CURRICULUM VITAE

PERSONAL DATA

Full name: Danilo Roccatano

Date of Birth: August 7 1967

Place of Birth Frosinone (Italy)

Marital Status: Not married

Nationality: Italian

Home address:
International University Bremen
Campus Ring 7
28759 Bremen
Germany

Work address:
International University Bremen
School of Engineering and Science
Campus Ring 1
28759 Bremen
Germany
Phone : +49 421 200-3144
Fax : +49 421 200-3249

E-mail : d.roccatano@iu-bremen.de

Web-page: www.iu-bremen.de/directory/faculty/32108

EDUCATION AND QUALIFICATIONS

1986: Diploma di maturità scientifica (High school degree)

1987-1992: Awarded the degree of "Dottore in Chimica" cum laude at the University of Rome, discussing a thesis on the *Structure determination of Aquatrisimidazolecopper (II) sulfate using Molecular Dynamics and XANES spectroscopy* [32] under the supervision of Prof. A. Di Nola and Prof. M. Barteri.

1993-1997: Awarded with the degree of "Dottore di ricerca in Chimica" (equivalent to PhD) at the University of Rome, with a thesis on *Study of complex molecular systems using molecular dynamics advanced techniques* [33].

WORK EXPERIENCES

1993: Received a grant from CASPUR (Consorzio per le Applicazioni di Supercalcolo per Università e Ricerca) for the developing of Molecular Dynamics program on parallel computer "Quadrics" (Alenia-Italy).

1996-1999: TMR European Community grant postodoc in the Prof. H.J.C. Berendsen MD group at University of Groningen on the projects *Structure and Dynamics of Intermediate States in Protein Folding* and PROMOD.

1999-2000: Postodoc on renewed Protein Folding TMR EC grant in the group of Prof. A.E. Mark at University of Groningen.

2000-2001: Postdoc in the group of Prof. A. Di Nola at the Dept. of Chemistry of the University of Rome "La Sapienza" (Italy).

2001-2003: Postdoc position in the group of Prof. F. Mazza Dipartimento di Chimica, Ingegneria Chimica e Materiali at the University of L'Aquila (Italy).

2003-2005 Postdoc position in the group of Prof. Martin Zacharias at School of Engineering and science of International University of Bremen (Germany).

COMPUTER SKILLS:

Platforms: Silicon Graphics, Sun, DEC Alpha, PC, Macintosh, Quadrics (APE 100).

Operative Systems: Unix, Windows, MSDOS.

Programming languages: Fortran 77, C, Awk, Perl, Unix shell scripting, MPI, HTML, Tcl/tk, LaTeX.

Software: GROMACS, GROMOS, AMBER, XPLOR, TINKER, GAUSSIAN94, GAMESS, QUANTA, INSIGHT, and several tools for scientific visualization and data analysis under Unix OS (VMD, MOLMOL, XMGRACE, SCILAB, etc).

Database: Swiss Prot, PDB, CSD.

Software development: I have modified MD codes, like GROMOS87 and GROMACS to implement new algorithms. I also wrote several programs in AWK, PERL, FORTRAN and C languages to perform specific analysis of MD data.

Furthermore, I have setup and provided to the maintenance of a PC cluster running Linux and Windows OS's at the Bioinformatics and Computational chemistry laboratory of the Dept. of Chemistry, Chemical Engineering and Materials of the University of L'Aquila.

FURTHER INFORMATION:

Languages:

Italian: Native language.
English: Fluent written and spoken.
German : Basic.

RESEARCH INTERESTS

Protein dynamics [6], protein folding [7], peptide stability in non aqueous solvent [17], developing new docking or conformational space sampling methods[11], parallel computing [26], force field development for solvents or small molecules [21], properties of ions and small molecules in solutions [10,25], simulation of inorganic compounds [32], statistical mechanics QGE theory applications [8].

