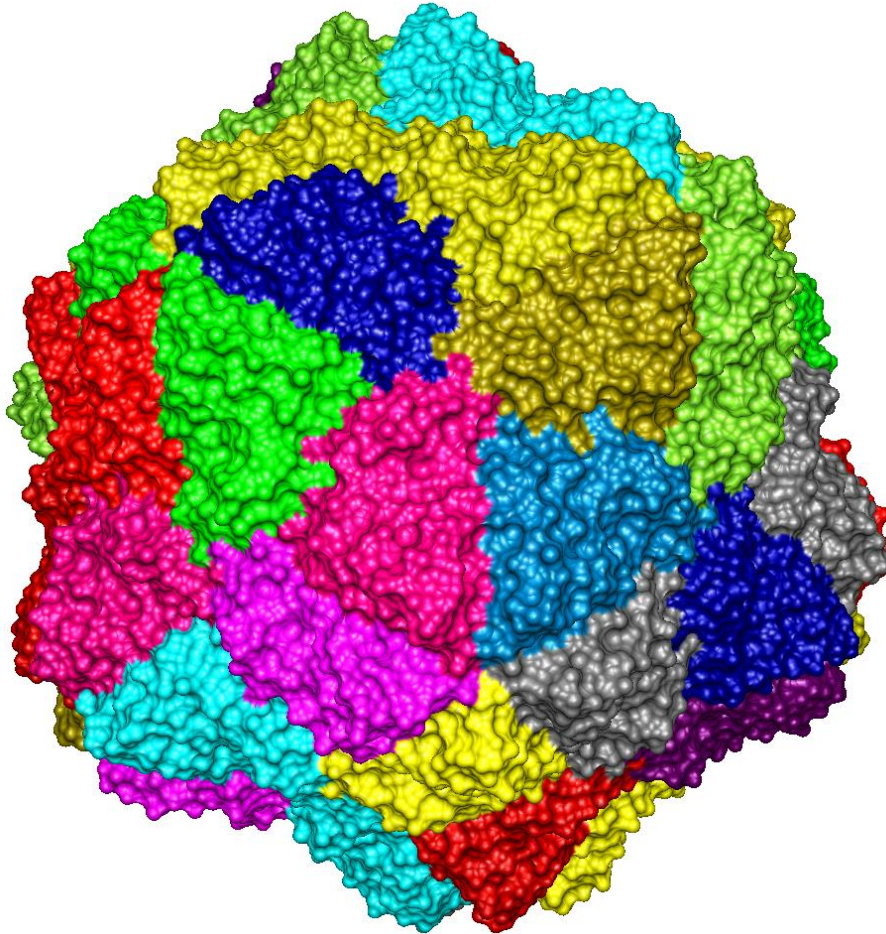




## ACTIVITY REPORT



AnTheProt 3D © 2007-2020

**Pr. Gilbert DELÉAGE**

[https://www.gdeleage.fr/prof/Dossier\\_English\\_G\\_Deleage.pdf](https://www.gdeleage.fr/prof/Dossier_English_G_Deleage.pdf)



**I**nstitut de **B**iologie et **C**himie des **P**rotéines -IBCP

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*The picture of the cover was performed with the help of the ANTHEPROT 3D software (Windows) that I developed in 2007-2009 at IBCP from the 3D structure of a viral capsid (pdb code: 2buk). The accessible surface was calculated using the MSMS program (Scripps Research Institute).*

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## I. CURRICULUM VITAE

### I.1. ADMINISTRATIVE SKILLS

#### GILBERT DELÉAGE

Born on November, 7th 1956 in Lyon, FRANCE

French

Married, 2 children

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### I.2. DIPLOMAS

Diploma	Year
Habilitation in PHD students supervision (HDR)	1993
PHD Biophysics and Bioinformatics	1988
Doctor in Biochemistry at Lyon University	1984
Master in Biochemisry	1981

### I.3. FUNCTIONS

- Professor exceptional class (64<sup>e</sup> CNU national concours) september, 2<sup>nd</sup> 2012
- Professor exceptional class (64<sup>e</sup> CNU national concours) september, 1<sup>st</sup> 2009
- Professor class 1 (64<sup>e</sup> CNU national concours) september, 1<sup>st</sup> 2001
- Professor class 2 (64<sup>e</sup> CNU) september, 1<sup>st</sup> 1998
- Associate professor class 1 (64<sup>e</sup> CNU) october, 1<sup>st</sup> 1991
- Associate professor class 1 (64<sup>e</sup> CNU) october, 1<sup>st</sup> 1989
- Assistant professor october, 1<sup>st</sup> 1984
- Doctoral fellowship 1982-1984

### I.4. LOCAL RESEARCH RESPONSABILITIES

- **Director** of “Molecular and Strcutural Bases of infectious systems” UMR 5086 (2011-2015)
- **Director** of Institute of Biology and Chemistry of Proteins (180 people) UMR 5086 CNRS- Lyon University (2007-2015)

- Deputy Director of Institute of Biology and Chemistry of Proteins UMR 5086 CNRS- Lyon University (2005-2006)
- Elected to the board of Chemistry/Biochemistry faculty council (1994-1998; 2004-2008)
- Elected member of recruitment commission (CSES) (1992-1996; 2000-2004 ; 2004-2007)
- Laureate of PEDR ("Prime Encadrement Doctoral et de Recherche") since 1995

### I.5. PARTICIPATION TO FRENCH NATIONAL COMMITTEES

- **Elected member** and **vice-chairman** of the National Council of Universities (CNU 64<sup>e</sup> section) (2011-2014)
- In charge of Bioinformatics at National Center for Scientific Research (INSB-CNRS) since 2009
- Member of Scientific Council of the GIS IBISA "Scientific Infrastructures for Biology, Health and Agronomy" (IBISA from Minister of Scientific Research) (2008-2009)
- Appointed member of the National Council of Universities (CNU 64<sup>e</sup> section) (2008-2011)
- Expert and Member of Scientific council of Région Lorraine: «Modeling, information and numerics systems» for Lorraine region. (2007-2010)
- Elected member at National Evaluation Committee of CNRS 21<sup>e</sup> section (2004-2007)
- Elected member at National Evaluation Committee of CNRS "Bioinformatics" 44<sup>e</sup> section (2006-2007)
- External member of Recruitment Committee 64<sup>e</sup> section at Strasbourg University (2004-2008)
- Vice-president of Bioinformatics Incitative Actions «IMPbio» of Minister of Scientific Research (2002-2003)
- Member of scientific council for Incitative Actions of Minister of Scientific Research (GRID computing ) (2001-2002)
- Member of national council for the allocation of CPU time on french supercomputer( IDRIS-CNRS, CINES-MESR, « Organized Molecular Systems in Biology « CP7 (1998-2004)
- Financial responsible of "Molecular Modeling and Graphics Group" (2001)
- Responsible for the animation (1999-2001) of a National Group: «Systemic analysis of 3D structures Interactions» in Bioinformatics Actions of Minister of Scientific Research.
- Secretary of "Molecular Modeling and Graphics Group" 1989
- Member of the Scientific Advisory Board to Oxford Molecular company (1992-1995)

### I.6. EXPERTISES – REPORTS – EVALUATIONS (SINCE 2003)

- Member of **Editorial Board** of "Advances in Bioinformatics" (2014-
- **Chairman of committee** for the AERES evaluation of the CNRS Laboratory UMR 8015 14/01/2009
- Expert for National Research Agency (Young researchers call) January 2009
- Expert for National Association for Research and Technology ANRT (doctoral fellowship call CIFRE) 2008, 2014
- Expert for « Royal Society Award » Price 2008

- Expert for National Research Agency (young researchers call) April 2008
- Scientific expert of AERES evaluation committee of IBMC Laboratory UPR 9002 CNRS Strasbourg (19-21/02/2008)
- Scientific expert of the AERES evaluation committee of the INSERM unit U665 Paris (13/02/2008)
- Member of the AERES evaluation committee of the IGBMC laboratory UMR 7104 Strasbourg (4-7/02/2008)
- Scientific expert for « Pays de Loire » Fundings call (2007)
- Scientific expert for CEFIPRA (Indo-French Research funding call) (2007)
- Chairman of the evaluation committee of IGS laboratory « Informatique et Génomique Structurale » UPR2589 (2006)
- Expert for the "Royal Irish Academy " Ireland (2006)
- Expert for Canadian Foundation of Innovation (FCI) 2006
- Expert for infrastructure RIO call In Structural Biology (2003-2006)
- Expert for National Research Agency (2005, 2006, 2009) PCV- Open and Young programs
- Member of the evaluation committee of the UMR 8015 laboratory 11/02/2005
- Participation to a report for the French Embassy in USA on Bioinformatics in california (February 2004)
- Expert for « Direction des Etudes Supérieures du Ministère de l'Education Nationale » (MSTP10) (2004-2005)
- Member of evaluation committee of UMR 6098 (2003)
- Régular reviewer for Bioinformatics, Applied Bioinformatics, J.Mol.Biol., Nucl Acids Res., Proteins, BMC Bioinformatics, BMC Genomics, Biochimie, Bioinformatics and Biology Insights, Microbial Pathogenesis, Nucleosides Nucleotides and Nucleic Acids.

## I.7. UNIVERSITY RESPONSABILITIES

My full teaching duties are performed (192 H Eq TD) since my appointment in 1984 (200H eqTD per year in average).

