K. Li, K. Wang, K. Houlihan, A. Sankovsky, W. Sinko, **C. A. F. Oliveira**, J. Andrew McCammon and Eric Oldfield  
JACS (submitted)
3. *Protecting High Energy Barriers: A New Equation to Regulate Boost Energy in Accelerated Molecular Dynamics Simulations.*  
W. Sinko, **C. A. F. Oliveira**, J. A. McCammon.  
J. Chem. Theor. Comp. (Article ASAP). (\* **joint first-author**)
4. *Guide to Virtual Screening: Application to the Akt Phosphatase PHLPP.*  
*In Methods in Molecular Biology: Computational Drug Discovery and Design.*

W. Sinko, E. Sierecki, **C. A. F. Oliveira**, J. A. McCammon (in press).  
COMPUTATIONAL DRUG DISCOVERY AND DESIGN  
Methods in Molecular Biology, 819, 561-73 (2012)

5. *Enhanced Lipid Diffusion and Mixing in Accelerated Molecular Dynamics.*  
Yi Wang, P. R. L. Markwick, **C. A. F. Oliveira**, J. A. McCammon  
J. Chem. Theor. Comp. 7, 3199-3207 (2011).
6. *Large-Scale Conformational Changes of Trypanosoma cruzi Proline Racemase Predicted by Accelerated Molecular Dynamics Simulation.*  
**C. A. F. Oliveira**, B. Grant, M. Zhou, J. A. McCammon  
PloS Comp. Biol. 7(10), e1002178 (2011).
7. *Pyrene-Based Inhibitors of Metalloproteinases Types 2 and 3 May Work as Conformation-Selective Inhibitors.*  
J. Durrant, **C. A. F. Oliveira\***, J. A. McCammon. (\* **joint first-author**)  
Chem. Biol. & Drug Design. 78, 191-198 (2011) (**Cover**)
8. *Applying Molecular Dynamics Simulations to Identify Rarely Sampled Ligand-bound Conformational States of Undecaprenyl Pyrophosphate Synthase, an Antibacterial Target.*  
W. Sinko, **C. A. F. Oliveira**, S. Williams, A. V. Wynsberghe, E. Oldfield, J. A. McCammon.  
Chem. Biol. & Drug Design. 77, 412-420 (2011) (**Cover**) (Faculty of 1000: <http://f1000.com/8311970>)
9. *POVME: An Algorithm for Measuring Binding-Pocket Volume.*  
J. Durrant, **C. A. F. Oliveira**, J. A. McCammon.  
J. Mol. Graph. Model. 29, 773-776 (2011).
10. *From Zn to Mn: The Study of Novel Manganese-Binding Groups in the Search for New Drugs against Tuberculosis.*  
S. L. Williams, **C. A. F. Oliveira**, H. Vazquez, J. A. McCammon.  
Chem. Biol. & Drug Design 77, 117-123 (2011)
11. *From Sensors to Silencers: Quinoline- and Benzimidazole-Sulfonamides as Inhibitors for Zinc Proteases.*  
M. Rouffet, **C. A. F. Oliveira**, J. A. McCammon, S. M. Cohen.  
J. Amer. Chem. Soc. 13, 8232-8233 (2010).
12. *Coupling Constant pH Simulations with Accelerated Molecular Dynamics Method*  
S. Williams, **C. A. F. Oliveira**, J. A. McCammon.  
J. Chem. Theory Comput. 6, 560-568 (2010)
13. *Design of MMP2 inhibitors: Including Receptor Flexibility and Induced fit-Effects into Drug Design.*  
J. Durrant, **C. A. F. Oliveira**, J. A. McCammon  
J. Mol. Recognition (2010) - Special Issue Article
14. *Thioamide hydroxythiopyrones supersede amide hydroxythiopyrones in potency against anthrax lethal factor.*  
A. Agrawal, **C. A. F. Oliveira**, Y. Cheng, J. A. Jacobsen, J. A. McCammon, Seth M. Cohen  
J. Med. Chem. 52, 1063-1074 (2009).
15. *Coupling Accelerated Molecular Dynamics Methods with Thermodynamic Integration Simulations.*  
**C. A. F. Oliveira**, D. Hammelberg, J. A. McCammon.  
J. Chem. Theor. Comp. 4, 1516-1525 (2008)
16. *Biomolecular Association of the E9 – Im9 Colicin Dnase – Immunity Protein recognition in Water: A Multiple Copy and Accelerated Molecular Dynamics Simulation Study.*  
R. Baron, S. Wong, **C. A. F. Oliveira**, J. A. McCammon.  
J. Phys. Chem. B. 112, 16802-16814 (2008)

