



Curriculum Vitae

1. Name, Gender, Nationality

Family Name	Name	Gender	Nationality
CHRETIEN	Jacques R.	Male	French



2. Overall Scientific Expertise

Computational Chemistry and Molecular Modelling

- Developing data bases and QSAR Models for Health and Medicinal Chemistry.
(e.g. Psychotropic compounds, Dopaminergic activity, Radioprotective compounds, anti-AIDS, Alzheimer, Phospholipase A2 inhibitors,...).

Virtual High Throughput (v-HTS) screening.

- *Acute toxicity prediction of organo-phosphorous compounds on Acetyl-cholinesterase*
- *Validated models for pharmacokinetic properties prediction (ADME).*
- *Olfaction*
- *Anti-carcinomic compounds screening among 8 different mechanisms.*

Alternative methods to animal testing

- *Cosmetics (skin sensitisation with integration of in vitro and in silico procedures).*
- *Developing in silico predictive procedures for ecotoxicity prediction (carcinogenicity, skin sensitization, developmental toxicity,...).*



3. Professional Experience

Professional Experience 1 (most recent)	
Occupation or position held	<i>President & co-founder</i>
Date (starting)	<i>08.02.2002</i>
Date (finishing)	<i>08.04.2009</i>
Main activities	<i>Computational Chemistry / Developing In silico Alternative Methods to Animal Testing for pharmacy, ecotoxicity & cosmetics</i>
Main responsibilities	<i>Scientific, administrative and financial management, in charge of national and international contacts and participation with lectures to a lot of symposia worldwide / From April 2009 up to now, acting as Scientific Vice-President to boost cutting edge technologies or procedures.</i>
Name of employing organisation	<i>BioChemics Consulting SAS</i>
Address of employing organisation (City, Country sufficient)	<i>111 Bld Duhamel du Monceau, 45166 Olivet, France</i>
Type of sector	<i>Contract Research Organisation</i>
Professional Experience 2	
Occupation or position held	<i>Full University Professor Founder & Head of the Laboratory of Chemometrics and Bioinformatics</i>
Date (starting)	<i>01.02.1980</i>
Date (finishing)	<i>01.09.2002</i>
Main activities	<i>Teacher in Analytical Chemistry and Chemometrics; Opening a Research Laboratory in Chemometrics and Bioinformatics in September 1986 devoted to Data Processing of physico-chemical data, and biological data; impulsing new strategies in Computational Chemistry and Molecular Modeling.</i>
Main responsibilities	<i>As a teacher in Anal Chem taking care finding a training period and a job in industry for all my students or for my Laboratory co-workers finding a position in industry in Europe or in US (e.g. two previous post doctoral fellows are now professors in US universities)</i>
Name of employing organisation	<i>University of Orleans (France)</i>
Address of employing organisation (City, Country sufficient)	<i>University of Orleans (France)</i>
Type of sector	<i>Academia</i>



Professional Experience 3	
Occupation or position held	<i>Emeritus University Professor and Head of Laboratory of Chemometrics and Bioinformatics</i>
Date (starting)	<i>01.09.2002</i>
Date (finishing)	<i>01.09.2005</i>
Main activities	<i>Developing new strategies and algorithm for biochemical Data Mining using fuzzy logics and genetic algorithm to deliver added values relatively to common software / Validation in olfaction, the most complex field of chemical bioactivity, and transposition to the area of ecotoxicity to address main REACH requirements</i>
Main responsibilities	<i>Training Ph'D students and post doctoral fellows while working on contracts</i>
Name of employing organisation	<i>University of Orleans (France)</i>
Address of employing organisation (City, Country sufficient)	<i>University of Orleans (France)</i>
Type of sector	<i>Academia</i>
Professional Experience 4	
Occupation or position held	<i>Director of the University Institute of Technology ("Institut Universitaire de Technologie" (I.U.T.))</i>
Date (starting)	<i>20.04.1982</i>
Date (finishing)	<i>20.04.1986</i>
Main activities	<i>Boosting the development of three existing Departments in Chemistry, Mechanics and Administration; launching a new Department in Computational Sciences; impulsing the development and use of various Computer Aided Technologies for Research and Industry.</i>
Main responsibilities	<i>Administrative, financial and Scientific Responsibilities of an Academic Establishment including ~100 teachers, ~50 technicians or engineers, ~750 students.</i>
Name of employing organisation	<i>University of Orleans (France)</i>
Address of employing organisation (City, Country sufficient)	<i>University of Orleans (France)</i>
Type of sector	<i>Public institution</i>
Professional Experience 5	
Occupation or position held	<i>Research Fellow and Senior Researcher</i>
Date (starting)	<i>01.09.1972</i>
Date (finishing)	<i>01.09.1993</i>