### **Undergraduate level in Biochemistry (since 2002)**

- UE IBIS "Introduction to Structural Bioinformatics" (3 credits)
- UE "Graphics Programming for Biochemist" (3 credits)

### **Master in Biochemistry (since 1998)**

- UE "Structural Bioinformatics" (6 credits)
- UE "Methods in Molecular Bioinformatics" (UE M2, resp. D. Mouchiroud & G. Deléage)

### **Doctorat:**

- Doctoral school Module in Bioinformatics

### **Ecole Normale supérieure of Lyon: (since 1994)**

- UE Statistics and Computer science for the Biologist (resp. D. Mouchiroud & G. Deléage)

### **Institut National des Sciences Appliquées (INSA) (since 2004)**

- Protein Bioinformatics for engineer school "Bioinformatics and Modeling" year 4 (resp. G. Deléage)

### I.8. SCIENTIFIC SOCIETIES MEMBERSHIPS

- Member of french society of Molecular Biology and Biochemistry (SFBBM)
- Member of French Bioinformatics Society (SFBI)

### I.9. DISTINCTION

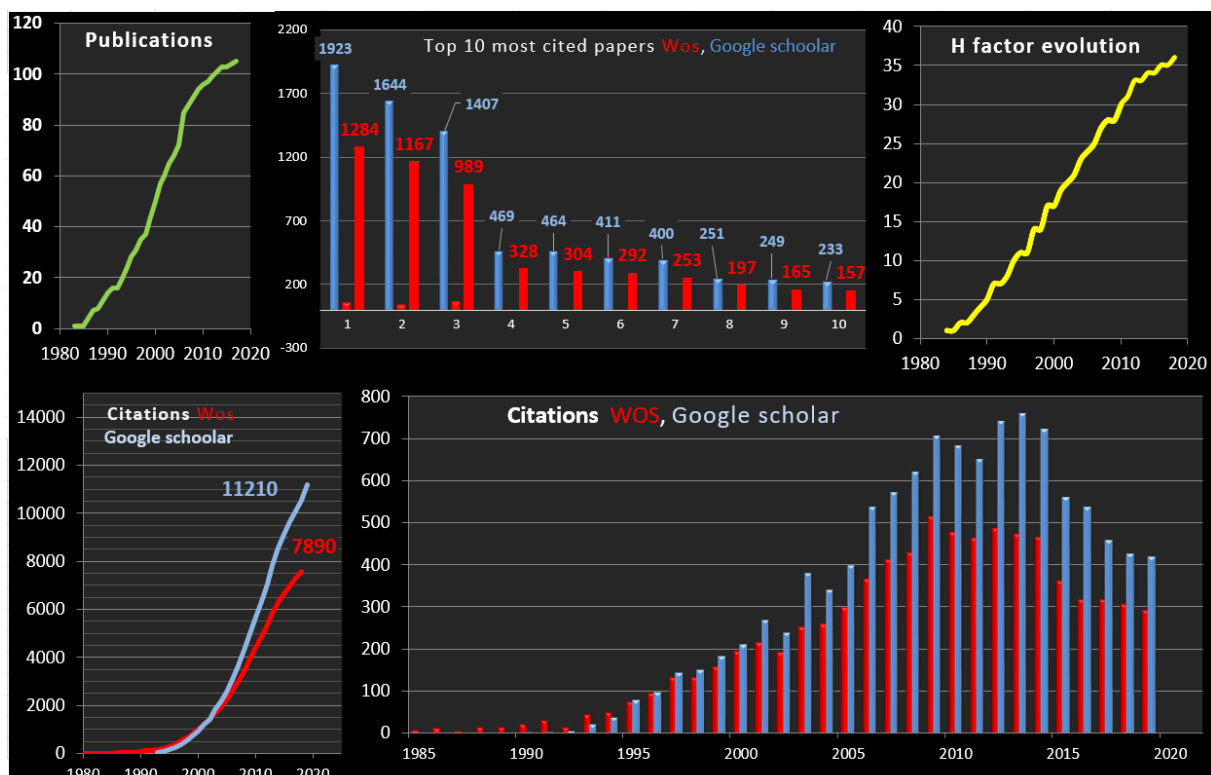
- Honored "Chevalier des Palmes académiques"

### I.10. OTHERS ACTIVITIES

- Setup in 1993 and maintaining of IBCP website (<http://www.ibcp.fr>) ranked as most visible web site of CNRS by [Webometrics](#) in 2007.
- Development of a databases for publications (realtime update of citations), stuff, PHD students, contracts, newsletter and theses defense at IBCP (up since 2005).
- Development of bioinformatics team website (<http://pbil.ibcp.fr>)

### I.11. SCIENTIFIC STATS AND POSITIONNING IN THE FIELD

Publication list and citation index are available at URL : <https://www.gdeleage.fr/prof/publis.php> or from Google scholar: <http://scholar.google.fr/citations?user=ijx5ISwAAAAJ&pagesize=100&hl=en>



The position of scientific research is 51 in the world and 1<sup>st</sup> in France (see WOS extract performed in May 2018)

At Lyon University, my main role was to introduce structural bioinformatics and structural biology in 1996 and to contribute to teach this field since my nomination as full professor in 1998. In addition, due to joined efforts of C. Gautier and myself, Lyon city was recognized as a national Bioinformatics Platform (RIO/IBISA label since 2003). In June 1998, M. Gouy and myself set up the Pôle Bioinformatique Lyonnais. This action contributes to the structuration of bioinformatics in Lyon thanks to our common volonte to coordinate the bioinformatics activities in the Rhône-Alpes region. Today, Lyon is an international place for bioinformatics research and services with a worldwide visibility.



**Results: ...**  
(from Web of Science Core Collection)

**You searched for:** TOPIC: (PROTEIN and ("molecular modelling" OR "secondary structure prediction" OR "sequence analysis" OR "web server")) [...More](#)

**Create Alert**

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**Refine Results**

Search within results for...

**Filter results by:**

- Highly Cited in Field (223)
- Hot Papers in Field (6)
- Open Access (16,935)

**Refine**

**Publication Years**

- 2018 (549)
- 2017 (1,475)
- 2016 (1,506)
- 2015 (1,526)
- 2014 (1,459)

[more options / values...](#)

**Authors** **Refine** **Exclude** **Cancel** Sort these by: Record Count

The first 100 Authors (by record count) are shown. For advanced refine options, use [Analyze results](#).

<input type="checkbox"/> WANG Y (144)	<input type="checkbox"/> KOONIN EV (49)	<input checked="" type="checkbox"/> DELEAGE G (39)	<input type="checkbox"/> LIU ZH (33)
<input type="checkbox"/> CHOU KC (141)	<input type="checkbox"/> LIU B (49)	<input type="checkbox"/> GRISHIN NV (39)	<input type="checkbox"/> SUZUKI K (33)
<input type="checkbox"/> ZHANG Y (133)	<input type="checkbox"/> KIM JH (48)	<input type="checkbox"/> JORNVALL H (39)	<input type="checkbox"/> WANG P (33)
<input type="checkbox"/> LI Y (116)	<input type="checkbox"/> ZHOU Y (47)	<input type="checkbox"/> WANG Q (39)	<input type="checkbox"/> XU D (33)
<input type="checkbox"/> LIU Y (112)	<input type="checkbox"/> BUJNICKI JM (46)	<input type="checkbox"/> XU J (39)	<input type="checkbox"/> XU Y (33)
<input type="checkbox"/> WANG J (105)	<input type="checkbox"/> LI M (46)	<input type="checkbox"/> CHEN X (38)	<input type="checkbox"/> BLUNDELL TL (32)
<input type="checkbox"/> LI J (103)	<input type="checkbox"/> WANG X (46)	<input type="checkbox"/> LI W (38)	<input type="checkbox"/> LEE SH (32)
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<input type="checkbox"/> LEE JH (70)	<input type="checkbox"/> LIU L (43)	<input type="checkbox"/> CALLEBAUT I (36)	<input type="checkbox"/> PUHLERA A (31)
<input type="checkbox"/> CHEN J (69)	<input type="checkbox"/> CHEN Y (42)	<input type="checkbox"/> KIM SJ (36)	<input type="checkbox"/> ZHANG W (31)
<input type="checkbox"/> LEE J (59)	<input type="checkbox"/> KUMAR R (42)	<input type="checkbox"/> KOBAYASHI M (36)	<input type="checkbox"/> JIANG Y (30)
<input type="checkbox"/> LI H (58)	<input type="checkbox"/> LI Z (42)	<input type="checkbox"/> TANAKA K (36)	<input type="checkbox"/> KOLINSKI A (30)
<input type="checkbox"/> RAGHAVA GPS (58)	<input type="checkbox"/> WANG XL (42)	<input type="checkbox"/> WATANABE M (36)	<input type="checkbox"/> LIN L (30)
<input type="checkbox"/> WANG L (58)	<input type="checkbox"/> ZHANG H (42)	<input type="checkbox"/> ZHANG Q (36)	<input type="checkbox"/> LIU H (30)
<input type="checkbox"/> CHEN L (57)	<input type="checkbox"/> COON JJ (41)	<input type="checkbox"/> GROMIHA MM (35)	<input type="checkbox"/> LIU X (30)
<input type="checkbox"/> HUANG Y (57)	<input type="checkbox"/> KIM J (41)	<input type="checkbox"/> LI B (35)	<input type="checkbox"/> MORNON JP (30)
<input type="checkbox"/> XIAO X (57)	<input type="checkbox"/> ROST B (41)	<input type="checkbox"/> MARTELLA V (35)	<input type="checkbox"/> WANG YJ (30)
<input type="checkbox"/> KUMAR S (55)	<input type="checkbox"/> HUNT DF (40)	<input type="checkbox"/> ZHANG X (35)	<input type="checkbox"/> ITO Y (29)
<input type="checkbox"/> WANG H (55)	<input type="checkbox"/> LOTTSPEICH F (40)	<input type="checkbox"/> BORK P (34)	<input type="checkbox"/> KIM YS (29)
<input type="checkbox"/> CHEN W (54)	<input type="checkbox"/> SUZUKI T (40)	<input type="checkbox"/> LIU Z (34)	<input type="checkbox"/> LEE JK (29)
<input type="checkbox"/> SHEN HB (51)	<input type="checkbox"/> CHEN H (39)	<input type="checkbox"/> LI C (33)	<input type="checkbox"/> LI XH (29)

