

CURRICULUM VITAE

Name François-Yves DUPRADEAU

Personal Address

5, rue Henri Bergson
80080 Amiens

Phone: +33-(0)3-2248-6964

Citizenship

French

Date of Birth

November 6, 1967

Marital Status

Married, two children

Professional Address

UMR CNRS 6219 & UFR de Pharmacie
Université de Picardie - Jules Verne (UPJV),
1-3, rue des Louvels,
80037 Amiens Cedex 1, France

Phone: +33-(0)3-2282-7498

Fax: +33-(0)3-2282-7469

E-mail: fyd@q4md-forcefieldtools.org

<http://q4md-forcefieldtools.org/FyD/>

Present Situation

Since Sept 2006

Professor of organic chemistry at the "UFR de Pharmacie", UPJV, Amiens,

Teaching: Organic chemistry 1st & 2nd years of University, "UFR de Pharmacie", UPJV, Amiens

Research Project: Bioinformatics and force field development: Application to molecular dynamics simulation of modified and chemically engineered biomolecules (peptides, glycoconjugates, oligonucleotides) and bioinorganic complexes.

Professional Appointments

1997-2006

Assistant Professor (Maître de Conférences) at the "UFR de Pharmacie", UPJV, Amiens,

Laboratory Director: Prof J. Rochette,

Research Project: Molecular modeling of proteins and nucleic acids (RESP/ESP charge and force field parameter development, molecular dynamics, free energy determination and homology modeling).

2004-2005

Two years Research Associate at The Scripps Research Institute, La Jolla, CA,

Laboratory Director: [Prof D.-A. Case](#),

Research Project: Study of electrostatic interactions in proteins and nucleic acids.

1996

Post-doctoral Fellow, Laboratoire des Bio-Molécules, CNRS, Université d'Orsay, Paris XI, France),

Adviser: [Prof J.-M. Beau](#),

Research Project: Study of a new method relevant to the reduction of azido-oligosaccharides based on a samarium diiodide-water system.

1994

16 months Post-doctoral Fellow (as part of my military obligation) in the Department of Synthetic Organic Chemistry at the "Bio-Membrane Institute" (University of Washington, Seattle, USA),

Advisers: [Prof S.-i. Hakomori](#) & Dr T. Toyokuni,

Research Project: Development of synthetic carbohydrate vaccines based on the tumor-associated Tn antigen (GalNAc- α -Ser/Thr).

Education

2003

Habilitation Thesis (Université de Picardie Jules Verne, Amiens),

Laboratory Director: Prof J. Rochette

Thesis title: Total synthesis and structural study of bio-molecules.

1993

Ph.D. Thesis (Université d'Orsay, Paris XI),

Advisers: Prof J.-M. Beau & Dr. J. Prandi

Thesis title: Synthesis of rare sugars: application to carbohydrate fragments of Esperamicins.

1990

D.E.A. de Chimie Organique (M. Sc. in Organic Chemistry) with honors, Université d'Orsay, Paris XI.

Advisers: Prof J.-M. Beau & Dr. J. Prandi

1989-1988

Maîtrise (4th year of University, B. Sc., Biochemistry major), Université d'Orléans, France.

Licence (3rd year of University, Biochemistry major), Université d'Orléans.

1987

D.E.U.G. B (1st two years of University, Biology major), Université d'Orléans.

1985

Baccalauréat D (High School Diploma, Sciences), Lycée Pothier, Orléans.

Professional skills

- Empirical force field development and bioinformatics.
- Molecular mechanics, molecular dynamics and quantum chemistry (DFT & WFT).
- Linux administration and knowledge in PERL, Shell, PHP, MySQL and HTML.
- Structure determination by using circular dichroism and N.M.R.
- Total synthesis: peptide, sugar, organic and asymmetric synthesis (former interests).
- Foreign language: English.

Teaching

- Organic chemistry (1st and 2nd years of university) at the "UFR de pharmacie", UPJV, Amiens.
- Molecular modeling (3rd year of university) at the "UFR de pharmacie", UPJV, Amiens.

Outside interests

Judo (black belt, 4th dan) and jogging.

Representative publications

C. Cézard, X. Trivelli, F. Aubry, F. Djedaini-Pilard & F.-Y. Dupradeau, Molecular dynamics studies of native and substituted cyclodextrins in different media: 1. Charge derivation and force field performances, *Phys. Chem. Chem. Phys.* **2011**, *13*, 15103-15121.

E. Vanquelef, S. Simon, G. Marquant, E. Garcia, G. Klimerak, J. C. Delepine, P. Cieplak & F.-Y. Dupradeau, R.E.D. Server: a web service for deriving RESP and ESP charges and building force field libraries for new molecules and molecular fragments, *Nucl. Acids Res. (Web server issue)* **2011**, *39*, W511-W517.

F.-Y. Dupradeau, A. Pigache, T. Zaffran, C. Savineau, R. Lelong, N. Grivel, D. Lelong, W. Rosanski & P. Cieplak, The R.E.D. tools: Advances in RESP and ESP charge derivation and force field library building, *Phys. Chem. Chem. Phys.* **2010**, *12*, 7821-7839.

F.-Y. Dupradeau, C. Cézard, R. Lelong, E. Stanislawiak, J. Pecher, J. C. Delepine & P. Cieplak, R.E.D.D.B.: A database for RESP and ESP atomic charges, and force field libraries, *Nucl. Acids Res. (Database issue)* **2008**, *36*, D360-D367.

F.-Y. Dupradeau, D. A. Case, C. Yu, R. Jimenez & F. Romesberg, Differential Solvation and Tautomer Stability of a Model Base Pair within the Minor and Major Grooves of DNA, *J. Am. Chem. Soc.* **2005**, *127*, 15612-15617.

Full list of publications at q4md-forcefieldtools.org/FyD/Pubs.htm

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