Main activities	<i>Project Controller in Computational Chemistry: (1) Relational Data Base Management System, (2) Two data bases on Psychotropic Compounds and on Radio-Protective Compounds, (3) Software and developments in Molecular Modelling and 2D or 3D QSAR.</i>
Main responsibilities	<i>In charge, part-time, of a multidisciplinary group including chemists, mathematician and computational science specialists / negotiating, managing and reporting corresponding contracts with support of public organizations.</i>
Name of employing organisation	<i>CNRS and Institut de Topologie et de Dynamique des Systèmes (ITODYS), University Paris VII</i>
Address of employing organisation (City, Country sufficient)	<i>University Paris VII (Paris, France)</i>
Type of sector	<i>Public Institution</i>

4. Educational Background

Educational qualification 1 (most recent)	
Description of qualification achieved (e.g. Bachelor of science in tissue engineering)	<i>Chemical Engineer from Ecole Nationale Supérieure de Chimie de Clermont Ferrand.</i>
Principal subject (e.g. Animal Physiology)	<i>Organic, Inorganic and Industrial Chemistry</i>
Date (starting)	<i>01.09.1961</i>
Date (finishing)	<i>30.06.1964</i>
Name of organisation (incl. city and country) awarding degree	<i>University of Clermont-Ferrand, France</i>
Title of degree awarded	<i>Chemical Engineer ENSCCF</i>
Educational qualification 2	
Description of qualification achieved (e.g. Bachelor of science in tissue engineering)	<i>Docteur es Sciences / (Ph'D)</i>
Principal subject (e.g. Animal Physiology)	<i>Physical Organic Chemistry</i>
Other subjects	
Date (starting)	<i>01.09.1966</i>
Date (finishing)	<i>07.06.1971</i>
Name of organisation (incl. city and country) awarding degree	<i>University of Orléans</i>
Title of degree awarded	<i>Docteur es Sciences</i>



5. Fellowships, Awards, Membership in Learned Societies, Editorial Boards and Advisory Bodies

5.1 Fellowships

Fellowship I	
Title of fellowship	<i>Member of the Admission Jury at Ecole Polytechnique</i>
Description of fellowship (type, maximal duration, prestige)	<i>Member of the Jury as Chemistry Expert during a period of five weeks each summer to contribute to the student selection of the most prestigious scientific school in France.</i>
Date (starting)	<i>01.01.1974</i>
Date (finishing)	<i>30.09.1979</i>
Funding/awarding organisation	<i>Ecole Polytechnique / Minister of French Armies.</i>
Address (city + country sufficient)	<i>Ecole Polytechnique, Palaiseau (France)</i>

5.2 Awards

Award I	
Title of award	<i>Officier de l'Ordre des Palmes Académiques</i>
Description of award (type, prestige etc.)	<i>In recognition of special efficiency in developing the Institute of Technology in Orleans, during the period 1982-1986 and for the implementation of Computational Sciences and Computer Aided Technologies.</i>
Date	<i>28.07.1988</i>
Awarding organisation	<i>Ministre de l'Education Nationale de la Jeunesse et des Sports</i>
Address (city + country sufficient)	<i>Ministère de l'Education Nationale, Paris (France)</i>

5.3 Membership in learned societies & professional associations & editorial boards

Society / Association / Editorial Board I	
Society / Association	<i>American Chemical Society (ACS)</i>
Description of society's / association's activities	<i>All areas, related to chemistry, member of the divisions: (1)computational chemistry, (2) chemical Information, (3)medicinal chemistry</i>



Membership from ...	<i>1978</i>
...to (if currently member, please state 'current')	<i>current</i>
Address (city + country sufficient)	<i>Washington D.C.(USA)</i>
Society / Association II	
Society / Association	<i>Société Chimique de France</i>
Description of society's / association's activities	<i>Informations about local meetings, or sponsored symposiums at national or European level</i>
Membership from ...	<i>01.01.1968</i>
...to (if currently member, please state 'current')	<i>current</i>
Address (city + country sufficient)	<i>Paris (F)</i>

5.4 Membership in advisory bodies / committees

Advisory body / committee I	
Name of advisory body	<i>ANSES (Agence Nationale de Sécurité Sanitaire, de l'Alimentation, de l'Environnement et du Travail)</i>
Description of the roles and responsibilities of the advisory body	<i>Scientific survey of alternative methods in the area of QSAR, modelling and in vitro tests (for their scientific bulletin). Member of the Scientific Committee in charge of the Research Programs (CSPR).</i>
Membership from ...	<i>16.03.2009</i>
...to (if currently member, please state 'current')	<i>current</i>
Address (city + country sufficient)	<i>Maisons-Alfort (France)</i>