Percentiles de citations*	Nombre d'articles
0,01% ≥ percentile	0
0,01% > percentile ≥ 0.1%	3
1% > percentile ≥ 0.1%	8
1% > percentile ≥ 10%	31
10% > percentile ≥ 20%	20
20% > percentile ≥ 50%	14

\*Indicates that 3 publications are in the top 0,1% most cited papers

## II. SUMMARY OF RESEARCH ACTIVITIES

My research activity deals with structural bioinformatics. It is a field I contribute to setup and develop in France. Indeed 25 years ago, we spoke about « Computer science applied to Biology » rather than Bioinformatics, a term introduced in 1990. At that time very few people thought that computer science will transform the strategy in biology. In 16 years, at IBCP, I have setup (2 people in 1992) and developed (15 people in 2009) a structural bioinformatics group which has acquired an international visibility. The attractiveness of the team contributed to the arrival of leading researchers to IBCP.

### II.1. DEVELOPMENT OF METHODS FOR PROTEINS SEQUENCES ANALYSIS AND PREDICTION OF SECONDARY STRUCTURES.

More than 15 predictive methods were developed among which the “Double Prediction Method”, 1987; “Self Optimised Prediction Method”, 1994; “Self Optimised Prediction Method from Alignments”, 1995 (each of the founding papers were cited over 200 times).

### II.2. DEVELOPMENT OF COMPUTER PROGRAMS FOR 1D, 2D ET 3D ANALYSIS OF PROTEINS

ANTHEPROT (ANalyze THE PROTEins), 1988-2007. This software was the first program mainly devoted to protein (with PC/Gene by A. Bairoch). About 250 citations, more than 8500 FTP and more than 1500 analysis requests each year. DicroProt, 1993. Still widely used today and the article has been cited over 100 times.

### II.3. WEB SERVERS

I have developed with C. Geourjon in 1994 the first mailserver in France to perform predictions of protein secondary structures (80,000 predictions). Thenafter, I integrated these prediction methods into the Network Protein sequence Analysis, 2000 (NPS@) webserver (release 1)). C. Combet is continuing its development and its maintenance. The paper describing NPS@ received over 640 citations; in 2009, 6471 analyses were performed each day thus summing more than 12,000,000 analyses in 10 years.

### II.4. VIRAL BIOINFORMATICS

With the increasing interest in molecular virology, I felt the need to develop new databases dedicated to virus. Thus, the development of

HCVDB (PHD work of C. Combet under my supervision) was initiated first at the french level (Réseau National Hépatites) then extended to Europe thanks to a European contract in FP5 [HepCVax] in the "workpackage" database I was in charge of. Finally, the EuHCVdb was supported by a FP6 Network of Excellence (VIRGIL). The database acquired a reputation and worldwide visibility.

### II.5. APPLICATIONS IN BIOLOGY

Methods should be developed only if they are usable by the scientific community of biochemists and biologists. Therefore, methods and tools have been applied most often in collaboration with groups of biologists (immunologists, virologists, molecular biologists, structural, microbiologists) leading to results very original. For example, by using molecular modeling at low level of identity, I proposed insertions sites for peptides in viral capsid so as to modify the virus tropism. This was the first demonstration that we are able to design virus for targeting new given cells. (Girod *et al.*, *Nature Medecine*, 1999).

R.Lavery, K. Zakrzewska, R. Terreux joined the bioinformatics group in 2007 and J. Martin in 2008 thus allowing to work in several directions.

- GRID computing [C. Blanchet]
- Molecular modeling and 3D Web [E. Bettler]
- Integration of tools and viral databases [C. Combet]
- Drug design and QSAR [R. Terreux]
- Molecular interactions [R. Lavery & K. Zakrzewska]

*Having developed in Lyon in 1986, structural bioinformatics (before the 'bioinformatics' word exists), I play a role in its development and in structuring the research on bioinformatics and structural biology (absent at that time in Lyon). This effort was completed in 1997 with the first determination of the 3D structure of a protein entirely conducted in Lyon (P33) and by obtaining a "Contrat de Plan Etat Region 2000-2006" to fund the extension of the IBCP building with an additional floor dedicated to bioinformatics (delivered in 2003).*

## II.6. SUMMARY OF SCIENTIFIC RECORDS

<b>OUVRAGES</b>				
Publications with peer review	96			
Averaged IF	4.87			
Publications with IF >4	50			
Publications with IF >10	8			
Publication with IF >= 25	1			
First authorship	12			
Last authorship	25			
Book chapters	13			
Communications	146			
Patents	4			
<b>CITATIONS (104 items)</b>				
Citations (All databases WoS)	7890			
Citations/paper	75.19			
Citations (Google scholar)	<u>11210</u>			
Articles with at least 100 citations	13			
Citations without self-citation (Wos)	7865			
H Index (Wos)	36			
H index (Google)	40			
G index	86			
<b>Others</b>				
PHD / HDR jurys defenses	79			
Research Contracts **	32			
Meetings organization	13			
Invited talks (or trainings)	38			
PHD directions	11			
		<b>Journal</b>	<b>Number</b>	<b>Impact factor 2009</b> <b>Source ISI</b>
		NAT MED	1	25.430
		HEPATOLOGY	3	10.885
		BLOOD	1	10.558
		TRENDS BIOCHEM SCI	2	10.364
		NUCLEIC ACIDS RES	6	7.479
		ONCOGENE	1	7.414
		CLIN CHEM	1	6.886
		MOL BIOL EVOL	1	5.51
		J BIOL CHEM	2	5.328
		J VIROL	7	5.189
		BIOCHEM J	1	5.016
		EUR J CANCER	1	4.944
		EUR J IMMUNOL	1	4.942
		BIOINFORMATICS+CABIOS	14	4.877
		MOL MICROBIOL	1	4.819
		BIOCHIM BIOPHYS ACTA	1	4.237
		DATABASE	1	4.020
		INSECT BIOCHEM MOLEC	1	4.018
		J MOL BIOL	2	4.008
		J UROLOGY	1	3.862
		J APPL CRYSTALLOGR	1	3.794
		BIOCHIMIE	1	3.787
		BIOCHIM BIOPHYS ACTA	1	3.587
		MATRIX BIOL	2	3.328
		BIOCHEMISTRY-US	2	3.226
		PROTEINS	1	3.085
		BMC BIOINFORMATICS	2	3.028
		J MED VIROL	1	2.895
		PROTEIN SCI	1	2.741
		J MOL RECOGNIT	3	2.286
		GENE	2	2.266
		COMPUT BIOL MED	1	1.112
		M S-MED SCI	1	0.486
		BIOFUTUR	1	0.038
		<i>Impact factors of publications (ISI 2010)</i>		

\* Given a set of articles ranked in decreasing order of the number of citations that they received, the g-index is the (unique) largest number such that the top g articles received (together) at least  $g^2$  citations.

\*\* 4 european contracts (2 NOE + 2 Projects)

\*\*\* among which 33 international

Ranking of publication by decreasing order of impact factor (from ISI 2009).

### III. RESEARCH ACTIVITIES

For better clarity the detailed activities of research are presented in chronological order: First, the work of theses (Bio / Biochemistry and Biophysics / Bioinformatics) prepared in different laboratories. Then all the work carried out or supervised at IBCP when I arrived in 1992 to IBCP.

#### III.1. 3<sup>EME</sup> cycle thesis (1982-1984)

The first part of my work was realised in the « Laboratoire de Biologie et Technologie des Membranes » (LBTM) directed by Pr. D.C. Gautheron. The research deal with mitochondrial ATPase-ATP synthase. This enzyme catalyses the reversible synthesis of ATP thanks to a proton gradient.



We established a correlation between ATP synthesis rate and proton flux use in order to localise the protons efficient for synthesis. To measure the setup of  $\Delta\mu\text{H}$ , a highly sensitive method based on fluorescence of 9-amino-6-chloro-2-méthoxyacridine was used. Our results suggested that efficient protons were not distributed in the bulk phase but rather clustered in a kinetic compartment. (P1, P2).

During this thesis, I also try to characterise the dicyclo-hexylcarbodiimide (DCCD) binding protein of the F0 part of ATP synthase complex. We purified this protein to homogeneity using liquid chromatography in chloroform/methanol mixtures after ether precipitation. Then I reconstituted the protein into liposomes and I demonstrated that this single protein was unable to constitute a proton pore (T1). This result has been confirmed by others authors thereafter.

Another protein of the F0 part has been studied "Oligomycin Sensitivity Conferring Protein" and we showed that the protein may have a structural role rather than functional in the proton pore (P4).