17. *Inhibition of Cathepsin B by Au(I) Complexes: A Kinetic and Computational Study.*  
S. S. Gunatilleke, **C. A. F. Oliveira**, J. A. McCammon, A. M. Barrios.  
J. Biol. Inorg. Chem. 13, 555-561, (2008)
18. *Sampling of Slow Diffusive Conformational Transitions with Accelerated Molecular Dynamics.*  
D. Hammelberg, **C. A. F. Oliveira**, J. A. McCammon.  
J. Chem. Phys. 127, 155102-155110, (2007).
19. *Estimating Kinetic Rates from Accelerated Molecular Dynamics Simulations: Alanine Dipeptide in Explicit Solvent as a Case Study.*  
**C. A. F. Oliveira**, D. Hammelberg, J. A. McCammon.  
J. Chem. Phys. 127, 175105-175112, (2007).
20. *Molecular Dynamics Simulations of Metalloproteinases Types 2 and 3 Reveal Differences in the Dynamic Behavior of the S1' Binding Pocket.*  
**C. A. F. Oliveira**, M. Zissen, J. Mongon, J. A. McCammon  
Curr. Pharm. Des. 13, 3471-3475, (2007).
21. *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)
22. *On the Application of Accelerated Molecular Dynamics to Liquid Water Simulations*  
**C. A. F. Oliveira**, D. Hammelberg, J. A. McCammon.  
J. Phys. Chem. B. 110, 22695-22701, (2006).
23. *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).
24. *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(1), 126-136 (2004).
25. *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(23), 8815-8822 (2003).
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.  
Proteins 52(4), 483-491 (2003).
27. *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).
28. *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(2), 786-791 (2002).
29. *Detecção em Tempo Real de Vazamentos em Redes de Escoamento para Fluidos Incompressíveis: Uma*

*Abordagem em Séries Temporais.*

**C. A. F. de Oliveira**, O. Q. F. de Araújo, J. L. Medeiros.  
Boletim Técnico da Petrobrás, Brasil, v.45, n. 2 (2002).

- 30.** Instantaneous Leak Detection in Pipe Networks for Incompressible Fluids: A Time Series Approach.

**C. A. F. de Oliveira**, O. Q. F. de Araújo, J. L. Medeiros.  
Proceedings of 3<sup>rd</sup> Enpromer, v. 1, p. 433-438 (2002).

- 31.** *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: Santos, Hélio F.; Coura, Pablo Z.; Dantas, Sócrates O.; Barone, Paulo M. V. B. (Org.). Escola Brasileira de Estrutura Eletrônica. São Paulo, p. 191-201 (2002).

- 32.** *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(4-5), 999-1006 (2000).

## REFERENCES

### **Prof. J. Andrew McCammon**

Department of Chemistry & Biochemistry  
University of California, San Diego  
9500 Gilman Drive  
La Jolla, CA 92093-0365  
e-mail: jmccammon@ucsd.edu

### **Prof. Ricardo Bicca de Alencastro**

Department of Chemistry  
Federal University of Rio de Janeiro (Brazil)  
Centro de Tecnologia, Bloco A, Sala 609  
Cidade Universitaria.  
e-mail: bicca@iq.ufrj.br

### **Dr. Cristiano R. W. Guimarães**

Pfizer, Inc.  
Cardiovascular and Metabolic Diseases Department  
Eastern Point Road  
Groton, CT 06340  
e-mail: cristiano.guimaraes@pfizer.com