6. Publications

Nr.	Citation
1	<i>CHRETIEN JR et al, (1985) Etudes S.A.R. et banques de données pharmacologiques: une méthode DARC de CAO appliquées aux neuroleptiques. Eur J Med Chem 20, 315-325.</i>
2	<i>BOUDON A, SZYMONIAK J, CHRETIEN JR (1988) A Molecular Electrostatic Potential Study of phenothiazine dopaminergic antagonists. Eur J Med Chem 23, 365 - 371.</i>
3	<i>BOUDON A, SZYMONIAK J, CHRETIEN JR, DUBOIS JE (1988) Modeling the Binding Step in Dopamine Receptor / Antagonist Interactions. Can J Chem 66, 2995-3002.</i>
4	<i>KIREEV DB, CHRETIEN JR, RAEVSKY OA (1995) The Molecular Modeling and QSAR Study of Anti-HIV-1 2-Heteroaryl-quinoline-4-amines. Eur J Med Chem 30, 395-402</i>
5	<i>KIREEV DB, CHRETIEN JR, GRIERSON DS, MONNERET C (1997) 3D QSAR Related to Conformational Changes for a Series of Anti-HIV1 HEPT Analogues. J Med Chem 1997, 40, 4257-4264</i>
6	<i>KIREEV DB, BERNARD P, CHRETIEN JR, ROS F (1998) Application of Kohonen Neural Networks in Classification of Biologically Active Compounds. SAR and QSAR in Environ Res, 8, 93-107.</i>
7	<i>BERNARD P, KIREEV DB, CHRETIEN JR, FORTIER PL, L. COPPET (1998) A 3D Model of the Acetylcholinesterase Catalytic Cavity Probed by Stereospecific Organophosphorous Inhibitors. J Mol Modeling 4, 323-334.</i>
8	<i>BERNARD P, KIREEV DB, CHRETIEN JR, FORTIER PL, COPPET L (1999) Automated Docking of 82 N-benzylpiperidine Derivatives to Mouse Acetylcholinesterase and Comparative Molecular Field Analysis with "Natural" Alignment. J Comput Aided Mol Design 13, 355-371.</i>
9	<i>BERNARD P, KIREEV DB, CHRETIEN JR, FORTIER PL, FROMENT D (2000) A Protein-Based Alignment 3D QSAR model of Stereospecific Organophosphorous Inhibitors of Acetylcholinesterase J Mol Model 6, 618-629.</i>
10	<i>GOLBRAIKH A, BERNARD P, CHRETIEN JR (2000) Validation of protein-based alignment in 3D Quantitative Structure-Activity Relationship (QSAR) with CoMFA models. Eur J Med Chem, 35, 123-136.</i>
11	<i>BERNARD P, BERTHON JY, CHRETIEN JR (2001) A Molecular Modeling and 3D QSAR study of a large series of Indole Inhibitors of Human Non-pancreatic Secretory Phospholipase A2. Eur J Med Chem 36, 1-19.</i>
12	<i>PINTORE M, BERNARD P, BERTHON JY, CHRETIEN JR (2001) Protein-Based Alignment in 3D QSAR of 26 Indole Inhibitors of Human Pancreatic Phospholipase A2. Eur J Med Chem 36, 21-30.</i>
13	<i>PINTORE M, PICLIN N, BENFENATI E, GINI G, CHRETIEN JR (2003) "Database mining with adaptive fuzzy partition (AFP): Application to the prediction of pesticide toxicity on rats". Envir Toxico and Chem 22 (5), 983-991.</i>



14	<i>PINTORE M, PICLIN N, BENFENATI E, GINI G, CHRETIEN JR (2003) Predicting toxicity against the fathead minnow by Adaptive Fuzzy Partition. QSAR Comb Sci 22, 210-219.</i>
15	<i>PINTORE M, van de WATERBEEMD H, PICLIN N, CHRETIEN JR (2003), Prediction of oral bioavailability by Adaptive Fuzzy Partitioning. Eur J Med Chem 38, 427-431.</i>
16	<i>PICLIN N, PINTORE M, WECHMAN C, CHRETIEN JR (2004), Classification of a large anticancer data set by Adaptive Fuzzy Partition. J Comp Aided Mol Design, 18, 577-586</i>
17	<i>PINTORE M, WECHMAN C, SICARD G, CHASTRETTE M, AMAURY N, CHRETIEN JR (2006) Comparing the information content of two large olfactory databases. J Chem Inf & Mod 46, 32-38</i>
18	<i>PINTORE M, MOMBELLI E, WECHMAN C, CHRETIEN JR (2006) 3D QSAR study of PLA2 inhibitors. A modeling approach to select new and specific anti-inflammatory drugs. Current Med Chem, Anti-inflammatory Agents in Med Chem 5, 175-187.</i>
19	<i>PICLIN N, PINTORE M, WECHMAN C, RONCAGLIONI A, BENFENATI E, CHRETIEN JR (2006) Ecotoxicity Prediction by Adaptive Fuzzy Partitioning. Comparing descriptors computed on 2D and 3D structures. SAR & QSAR in Environ Res 17, 225 – 251</i>
20	<i>CHAUDHRY Q, CHRETIEN JR et al (2007) Algorithms for (Q)SAR model building, In Quantitative Structure-Activity Relationships (QSAR) for Pesticides Regulatory Purposes. Benfenati E, Editor, Elsevier, Amsterdam, p 111-147.</i>
21	<i>Q. CHAUDHRY, N. PICLIN, J. COTTERILL, M. PINTORE, N.R. PRICE, J.R. CHRÉTIEN, A. RONCAGLIONI. Global QSAR models of skin sensitizers for regulatory purposes. Chemistry Central Journal 2010, 4(Suppl 1):S5, 1-6.</i>