#### III.2. PHD RESEARCH WORK (1985-1988)

The second part of my work still concerns ATP synthase complex and it was carried out in the Physico Biochemistry Laboratory directed by Pr. Roux B in collaboration with D.C. Gautheron team. Electrical properties of ATPase F1 were investigated by electrical birefringence with a home made apparatus. The sign was negative indicating that the permanent electric dipole was perpendicular to the longest axis of the protein. Analysis of signal decay permits to determine protein dimensions of 140 Å

(making the hypothesis of an oblate ellipsoid (P3). These dimensions were confirmed by X-ray crystallography 15 years later!

We also studied the effect of the IF1 natural inhibitory peptide that decreased the signal magnitude. Globally speaking, this method has revealed useful to precise the electro-optic properties of FO-F1 ATP synthase.

At that time, I also developed intrinsic fluorescence study of Fo-F1 ATPase by quenching measures of aromatic groups (T2). The study suggested that these important groups were located at the interface of subunits or buried within the molecule. The difference in accessibility was abolished when the protein was denaturated.

At the same time, the F1-ATPase sequences became available. This corresponds to the period in which I progressively switch to bioinformatics (even if the bioinformatics term did not exist). Indeed, very few tools were present and I began to develop a computer version of the well known Chou & Fasman method for predicting the secondary structure of proteins (P6). In the same time, I propose to take into account the predicted class of proteins from amino acids composition to improve the prediction accuracy. This method was called the double prediction method (P7). The improvement in the method was recognised by G.D. Fasman who invites me to write a full chapter of a book entitled "Prediction of Protein Structure and Principles of Protein Conformation" (L6).

As an illustration of the work, these predictive analyses allow to predict the very long  $\alpha$  helix in the  $\gamma$  subunit which was demonstrated by Walker to constitute the rotor axis of the molecular turbine.

#### III.3. WORK AFTER THE THESES (1989-1992)

The work combined both experimental and theoretical approaches onto mitochondrial F1 ATPase. Firstly, biophysics experiments were carried out in collaboration with A. Di Pietro, F. Penin and G. Divita. Intrinsic fluorescence coupled to circular dichroism allow us to precise the role of a Trp in the  $\epsilon$ , subunit in interaction with the  $\delta$  subunit. (P13, L7). Moreover an heterogeneity in Trp behavior located on  $\alpha$  subunits has been found (P15). My interest for bioinformatics still increase and I completely switched to bioinformatics and developed this activity since that period.

I started the development of ANTHEPROT software for protein sequence analysis in 1988 and established a contract with IBM company to adapt the program for IBM 5080 graphic workstation (P8, P9, G1).

This work was realised with C. Geourjon (DEA) with the help of R. Lahana who was the author of MAD (Molecular Advanced Design) at Pierre Fabre Laboratories. Thanks to this success story we made an interface of ANTHEPROT with MAD (G2) (P16). This development was done by C. Geourjon during his PHD work (under my supervision) and he won the "Lyon young researcher price" in 1995. Due to the restructuration of biochemistry labs in Lyon, Christophe Geourjon and I join the Institut of Biology

and Chemistry of Proteins in June 1992. Our job fixed by the director was to install and develop bioinformatics and molecular modeling at IBCP.

### III.4. RESEARCH AT IBCP(1992- TODAY)

Arriving at IBCP with one PHD student, I progressively set up a molecular modeling unit which was associated with the structural NMR one (animated by F. Penin) to constitute an individual team. Its composition (2 DR, 2 CR, 2 MC, 1 IR, 1 PR) is given and its activity comprises 5 directions in 2020 described at URL : <http://pbil.ibcp.fr>.

#### III.4.1. IMPROVING ANTHEPROT

The main idea was to provide biologists with a powerful computing software. Thus we include a lot of functions such as signature detection in biological sequences (P17). An additional module devoted to circular dichroism was developed (P18). This module was then extended so as to include several methods for CD spectra analysis (CONTIN, K2D,VARSELEC, SELCON).

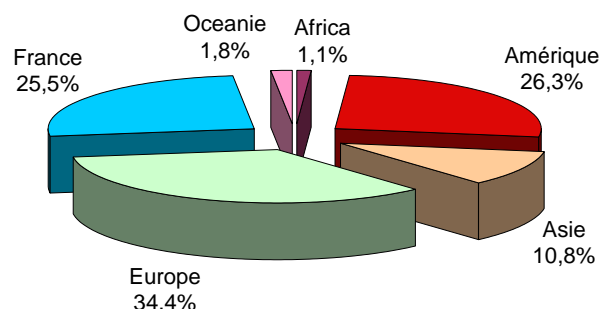
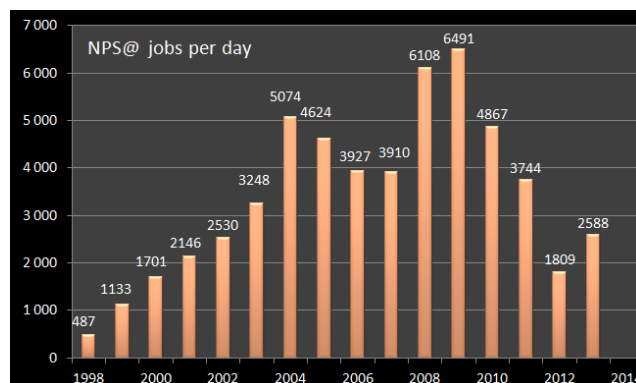
Finally, we added a completely new NMR module which facilitated molecular modeling from NMR restraints (P28) and offers a lot of 3D features such as structure superimposition or Ramachandran plots (P25). Since that time, I completely wrote a new program specially designed for PC under windows.

#### III.4.2. NEW METHODS

We propose a completely new predictive scheme for protein secondary structure prediction (P20). A improvement by 7% in prediction accuracy was reached thus leading to the best available method at that time 73,2% for 3 structural states (P26).

#### III.4.3. WEB SERVER FOR SEQUENCE ANALYSIS

After the development of several methods, we install (in 1994) one of the first mailserver for protein secondary structure prediction and proposed our programs on anonymous ftp site (<ftp://ftp.ibcp.fr>). This mailserver performed more than 80000 predictions! It has to be kept in mind that Internet servers only began in 1993. We setup one of the very first web server in 1998 of France. We wrote a review on structure prediction for the biologist in 1997! (P34). On January 1998 we created the « pôle bioinformatique Lyonnais (PBIL) » with M. Gouy at Villeurbanne. This webserver is able to analyse both nucleic and protein sequences (Blast, Fasta, Ssearch, Clustalw, Multalin) in a fully interactive manner. Today in 2009 our NPS@ server (<http://npsa-pbil.ibcp.fr>) is still running and performed in average 6491 analyses per day in 2009 (P43, P61). The basic paper was cited over 592 times.



Usage statistics of NPS@ server. Number of jobs per day (upper panel) and country usage (lower panel).

#### III.4.4. WEB SERVER FOR MODELING

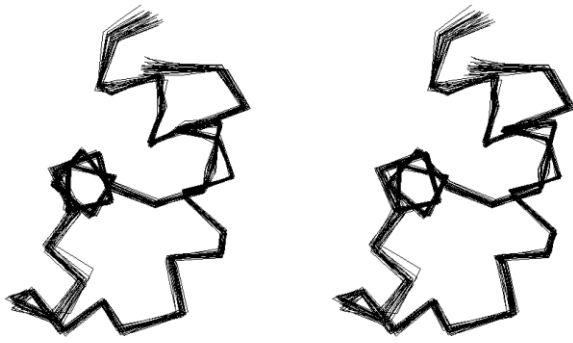
Identification of homogenous protein with known structure allows to build a 3D model of a query protein. This building process is called homology modeling. We develop in february 2002 a new web server [geno3D](http://geno3d-pbil.ibcp.fr) (<http://geno3d-pbil.ibcp.fr>) to perform automatic homology modeling. The originality of this program is the possibility to construct 3D models even using remote homologous protein as templates (P54).

In the PHD work of M. Errami (under my supervision) we exploit the comparison of the predicted secondary structures of templates and query protein to improve the choice of templates (P50). Then, we extend this discovery with M. Errami, to the detection of badly aligned sequences into multiple alignments (P57) and we showed that residues conservation into multiple alignment corresponds to interacting residues in 3D structures (P60). Geno3D was interfaced with Expasy, Prodom and Esript well known servers.