TEACHING ACTIVITIES

- Teaching in the course of Advanced Bioinformatics Lab I, idelivered by Prof. Zacharias at IUB on September 2004, Lectures on "Introdution to Perl Programming for Bioinformatics" and computer exercitations.
- Lecturing on "Targeted Molecular Dynamics Simulations to Study the Function of Biomolecules" at the summer School at International University Bremen: *Advanced Modelling of Biological Function*, Bremen, Aug, 13th 2004.

- Lecturing on "Molecular Dynamics Simulation of Biomolecules" in the course "Methods and research strategies in Life science" at International University of Bremen, November 2003.
- Lecturing on "Introduction to molecular dynamics simulations", in the Master course of Bioinformatics at the University of Rome "La Sapienza", on May 2003.
- Teaching Assistant in the course of Computational chemistry, delivered by Prof. M. Aschi at University of L'Aquila, on February 2003. Lectures on "Introduzione ai metodi della Dinamica Molecolare" and laboratory course on MD simulations. (o2.univaq.it/ roccata/ChimicaComp/ChimicaComp.html in italian)
- Teaching assistant for course in General and Inorganic Chemistry, delivered by Prof. F. Mazza, at University of L'Aquila, on February 2003. (o2.univaq.it/ roccata/Esercitazioni.html in italian)
- Teaching assistant in courses of General and Inorganic Chemistry, delivered by Prof. F. Mazza and Prof. M. Aschi, at University of L'Aquila, on June-July 2002.
- Lectures on "Introduction to the Molecular Modeling", in the course of Pharmaceutical chemistry, delivered by Prof. G. Arcadi at University of L'Aquila on May 2002.
- Lectures with title "Introduction course to the use of GROMACS package" with practical, in the *College Course on Molecular Modeling* delivered by Prof. A. E. Mark at the University of Groningen on May 2000.

I have also supervised the research activity of different undergraduate and PhD students in the groups of Prof. A. Di Nola (at University of Rome "La Sapienza") and Prof. K. Bruger (at University of Leipzig in Germany).

RESEARCH FOUNDINGS

- 2001-2003: Young research grant from University of L'Aquila on *Molecular Dynamics simulations study of protein-substrate interactions* .
- 2002: "Progetto Vigoni 2001-2002" research grant on *Optimization of fluorinated alcohols/water mixture models for molecular simulations study of stability and folding of peptides in solution.* The project was an interchange researcher project between the University of L'Aquila and the University of Leipzig (group of prof. K Bruger).

OTHERS ACTIVITIES

- Member of the organizing Committee of the *1st and 2nd Workshop on Molecular Theories and Simulations*, Gaeta, May, 2002-2003.
- Referee of papers for the journals: J. Am. Chem. Soc., J. Phys. Chem., J. of Molecular Graphics and Modelling, and Chemical Physics.

CONFERENCES AND MEETINGS

1. *Algorithms for Macromolecular Modelling IV*, Leicester, Aug, 18th 2004. Poster Presentation.

2. *Life Science Seminar, IUB*, Bremen, Nov., 27th 2003. **Lecture :**. In Silico *Simulations of Peptides Stability and Folding.*

3. *Lincei EMBO Symposium: Protein Folding and Misfolding*, Roma, 3-5, Aprile 2003.

4. *2nd Workshop on Molecular Theories and Simulations*, Gaeta, May, 10-12th 2003. **Oral presentation:**. *A statistical mechanics approach to the protein folding problem.*

5. *The 2002 COE Conference of IMS: Dynamical Structures and Molecular Design of MetalloProteins.* , Okazaki, Japan, November 2002.
   Poster Presentation.

6. *Proteine 2002*, L'Aquila, Italy, June 6-8, 2002.
   Poster Presentation.

7. *ESS Workshop: Flexibility and Function of Proteins*, Heidelberg, Germany, January 25-27 2002. Poster presentation.

8. *EU Training & Mobility of Researchers Network. "Structure and Dynamics of Intermediate States in Protein Folding." Final meeting* , Granada, Spain, 2001. **Oral presentation**.

