

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: 858-534-0956
e-mail: cesar@mccammon.ucsd.edu

PROFESSIONAL EXPERIENCE

2005 – Present: University of California, San Diego

Postdoctoral Research Associate.

Howard Hughes Medical Institute

Research Advisor: Professor J. Andrew McCammon

- Development and Application of Accelerated Molecular Dynamics Simulation.
- Free Energy methods
- Drug Design/Discovery.

EDUCATION

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

Ph.D.

Research Advisor: Professor Ricardo Bicca de Alencastro.

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.
- QM/MM Study of the Role of His157 in the Catalytic Triad of Herpesvirus Proteases.

1996 – 2001: Federal University of Rio de Janeiro (Rio de Janeiro, Brazil)

B.S. in Chemical Engineering *with distinction*

- Evaluation of the Relative Octanol/Water Partition Coefficients of Thrombin Inhibitors via Free-Energy Perturbations.
- A Molecular Dynamics Study on Liquid 1-Octanol and Its Water-Saturated Solution.
- Development of a Molecular Dynamics Code for the Simulation of Atomic and Molecular Systems.
- 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)**

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

GRANTS AND HONORS**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****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.*23th 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

PUBLICATIONS

1. *Coupling Constant pH Simulations with Accelerated Molecular Dynamics Method.*
S. Williams, **C. A. F. Oliveira**, J. A. McCammon (in preparation).
2. *Studying the Cross-Reaction Between Trypanosoma Cruzi Antibodies and Human Beta-1 Adrenergic Receptor.*
C. A. F. Oliveira, J. A. McCammon (in preparation).
3. *Inclusion of Receptor Flexibility in Docking Analyses of Metalloproteinases types 2 and 3 Reveals that Pyrone-Based Molecules Work as Conformation Selective Inhibitors*
C. A. F. Oliveira, J. A. McCammon (in preparation).
4. *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. Recog. (accepted)
5. *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).
6. *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)
7. *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)
8. *Reversible Folding of Trp-Cage Protein from Accelerated Molecular Dynamics Simulation.*
C. A. F. Oliveira, D. Hammelberg, J. A. McCammon (submitted)
9. *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. Inoorg. Chem. 13, 555-561, (2008)
10. *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).
11. *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).
12. *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).

13. 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)

14. 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).

15. 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).

16. 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).

17. 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).

18. 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).

19. 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).

20. 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).

21. 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).

22. 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 3rd Enpromer, v. 1, p. 433-438 (2002).

23. *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).

24. *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).

MEETING ABSTRACTS

1. Accelerated Molecular Dynamics Simulations: Extending the Time Scale os All-Atom Simulations of Biological System.
C. A. F. Oliveira, D. Hammelberg, J. A. McCammon.
European Protein Society, Zurich, 2009.
2. *Estimating Kinetic Rates from Accelerated Molecular Dynanics Simulation: Alanine Dipeptide in Explicit Solvent as a Case Study.*
C. A. F. Oliveira, D. Hammelberg, J. A. McCammon.
American Chemical Society Meeting, Boston, 2007.
3. *Full Length Zinc Selective Inhibitors of Matrix Metalloproteinases.*
F. E. Jacobsen, **C. A. F. Oliveira**, J. A. McCammon, S. M. Cohen.
American Chemical Society Meeting, Chicago, 2007.
4. *On the Application of Accelerated Molecular Dynamics to Liquid Water Simulations.*
C. A. F. Oliveira, D. Hammelberg, J. A. McCammon.
American Chemical Society Meeting, San Fracisco, 2006.
5. *Molecular Basis of the Interaction between Parabutoxin 1 and Voltage-Gated Potassium Channel Kv1.1.*
F. P. Fleming, **C. A. F. Oliveira**, C. R. W. Guimarães, G. Barreiro, R. Bicca de Alencastro.
2nd Brazilian Symposium on Medicinal Chemistry, Current Trends in Drug Discovery and Development, RJ, Brazil, 2004.
6. *Investigation of the Catalytic Activity of the Human Cytomegalovirus Protease via Molecular Dynamics Simulations.*
C. A. F. Oliveira, C. R. W. Guimarães, G. Barreiro, R. Bicca de Alencastro.
2nd Brazilian Symposium on Medicinal Chemistry, Current Trends in Drug Discovery and Development, RJ, Brazil, 2004.
7. *Molecular Dynamic Simulations on Polyamidoamine Dendrimers.*
E. R. A. Oliveira, **C. A. F. Oliveira**, V. Furtado, R. Bicca de Alencastro.
2nd Brazilian Symposium on Medicinal Chemistry, Current Trends in Drug Discovery and Development, RJ, Brazil, 2004.
8. *A Molecular Dynamics Investigation of the Responsible Factors for the Selectivity of the HSV-2 Protease in the Catalysis of its Natural Substrate.*
P. A. P. Neto, **C. A. F. Oliveira**, R. Bicca de Alencastro.
2nd Brazilian Symposium on Medicinal Chemistry, Current Trends in Drug Discovery and Development, RJ, Brazil, 2004.
9. *Molecular Basis of the Interaction between Parabutoxin 1 and Voltage-Gated Potassium Channel Kv1.1.*
F. P. Fleming, **C. A. F. Oliveira**, C. R. W. Guimarães, G. Barreiro, R. Bicca de Alencastro.