##### III.4.4.1. 3D structures determination

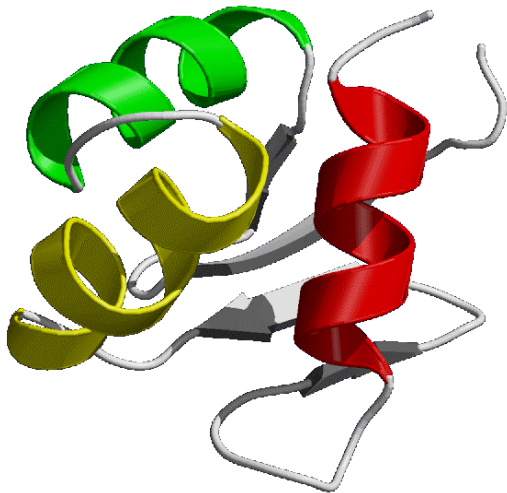
On the experimental level,our team "Structural bioinformatics and NMR" determined by NMR and molecular modeling the 3D structure of several proteins domains that interact with DNA:

- 1) FruR (57 amino acids, 7380 Da) transcription factor involved in fructose metabolism (P33)



34 superimposed structures (pdb code:1UXC) from NMR data (NMR experiments carried out by R. Montserret and F. Penin)

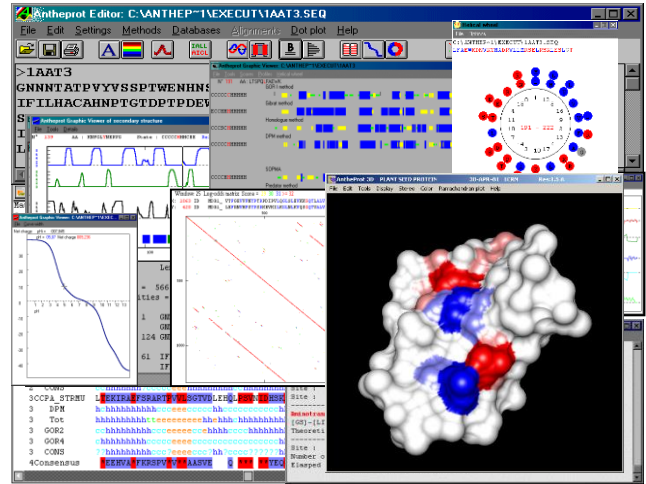
- 2) Antigenic peptides from hepatitis C virus nucleocapsid (44 amino acids).
- 3) HSF (125 acides aminés, 13690 Da) transcription factor involved in the regulation of heat shock protein.



HSF NMR structure (experiments carried out by Y.S. Yang and F. Penin).

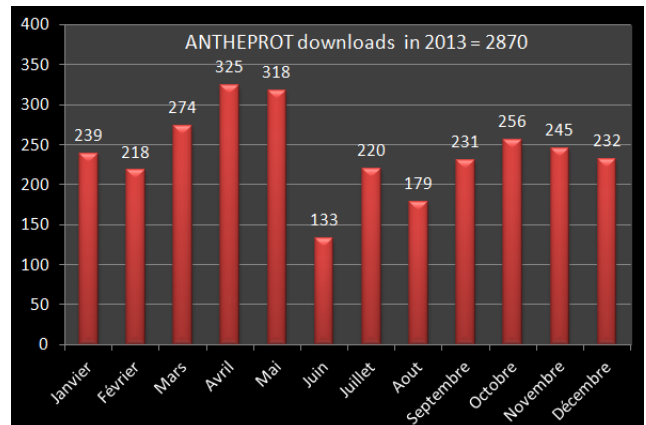
#### III.4.5. SOFTWARE DEVELOPMENTS (1988-2020)

I am developing since 2001 a completely new release of ANTHEPROT <http://antheprot-pbil.ibcp.fr> that run under Windows 3.1, Win95 and Win NT operating systems. The software supports client-server capabilities (P49); thus the user may perform sequence comparison against remotely installed databanks.



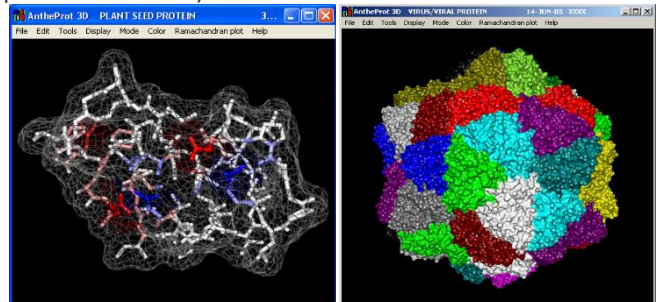
ANTHEPROT Windows release 5.2

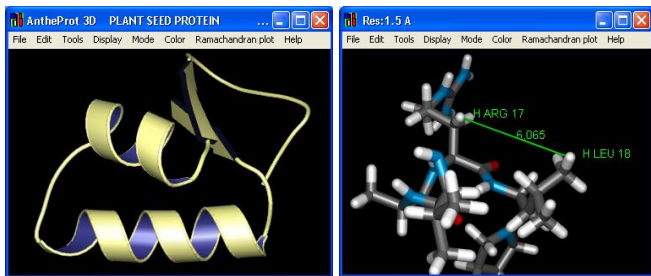
More recently, I develop a 3D viewer of macromolecules for Windows called AnTheProt 3D (see illustrations, cover of the document and examples <http://antheprot-pbil.ibcp.fr/3D/>) with the help of OpenGL library. This viewer supports different representation mode (CPK, ball and sticks, wireframe, backbone, alpha trace, surfaces, ribbons) with fully interactive manipulation.



ANTHEPROT downloads(2013)

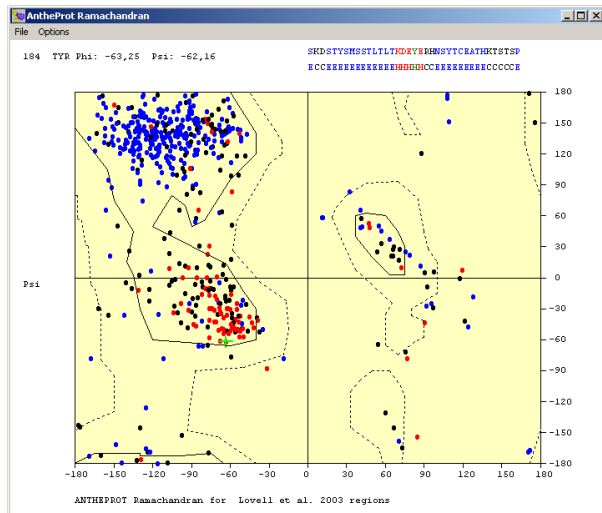
The program is interfaced with Molscript (ribbons), Delphi (electrostatic potentials), MSMS (molecular surfaces) and REDUCE (hydrogens addition/removal). Moreover, AntheProt3D offers to monitor videos and to view in several stereoscopic modes (green/red anaglyph, or quadbuffer modes).





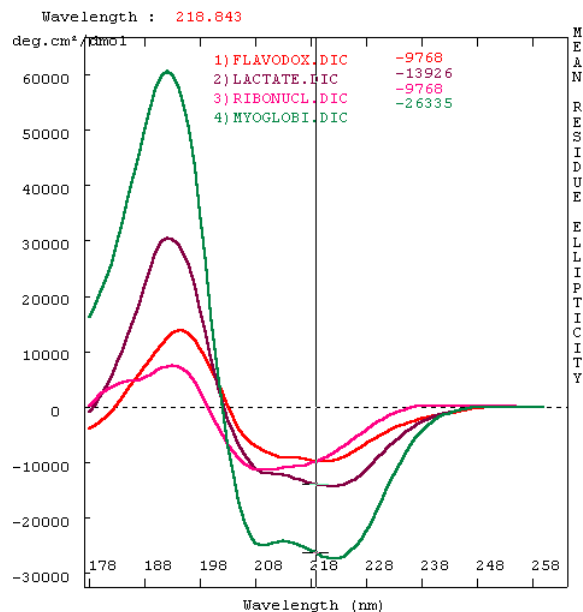
AnTheProt 3D

AntheProt 3D is also able to display interactive Ramachandran plot. This viewer has been used in a recent study in molecular modeling of melanocortin mutants (P84).



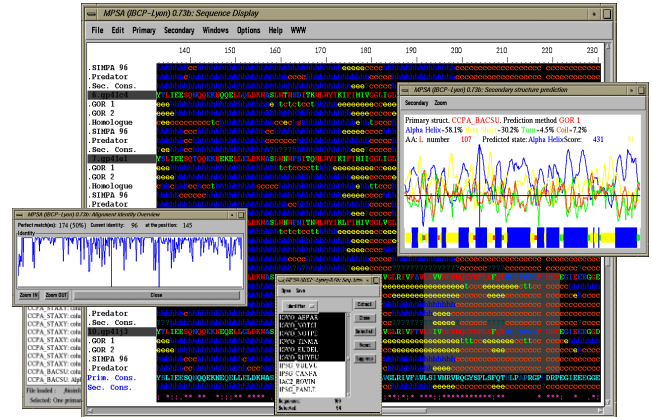
Ramachandran plot within AnTheProt 3D

Another program called Dicroprot integrates several methods for the deconvolution of circular dichroism spectra <http://dicroprot-pbil.ibcp.fr>. In addition this program allows the management of raw CD spectra as monitored by Jobin Yvon apparatus.



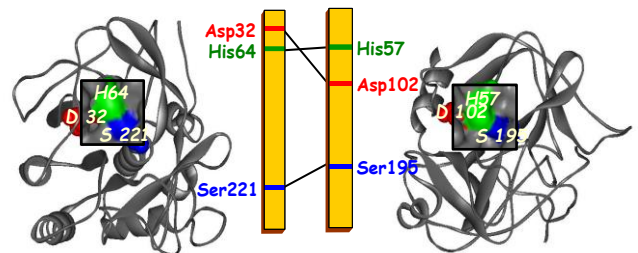
DICROPROT release 2.5

During the PHD work of C. Blanchet (under my supervision), a normalised interface for multiple alignment has been developed (P44). This new software (MPSA for Multiple Protein Sequence Analysis) has no limitation in number and length of sequences compatible with the memory of the machine.



MPSA : multiple alignment edition

The modeling of the GP41 protein (C. Combet DEA work) has been performed and lead us to develop new methods to compare the surfaces properties shared by different proteins. To that goal, M. Jambon developed SUMO (P58) during his PhD work (supervised by C. Geourjon and me in the team) and a patent has been deposited on this new bioinformatics method. The program has been the subject of a licensing agreement with **MEDIT** and a web server for academic users has been developed (P67).