9. *Third International Workshop on Methods for Molecular Modeling* New York City, 2000. Poster presentation.

10. *The Molecular Graphics and Modeling Society 18th International Meeting and AGM: Modelling Biomolecular Mechanism: From States to Processes at the Atomic Level* , York (UK), 2000. Poster presentation.

11. *Nederlandse Organisatie voor Werenschappelijk Onderzoek:* Tweedaagse wetenschappelijke bijeenkomst van de CW studiegroep Bio-Moleculaire Chemie *, Lunteren, 2000.* **Oral presentation**.

12. XIII International Biophysics Congress *, New Delhi, India, 1999.*
   Poster Abstracts:

   - **D. Roccatano**, A. Amadei, A. Di Nola and H.J.C Berendsen, *Study of a β-hairpin forming peptide in aqueous solution using Molecular Dynamics simulations* Journal of Bioscience, **24/S1**,49, (1999).
   - M. Mangoni, **D. Roccatano**, A. Di Nola *Docking of flexible ligands to flexible receptors in solution by molecular dynamics simulations* Journal of Bioscience, **24/S1**,69, (1999).

13. *EU Training & Mobility of Researchers Network. "Structure and Dynamics of Intermediate States in Protein Folding." 2st Annual meeting, Rome* , Italy, 1999. **Oral presentation**.

PUBLICATIONS

IN REFEREED JOURNALS

1. T.S Wong, N. Wu, **D. Roccatano**, M. Zacharias and U. Schwaneberg *Sensitive assay for laboratory evolution of hydroxylases toward aromatic and heterocyclic compounds* Applied and Environmental Microbiology, submitted.

2. **D. Roccatano**, G. Sbardella, M. Aschi, G. Amicosante, A. Di Nola, F. Mazza *Effect of D214-D233 dyad protonation state on TEM-1 β-Lactamase probed by Molecular Dynamics Simulations.* PROTEINS:Struct., Funct. and Bioinf., submitted.

3. M. D'Abramo, M. D'Alessandro, A. Di Nola, **D. Roccatano**, A. Amadei. *Characterization of liquid behavior by means of local density fluctuations* J. Mol. Liqu., submitted.

4. **D. Roccatano***, W. M. Nau and M. Zacharias *Structural and dynamics properties of CAGQW peptide in water: comparison of the GROMOS96 and OPLS force fields.* J. Phys. Chem. B, accepted.

5. V.M. Coiro, A. Di Nola, M.A. Vanoni, M. Aschi, A. Coda and **D. Roccatano**, *Insights into the ammonium channeling mechanism in Azospirillum brasilense glutamate synthase by Molecular Dynamics simulation.* Prot. Sci., in press.

6. I. Daidone, **D. Roccatano***, S. Hayward *Investigating the accessibility of the Closed and Open Domain Conformations of Citrate Synthase using Essential Dynamics Sampling* J. Mol. Biol., **339**, 515-525 (2004).

7. I. Daidone, F. Simona, **D. Roccatano**, R. A. Broglia, G. Tiana, G. Colombo, and A. Di Nola *The mechanism of α to β conformational transition of fibrillogenic peptides revealed by molecular dynamics simulations* PROTEINS:Struct., Funct. and Bioinf., **57**, 198-204 (2004).

8. **D. Roccatano**, A. Di Nola and A. Amadei, *Investigation on the folding/unfolding thermodynamics of single domain proteins using the Quasi-Gaussian entropy theory.* J. Phys. Chem. B, **108**, 5756-5762 (2004).

9. C. Bossa, M. Anselmi, **D. Roccatano**, A. Amadei, B. Vallone, M. Brunori and A. Di Nola. *Extended Molecular Dynamics simulation of the Carbon Monoxide migration in sperm whale Myoglobin* Bioph. J., **86**, 3855-3862 (2004).