XXVI Meeting of the Federal University of Rio de Janeiro, Rio de Janeiro, RJ, Brazil, 2004.

10. *Molecular Dynamic Simulations on Polyamidoamine Dendrimers.*
E. R. A. Oliveira, **C. A. F. Oliveira**, V. Furtado, R. Bicca de Alencastro.
XXVI Meeting of the Federal University of Rio de Janeiro, Rio de Janeiro, RJ, Brazil, 2004.
11. *A Molecular Dynamics Investigation of the Responsible Factors for the Selectivity of the HSV-2 Protease in the Catalysis of its Natural Substrate.*
P. A. P. Neto, **C. A. F. Oliveira**, R. Bicca de Alencastro.
XXVI Meeting of the Federal University of Rio de Janeiro, Rio de Janeiro, RJ, Brazil, 2004.
12. *Dendrimers in Drug Delivery Systems.*
E. R. A. Oliveira, **C. A. F. Oliveira**, V. Furtado, R. Bicca de Alencastro.
XXV Meeting of the Federal University of Rio de Janeiro, Rio de Janeiro, RJ, Brazil, 2003.
13. *Dendrimers in Drug Delivery Systems. A Molecular Dynamics Study.*
E. R. A. Oliveira, **C. A. F. Oliveira**, V. Furtado, R. Bicca de Alencastro.
26th Annual Meeting of the Brazilian Chemical Society, Poços de Caldas, MG, Brazil, 2003.
14. *Theoretical Study of Solvent Effects on the Diastereoselectivity of Michael Additions to Nitro-Olefins.*
T. M. Cardozo, **C. A. F. Oliveira**, C. R. W. Guimarães, J. Jones Jr., R. Bicca de Alencastro.
26th Annual Meeting of the Brazilian Chemical Society, Poços de Caldas, MG, Brazil, 2003.
15. *Dendrimers in Drug Delivery Systems. A Molecular Dynamics Study.*
E. R. A. Oliveira, **C. A. F. Oliveira**, V. Furtado, R. Bicca de Alencastro.
XII Brazilian Symposium of Theoretical Chemistry, Caxambu, MG, Brazil, 2003.
16. *Dendrimers in Drug Delivery Systems. A Molecular Dynamics Study.*
E. R. A. Oliveira, **C. A. F. Oliveira**, V. Furtado, R. Bicca de Alencastro.
9th Annual Regional Meeting of the Brazilian Chemical Society, Poços de Caldas, MG, Brazil, 2003.
17. *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.
XII Brazilian Symposium of Theoretical Chemistry, Caxambu, MG, Brazil, 2003.
18. *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.
43th Sanibel Symposium, St Augustine, FL, 2003.
19. *Molecular Modeling of the Chemotatic Tripeptide Formyl-Met-Leu-Phe-Oh via Molecular Mechanics.*
F. P. Fleming, **C. A. F. Oliveira**, R. Bicca de Alencastro.
XXV Meeting of the Federal University of Rio de Janeiro, Rio de Janeiro, RJ, Brazil, 2003.
20. *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.

- 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.
Workshop on Molecular Modeling in Biophysics: Methods and Applications, Rio de Janeiro, RJ, Brazil, 2002.
- 22.** *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.
- 23.** *Estimation of the Preorganization Free Energy for the Human Cytomegalovirus Protease.*
C. A. F. Oliveira, C. R. W. Guimarães, G. Barreiro, R. Bicca de Alencastro.
Workshop on New Concepts and Applications of Physical Organic Chemistry, Rio de Janeiro, RJ, Brazil, 2002.
- 24.** *Methodologies in Molecular Modeling of Biological Molecules*
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**.
VIII Brazilian Electronic Structure School, Juiz de Fora, MG, Brazil, 2002.
- 25.** *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, 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.
- 26.** *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, 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.
- 27.** *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.
- 28.** *Development of a Molecular Dynamics Program for the Simulation of Atomic and Molecular Systems.*
C. A. F. de Oliveira, C. R. W. Guimarães, and R. Bicca de Alencastro.
XXII Meeting of the Federal University of Rio de Janeiro, Rio de Janeiro, RJ, Brazil, 2000.
- 29.** *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.
- 30.** *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.

31. *Molecular Dynamics of the 1-Octanol Liquid State.*
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.
32. *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.
33. *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.
34. *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.
35. *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.
36. *Theoretical Studies on the Reduction of Disubstituted 3-Methyleneoxindoles by the NADH Hantzsch Ester Model.*
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.
37. *Theoretical Studies on the Reduction of Disubstituted 3-methyleneoxindoles by the NADH Hantzsch Ester Model.*
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.

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

Dr. Cristiano R. W. Guimarães

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