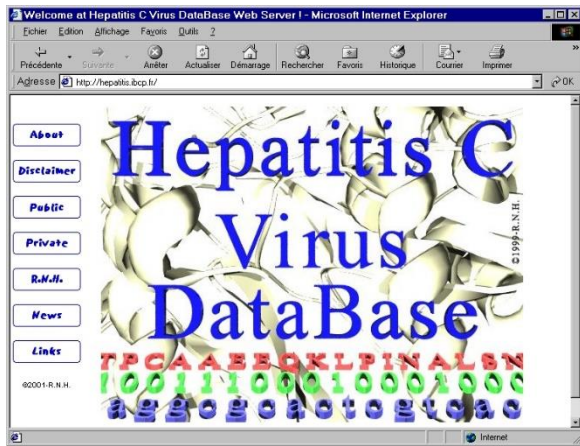


Comparison of Ser proteases with different fold. The amino acids of active sites are inverted into sequences hindering their alignment.

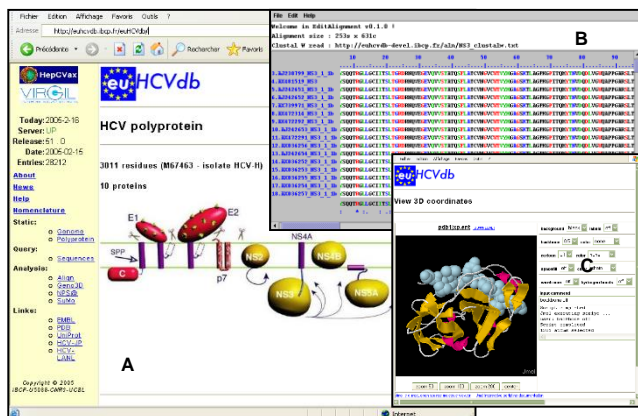
### III.4.6. EUROPEAN HEPATITIS C VIRUS DATABASE

Hepatitis C Virus was the main research domain of our team. Therefore, I decided to develop a bioinformatics activity related to this field. This part represents the PHD work of C. Combet (under my supervision). The project consists in the development of HCV database (P55, P64) aiming to put in relation protein and nucleic sequences with biological and clinical data (Réseau National Hépatites) animated by Dr. G. Inshaus and Pr. C. Bréchet. The main features of the database (<http://euhcvdb.ibcp.fr>) are :

1. Exhaustive collection of HCV genomic sequences.
2. Regular and automatic update.
3. Data confidentiality and secure access.
4. Coupling of the database with analysis tools.



HCVDB (french original databank)



euHCVdb European sequence database (<http://euHCVdb.bcp.fr>)

It is monthly updated from the EMBL Nucleotide sequence database and maintained in a relational database management system (PostgreSQL). Programs for parsing the EMBL database flat files, annotating HCV entries, filling up and querying the database used SQL and Java programming languages. Great efforts have been made to develop a fully automatic annotation procedure thanks to a reference set of HCV complete annotated well characterized genomes of various genotypes. This automatic procedure ensures standardisation of nomenclature for all entries and provides genomic regions/proteins present in the entry, bibliographic reference, genotype, interesting sites (e.g. HVR1) or domains (e.g. NS3 helicase), source of the sequence (e.g. isolate) and structural data that are available as protein 3D models. Two EU contracts (FP5 HepCvax and FP6 Virgil), now ended, funded software development of the euHCVdb project. A unified numbering system has been proposed in collaboration with an international HCV annotation consortium (P66, P70, P73, P86). This database (release 101 at 01/05/2009) contains more than 80000 entries. In case of modification of an entry this entry is automatically updated. The NPS@ tools have been adapted and integrated to euHCVdb (P43) in such a way that NPS@ programs can be launched directly from within euHCVdb. For example, starting with a given sequence, it is possible to perform a similar search by using BLAST, FASTA, PSI-BLAST, SSEARCH. From the list of hits, the user may align all sequences with MULTALIN or CLUSTALW. Then, predicted

secondary structures (SOPMA, PHD, DSC, etc.) can be inserted into the multiple alignment and a structure consensus can be calculated. Other tools developed in the team (PATTINPROT or PROSCAN) for pattern searching are available as well as profiles (hydrophobicity, antigenicity, solvent accessibility, transmembranous regions), HTH or "coiled-coil" motif detection. More than 46 methods are available today. Finally, all data generated by these programs can be downloaded into ANTHEPROT or MPSA programs (P55). Our team has now the responsibility of the European HCV database euHCVdb and established an international collaboration with american (C. Kuiken, Los Alamos Laboratory) and japanese (M. Mizokami, Université de Nagoya) databanks for the definition of new genotypes.

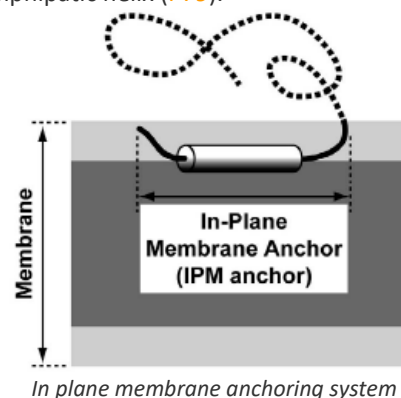
### III.4.7. GRID COMPUTING

Taking into account the huge demand in calculation generated by modern biology, C. Blanchet investigated the possibility of distributed computing with the help of GRID technologies.

Although being an emerging field, we address security problems (P76) in collaboration with CNRS Grid Institute and CC-IN2P3. We aimed at migrating the NPS@ server as a GPS@ (Grid Protein sequence, Analysis). This grid activity is supported by a GenHomme (Bioingénierie 2002) grant and by 2 european FP6 contracts: EGEE for grid infrastructure and EMBRACE for gridification of bioinformatics algorithms thus placing IBCP as a leader of biology labs involved in GRID technologies (P75) since it is the IDG node in biology. Finally, we applied these developments to refine all PDB files in collaboration with CMBI (Vriend' group in Nijmegen, Pays-Bas) (P85).

### III.4.8. PREDICTIONS OF AMPHIPATIC HELICES

The PHD work of N. Sapay (P69) (co-supervised by F. Penin and me in the team) consisted in the elaboration of a tool able to predict if a protein has an amphipatic helix associated with membrane by in plane insertion. This tool has been developed in collaboration with LORIA (Y. Guerneur) by using Support Vector Machines technologies. It was found to be efficient and allows us to demonstrate that both NS5A protein from HCV and 2C proteins from poliomyelitis virus, although not related, have a typical amphipatic helix (P79).



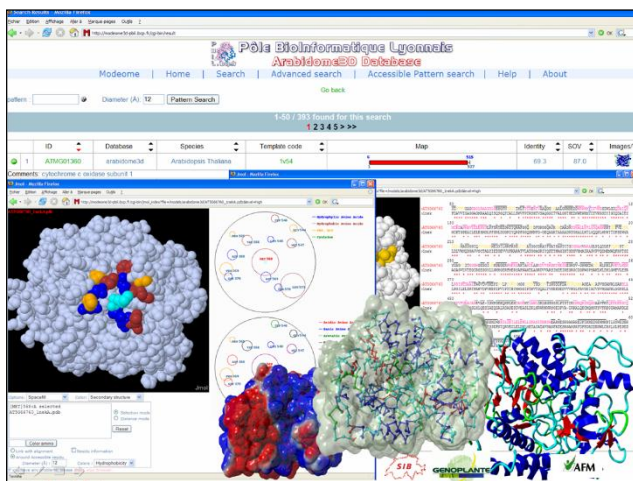
In plane membrane anchoring system



This feature has been found in all picornavirus family. Thus based on this discovery, we develop the amphipaseek algorithm (P72), a method which predicts correctly 60% of amphipatic anchor helices.

### III.4.9. 3D MODELS DATABASE

The PHD work of Nicolas Garnier (supervised by E. Bettler and me in the team) aimed at developing a management and storage system of 3D structure model generated by geno3D (cf page 9). This tool called Modeome3D (<http://modeome3D-pbil.ibcp.fr>) (P74) is able to manage full proteome modeling projects and has been validated onto HCV and *A. thaliana* proteomes. This tool was extended in MS2PHdb (Erreur ! Source du renvoi introuvable.) so as to estimate the impact of mutants in 3D models in relation to phenotypes.



Modeome3D

### III.4.10. MSX-3D

The PHD work of M. Heymann (supervision by C. Geurjon and me) consists in the development of a bioinformatics tool for model validation. The program uses cross links data and mass spectrometry identification to monitor and measure experimental distances that are compared with those deduced from homology models (P82).