10. M. Fioroni, K. Burger, and **D. Roccatano**, *Chiral Discrimination in 1,1,1-Trifluoropropan-2-ol: a molecular dynamics study.* J. Chem. Phys., **119**, 1-8 (2003).

11. I. Daidone, **D. Roccatano**, A. Amadei, and A. Di Nola, *Exploring the Folding Landscape of Horse Heat Cytochrome C by Essential Dynamics Sampling Simulations.* Bioph. J., **85**, 2865-2871 (2003).

12. M. Fioroni, K. Burger, A. E. Mark and **D. Roccatano**, *Insights into the nature of the hydrophobic interactions: a molecular dynamics simulation study of the 1,1,1-Trifluoropropan-2-ol and its aqueous solutions.* J. Phys. Chem. B,**107**, 4855-4861 (2003).

13. M. F. Gerini, **D. Roccatano***, E. Baciocchi, A. Di Nola. *Molecular dynamics simulation of Lignin peroxidase.* Bioph. J.,**84**, 3883-3893 (2003).

14. G. Colombo, G.M.S De Mori, **D. Roccatano** *Interplay between hydrophobic cluster and loop propensity in β-hairpin formation: a mechanistic study.* Prot. Sci., **12**, 538-550 (2003).

15. **D. Roccatano**, I. Daidone, M.-A. Ceruso, C. Bossa and A. Di Nola, *Selective excitation of native fluctuations during thermal unfolding simulations: horse heart cytochrome c as a case study.* Bioph. J.,**84**, 1876-1883 (2003).

16. M. Aschi,**D. Roccatano**, A. Di Nola, C. Gallina, E. Gavuzzo, G. Pochetti, M. Pieper, H. Tschesche, and F. Mazza *Molecular Dynamics study of the catalytic domain of human neutrofil collagenase. Specific role of the S_3 and S'_3 subsites in the interaction with a phophonate inhibitor.* J. Comp. Aided Mol. Des., **16**, 213-225 (2002).

17. **D. Roccatano***, G. Colombo, M. Fioroni and A. E. Mark, *The mechanism by which 2,2,2-trifluorethanol/water mixtures stabilize secondary structure formation in peptides: A molecular dynamics study.* PNAS **99** (19), 12179-12184 (2002).

18. G. Colombo, **D. Roccatano**, A. E. Mark *Folding and Stability of the Three-Stranded β-sheet Peptide Betanova: Insights from Molecular Dynamics Simulations* Proteins: Struct., Funct., Genet., **46**, 380-392 (2002).

19. M. Fioroni, K. Burger, A. E. Mark and **D. Roccatano*** *Model of 1,1,1,3,3,3-hexafluoropropan-2-ol for Molecular Dynamics simulations.* J. Phys. Chem. B, **105**, 10967-10975 (2001).

20. **D. Roccatano**, A. E. Mark, S. Hayward *Understanding the functional movement of citrate synthase using molecular dynamics simulations.* J.Mol.Bio. , **310**, 1039-1053 (2001).

21. M. Fioroni, K. Bruger, A. E. Mark, **D. Roccatano*** *A new 2,2,2-trifluorethanol model for molecular dynamics simulations.* J. Phys. Chem. B, **104**, 51, 12347-12354 (2000).

22. **D. Roccatano**, A. Amadei, A. Di Nola, H.J.C. Berendsen *A Molecular Dynamics study of the 41-56 β-hairpin from B1 domain of Protein G.* Protein Sci., **8**, 2130-2143, (1999).

23. M. Mangoni, **D. Roccatano**, A. Di Nola *Docking of flexible ligands to flexible receptors in solution by molecular dynamics simulations.* Proteins: Struct., Funct., Genet.,**35**, 153-162, (1999).

24. **D. Roccatano**, A. Amadei, M. E. F. Apol, A. Di Nola, H. J. C. Berendsen. *Application of the quasi-Gaussian entropy theory to molecular dynamics simulations of Lennard-Jones fluids.* J. Chem. Phys., **109**, 6358-6363, (1998).