### III.4.11. « TYROSINE KINASES BACTÉRIENNES » FAMILY (BYK)

Most of the protein tyrosine kinases found in bacteria have been recently classified in a new family, termed BY-kinase. In collaboration with C. Grangeasse (A Cozzone team), we setup a bioinformatics procedure to identify (and then extract) « Bacterial tyrosine kinases proteins » (P83). Indeed, they share no sequence homology with their eukaryotic counterparts and have no known eukaryotic homologues. They are involved in several biological functions (e.g. capsule biosynthesis, antibiotic resistance, virulence mechanism). Thus, they can be considered interesting therapeutic targets to develop new drugs to treat infectious diseases. However, their identification is

hindered due to slow progress in their structural characterization and comes most often from biochemical experiments. Moreover BY-kinase sequences are related to many other bacterial proteins involved in several biological functions (e.g. ParA family proteins). Accordingly, their annotations in generalist databases, sequence analysis and classification remain partial and inhomogeneous and there is no bioinformatics resource dedicated to these proteins. The combination of similarity search with sequence-profile alignment, pattern matching and sliding window computation to detect the tyrosine cluster was used to identify BY-kinase sequences in UniProt Knowledgebase. Cross-validations with keywords searches, pattern matching with several patterns and checking of motifs conservation in multiple sequence alignments were performed. Our pipeline identified 640 sequences as BY-kinases and allowed the definition of a PROSITE pattern that is the signature of the BY-kinases. The sequences identified by our pipeline as BY-kinases share a good sequence similarity with BY-kinases that have already been biochemically characterized, and they all bear the characteristic motifs of the catalytic domain, including the three Walker-like motifs followed by a tyrosine cluster. A database collecting the BY-Kinase sequences is under development and will be made available soon.

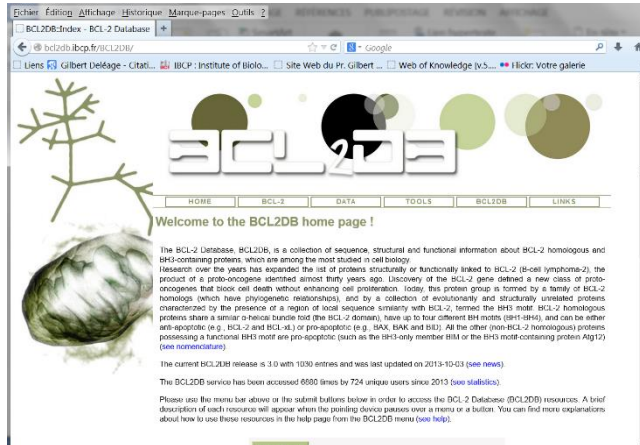
### III.4.12. BASE DE DONNÉES HBVDB

The PHD work of J. Hayer (supervision by C. Combet and myself) consisted in the development (P92) of an hepatitis B virus database (<http://hbvdb.ibcp.fr>) in close collaboration with Pr Fabien Zoulim team at CRCL.

The screenshot shows the HBVdb website home page. At the top, the logo 'HBVdb The Hepatitis B Virus database' is displayed. Below the logo is a navigation bar with buttons for 'HOME', 'HBV', 'QUERY', 'ANALYSIS', 'HBVDB', and 'LINKS'. A welcome message reads 'Welcome to the HBVdb home page !'. The main content area contains several sections: 'Genome' with a 'Genome' button; 'HBV Nomenclature' with a 'Nomenclature' button; 'Proteins' with buttons for 'Core', 'HBx', 'Surface', and 'Polymerase'; 'Query' with buttons for 'Dataset', 'Nucleotide', and 'Proteins'; 'Generic N' with buttons for 'Blast N', 'ClustalW N', and 'FASTA N'; 'Analysis Generic P' with buttons for 'Blast P', 'ClustalW P', and 'FASTA P'; 'Specialized' with buttons for 'Annotate', 'Genotype', and 'Resistance'; 'About' with an 'About' button; 'Contact' with a 'Contact' button; 'HBVdb Help' with buttons for 'Annotate', 'Genotype', 'Home', and 'Resistance'; 'News' with a 'News' button; and 'Statistics' with a 'Statistics' button. At the bottom, there is a footer with logos for BMS, IBP, and IBCP, and the text '© 1999-2012 PRAB/BMSSI/UMR5086/IBCP/CRNU/CBL'.

### III.4.13. BASE DE DONNÉES HBVDB

The PHD work of V. Rech de Laval under my direction (supervision by C. Combet and A. Aouacheria) conducted to the delivery of the BCL2-DB database (<http://bcl2db.ibcp.fr>). This work was carried out in close collaboration with A. Aouacheria at LBMC (**Erreur ! Source u renvoi introuvable.**).



BCL2DB Home page

## III.5. APPLICATIONS AND COLLABORATIONS

From a general point of view we always try to validate and apply our methods with biological experiments. Thus, we collaborate with numerous laboratories involved in general biology (P5, P10, P14, P30, P66, P77, P81), virology (P11, P12, P45, P46, P62, P63), molecular genetics (P4, P19, P23, P27, P32, P33) or vegetal (P65) or animal (P84) genomics. Some examples of such work are given thereafter.

### III.5.1. COLLABORATION WITH A.J. COZZONE GROUP

IBCP-CNRS UPR 412,7, passage du Vercors, 69 367 Lyon cedex

One of the research topics of this group is the FruR protein from *E. coli*. That protein is able to regulate the transcription of gene involved in neoglucogenesis as *pps*, *pck*, *aceBAK*, by DNA binding. In its N-terminal part, that protein presents high sequence similarity with LacI and GalR repressors.

The aim of our work was to modulate by site directed mutagenesis the affinity of the protein for DNA. Two approaches were used:

First, ANTHEPROT and homology modeling techniques allows us to build a 3D model that was used to propose mutants that must not alter the structure integrity.

Besides, overexpression of "hpF" *i.e.* FruR(1-57)\* were performed in Cozzone group (Scarabel *et al.*, 1994) in order to determine the 3D structure by liquid state NMR. These experiments were carried out in our team by R. Montserret and F. Penin. The collected data from NMR <sup>1</sup>H 2D spectra were used to determine the first 3D structure

of a protein entirely performed in Lyon. Refinement includes X-Plor protocols and development of specific modules in ANTHEPROT.

A set of 50 similar structures was obtained that exhibit 0,37Å RMSD for 47 first residues on secondary structures. The consensus site for DNA binding and recognition has been precised (P31). A collaboration to work on an other gene of a pathogenic bacteria has also been realised (P35).

### III.5.2. COLLABORATION WITH DR A. DI PIETRO GROUP

IBCP-CNRS UPR 412, 7, passage du Vercors, 69 367 Lyon cedex

The structure of nucleotides binding sites was analysed by mutation and molecular modeling. A "domain design" study of MDR sequences was performed in order to choose the regions to be cloned and overexpressed. These domains were obtained and a fluorescence characterisation was performed within A. Di Pietro group (P29). At the same time, a circular dichroism study was performed as well as a sequence analysis. This permits to cross validate these methods and to establish a 3D model built by analogy with nucleotidic sites (P37). Finally, molecular modeling suggested a similar mechanism between ABC proteins and helicase family (P52).

### III.5.3. COLLABORATION WITH PR. M. VAN DER REST GROUP

IBCP-CNRS UPR 412, 7, passage du Vercors, 69 367 Lyon Cedex

This group worked on extracellular matrix proteins and more precisely on collagens. These proteins play an important role in muscular, epidermic tissues of mamalian. Collagen constitutes a protein family with a repetitive motif made of a triple helix with succession of G-x-y flanked by non collagenic regions. We studied the secondary structure of N-terminal part of collagen suggesting antiparallel  $\beta$  sheets as in fibronectin or immunoglobulin. This organisation may suggest accessible interaction sites (P21). NMR experiments confirmed this observation.

We also solved by NMR the NC1 domain of collagen type XIV alpha1 which is the heparin binding site (P40).

### III.5.4. COLLABORATION WITH DR G. VERDIER GROUP

Laboratoire de Biologie Cellulaire Fongique, UMR CNRS 106, Université Lyon I, 43 Bd du 11 novembre 1918, 69622 Villeurbanne Cedex

Infection of a cell by a retrovirus needs the recognition of a receptor by viral proteins. The aim of their group research is to build and use retroviral vector for transgene of birds. Indeed, a better knowledge of viral binding region should allow genetic modification in order to build retroviral vectors with new tropism capabilities.

The chimeric virus could be able to infect new cells which is a prerequisite step in genic therapy

In a collaborative work, we performed theoretical studies on binding regions of retroviral proteins. By using the models we constructed, this team succeeds in the modification of virus tropism towards particular receptor of integrins or epidermal growth factor receptor (P22).

### III.5.5. COLLABORATION WITH PR. R. GOODY GROUP

Max Planck Institut, Dordmund Allemagne

The SOPM method we developed was used to locate a region involved in RT dimerisation of HIV1 RT. From this study synthetic peptides proved to inhibit reverse transcriptase dimerisation (P24).

### III.5.6. COLLABORATION WITH PR. C. DUMAS GROUP

Laboratoire de Reconnaissance Cellulaire et d'Amélioration des Plantes, UMR CNRS-INSA-ENSL

In collaboration with D. Gagliardi, our team determined the 3D structure of DNA binding domain (116 amino acids) of heat shock factor (Heat Shock Factor from Maize) by NMR. This result was also obtained by other teams either by NMR or by Xray crystallography. The structure is composed of 3 helices and 4  $\beta$  sheets. Helix 2 (in yellow page 9) is curved and secondary structures are well defined contrarily to aperiodic regions. Superimposition of 25 structures exhibits a 0.73 Å RMSD on secondary structures. This topology looks like that of CAP protein.

### III.5.7. COLLABORATION WITH DR M. HALLECK GROUP

Université de Munich, Allemagne

During the post doctorate of Dr. A. Girod we helped in defining the insertion sites of peptides into viral capsid in order to modify the tropism of adeno-associated virus (P22). The approach consisted in the insertion of a 14 mer peptide in the external (and exposed) regions of the capsid protein. Our work was to predict the best insertion sites so as to keep the structure integrity as well as its capacity to form virions. Thus we proposed 6 insertion sites and experiments will show that one of these sites make the virus able to bind to cell exhibiting specific receptor of the 14 mer peptide. (P41, P42).