25. **D. Roccatano**, H.J.C. Berendsen, P. D'Angelo. *Assessment of the validity of intermolecular potential models used in molecular dynamics simulations by extended X-ray absorption fine structure spectroscopy: A case study of Sr^{2+} in methanol solution.* J. Chem. Phys., **108**, 9487-9497, (1998).

26. **D. Roccatano**, R. Bizzarri, G. Chillemi, N. Sanna and A. Di Nola. *Development of a parallel Molecular Dynamics code on SIMD computers:an algorithm for the use of the pair list criterion.* J. Comp. Chem., **19**, 685-694, (1998).

27. A. Amadei, **D. Roccatano**, M. E. F. Apol, H. J. C. Berendsen, A. Di Nola. *Prediction of the liquid-vapor equilibrium pressure using the quasi-Gaussian entropy theory.* J. Chem. Phys., **105**, 7022-7025, (1996).

28. P. D'Angelo, N.V. Pavel, H.-F. Nolting, **D. Roccatano**. *Multielectron excitations at the L-edges of barium in aqueous solution.* Phys. Rev. B, **54**, 12129-12138, (1996).

29. A. Di Nola, E. Gavuzzo, F. Mazza, G. Pochetti, **D. Roccatano**. *Internal β-turn hydration: crystallographic evidence and Molecular Dynamics simulation.* J. Phys. Chem., **99**, 9625-9631, (1995).

30. P. D'Angelo, A. Di Nola, A. Filipponi, N.V. Pavel, **D. Roccatano**. *An extended X-ray adsorption fine structure study of aqueous solutions.* J. Chem. Phys., **100**, 985-994, (1994).

31. A. Di Nola, **D. Roccatano**, H.J.C. Berendsen. *Molecular dynamics simulation of the docking of substrates to proteins.* Proteins: Struct., Funct., Genet., **19**, 174-182, (1994).

OTHER PUBLICATIONS

32. Graduation Thesis: *Determinazione della struttura dello Cu(II) aquatrisimidazolo solfato mediante dinamica molecolare e spettroscopia XANES* , with supervisors: Prof. A. Di Nola e il Prof. M. Barteri, Roma 1992.

33. PhD Thesis: *Studio di sistemi molecolari complessi mediante l'uso di tecniche avanzate di Dinamica Molecolare,*with supervisor: Prof. A. Di Nola, Roma 1997.

IN PREPARATION

34. **D. Roccatano**, W. M. Nau and M. Zacharias *Study of the end-to-end contact kinetics of small peptides by molecular dynamics simulations.*

35. **D. Roccatano**, T. S. Wong, U. Schwaneberg and M. Zacharias *Cosolvent effect on cytochrome P450 BM3*

36. **D. Roccatano**, M. Fioroni, G. Colombo and M. Zacharias *Fluorinated alcohol co-solvent effects on the structural and dynamic properties of trialanine peptides.*

37. **D. Roccatano**, M. Fioroni, G. Colombo and M. Zacharias *Insights into the Structural and Dynamics Behaviour of Melittin Peptide in Solution from Molecular Dynamics Simulations.*

REFEREES

- Prof. Martin Zacharias
  International University Bremen
  School of Engineering and Science
  Campus Ring 1
  28759 Bremen
  Germany
  email : m.zacharias@iu-bremen.de

- Prof. Alan E. Mark
  Department of Biophysical Chemistry
  University of Groningen
  Nijenborgh 4, 9747 AG Groningen
  The Netherlands
  email: mark@chem.rug.nl

- Prof. A. Di Nola
  Dipartimento di Chimica,
  Università di Roma (La Sapienza)
  P. le A. Moro 5, 00185 Rome
  Italy
  email : dinola@degas.chem.uniroma1.it

- Dr. S. Hayward
  Royal Society Wolfson
  Bioinformatics Laboratory
  School of Information Systems
  University of East Anglia
  Norwich NR2 7TJ, UK
  email: sjh@sys.uea.ac.uk