**This work was the first demonstration that we are now able to target chimeric virus to new cell types.**

This innovative work has been published in Nature Medicine (P41) and leads to a patent deposited by Medigene company.

### III.5.8. COLLABORATION WITH DR JOLIVET GROUP

Laboratoire mixte UMR 103 CNRS-bioMérieux  
46, allée d'Italie, 69364 Lyon cedex

In the study of specific glycoprotein from prostate (Hk3) antigen with antibodies we have been able to

locate by molecular modeling technique the conformational epitopes of "phage display" experiments. The localisation of epitopes close to the catalytic sites of the protease explains the loss of activity and the competition with natural proteic inhibitor (P38). Moreover, an antibody against antipeptide PSA is able to recognise the whole protein even after fixation of the antibody to plastic support (P48, P53, P71). Another collaboration was performed on the epitope characterisation of NS3 protein from hepatitis C virus (P63).

### III.5.9. COLLABORATION WITH PR GALLINARI GROUP

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A combination of methods to predict the secondary structure of proteins was established by estimating *a posteriori* probabilities of isolated methods. This combination used a neural network and a multivariate linear regression. It was shown that the combination of methods always improved the prediction accuracy even with methods of different level of quality (P39). This method was implemented into the NPS@ web server.

### III.5.10. COLLABORATION WITH PR GILLET GROUP

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A molecular model of Nr13 protein (expressed in *Coturnix japonica*) which is involved into protection against cellular death (apoptosis) was built in our team by M. Jambon. The main difference in Nr13 protein is the absence of a long loop which is present into other homologous proteins and which connects BH3 to BH4 domain. This modeling study was performed in order to see if a BH4 domain may exist in Nr13 protein. The model shows:

1. The possibility of a BH4 domain in Nr13 protein since the connection between BH3 and BH4 domains is possible in spite of the very short loop.
2. The probable existence of 2 salt bridges. Mutations experiments (single or double mutations) confirmed the existence of salt bridges (P56).

### III.5.11. COLLABORATION WITH PR PAWLOTSKY GROUP

Hôpital Henri Mondor, Université Paris 12 Créteil, Paris

The study of hypervariable regions of envelope E2 glycoprotein (HVR1) shows a good conservation of physico-chemical properties in spite of highly variable sequences (P51).

### III.5.12. COLLABORATIONS WITH DR POCH GROUP

IGBMC, Illkirch

The collaboration with O. Poch's group consisted in the interface of our Geno3D modeling tool with PipeAlign (developped at IGBMC). This lead to MAGOS (P74) program: a modeling server on the Web with geno3D coupled with sequence facilities (MACSIMS). Moreover, another application for exploiting BLAST results has been developped (P80). This collaboration was supported by AFM grant for PHD N. Garnier work. Finally, an information system called MS2PH-DB coupling sequence data, multiple alignment and 3D models was developped.

### III.6. BIBLIOGRAPHY

- Chen, Y.H., Yang, J.T. & Chau, K.H., Determination of the helix and a form of proteins in aqueous solution by circular dichroism. *Biochemistry*, 1974, **13**, 3350-3359
- Chou, P.Y. & Fasman, G.D., Prediction of secondary structure of proteins from amino acid sequence, *Adv. Enzymol. Relat. Subj. Biochem.*, 1978, **47**, 45-148.
- Cortay, J.C., Bleicher, F., Duclos, B., Cenatiempo, Y., Gauthier, C., Prato, J.L. & Cozzone, A.J., Utilization of acetate in *Escherichia coli*: structural organization and differential expression of the ace operon., *Biochimie*, 1989, **71**, 1043-1049
- Cortay, J.C., Nègre, D., Scarabel, M., Ramseier, T.M., Vartak, N.B., Reizer, J., Saier, M.H. & Cozzone, A.J., Regulation of the acetate operon : overproduction, purification and characterization of the FruR protein. *J. Biol. Chem.*, **269**, 14885-14891
- Delisi, C., Computers in molecular biology : current applications and emerging trends, *Science*, 1988, **240**, 47-52
- Feng, D. F. & Doolittle, R. F., Progressive Alignment and Phylogenetic Tree Construction of Protein Sequences, *in Methods in Enzymology*, 1990, **183**, 375-387
- Garnier, J. Osguthorpe, D.J. & Robson, B. Analysis of the accuracy and implications of simple methods for predicting the secondary structure of globular proteins, *J. Mol. Biol.*, 1978, **120**, 97-120
- Gibrat, J. F., Garnier, J. & Robson, B. Further developments of protein secondary structure prediction using information theory, *J. Mol. Biol.*, 1987, **198**, 425-443
- Higgins, D.G. & Sharp, P.M., Clustal: a package for performing multiple sequence alignment on a microcomputer. *Gene*, 1988, **73**, 237-244
- Kabsch, W. & Sander, C., Dictionnary of Protein Secondary Structure : Pattern Recognition of Hydrogen-Bonded and Geometrical Features, *Biopolymers*, 1983, **22**, 2577-2637
- Levin, J.M., Robson, B. & Garnier, J., An algorithm for secondary structure determination in proteins based on sequence similarity, *FEBS Lett.*, 1986, **205**, 303-308
- Matthews, B.W., Comparison of the predicted and observed secondary structure of T4 phage lysozyme., *Biochim. biophys. Acta.*, 1975, **405**, 442-451
- Pearson, W.R. & Lipman, D.J., Improved tools for biological sensitive sequence comparison, *Proc. Natl. Acad. Sci.*, 1988, **85**, 2444-2448
- Provencher, S.W. & Glöckner, J., Estimation of globular protein secondary structure from circular dichroism. *Biochemistry*, 1981, **20**, 33-37
- Scarabel, M., Penin F., Bonod, C., Nègre, D., Cozzone, A.J. & Cortay, J.C., 1994, Overproduction, purification and structural characterization of the functional N-terminal DNA-binding domain of the FruR protein from *Escherichia coli* K-12 *Gene*, 1995, **153**, 9-15
- Xu X.Q., Leow C.K., Lu X., Zhang X., Liu J.S., Wong W.H., Asperger A., Deininger S., Eastwood Leung H.C. (2004) Molecular classification of liver cirrhosis in a rat model by proteomics and bioinformatics, *Proteomics*, 4, 3235-3245.

## IV. SCIENTIFIC RECORDS

### IV.1. THESES & HDR

- T1. University thesis  
Study of Proton fluxes catalyzed by the ATPase-ATP synthase complex either integrated or isolated from internal membrane of pig heart mitochondria.  
Lyon, July 1984
- T2. PHD  
Methods to predict protein secondary structures. Application to a model: the mitochondrial ATPase-F1. Studies of electrical and optical properties of F1-ATPase.  
Lyon, July 1988
- H1. Habilitation à diriger des recherches HDR. Lyon, July 1993

### IV.2. PEER REVIEW PUBLICATIONS

- P1. Correlations between ATP hydrolysis, ATP synthesis, generation and utilization of  $\Delta$ pH in mitochondrial ATPase-ATP synthase.  
Deléage G, Penin F, Godinot C & DC. Gautheron  
**Biochim. Biophys. Acta** (1983) 725, 464-471. [[PubMed](#)] [IF = 4.431]
- P2. Preparation of a highly coupled H<sup>+</sup>-ATP synthetase from pig heart mitochondria  
Gautheron DC, Penin F, Deléage G & C. Godinot  
**Methods Enzymol.** (1986) 126, 417-427. [[PubMed](#)] [IF = 1.618]
- P3. Structural aspects and orientation mechanism of mitochondrial F1-ATPase. Evidence for a negative electric birefringence due to a permanent moment perpendicular to the long axes of the particle.  
Deléage G, Roux B & C. Marion  
**Biochemistry** (1986) 25, 2854-2858. [[PubMed](#)] [IF = 3.922]
- P4. Efficient reconstitution of mitochondrial energy transfer reactions from depleted membranes and F1-ATPase as a function of the amount of bound oligomycin sensitivity conferring protein (OSCP)  
Penin F, Deléage G, Godinot C & DC. Gautheron  
**Biochim. Biophys. Acta** (1986) 852, 55-67. [[PubMed](#)] [IF = 4.431]
- P5. Amino acid sequence and putative conformational characteristics of the 25 kDa silk protein of *Bombyx Mori*.  
Chevallard M, Deléage G & P. Couble  
**Sericologia** (1986) 26, 435-449
- P6. A computerized version of the CHOU and FASMAN method for predicting the secondary structure of proteins.  
Deléage G, Tinland B & B. Roux  
**Anal. Biochem.** (1987) 163, 292-297. [[PubMed](#)] [IF = 2.174]
- P7. An algorithm for protein secondary structure prediction based on class prediction.  
Deléage G & B. Roux  
**Protein Engineering** (1987) 1, 289-294. [[PubMed](#)] [IF = 2.065]
- P8. ANTHEPROT : A package for protein sequence analysis using a microcomputer.  
Deléage G, Clerc FF, Roux B & DC Gautheron  
**Comp. Appl. Biosc.** (1988) 4, 351-356. [[PubMed](#)] [IF=6,701]
- P9. ANTHEPROT : IBM PC and Apple Macintosh versions.  
Deléage G, Clerc FF & B. Roux

- Comp. Appl. Biosc.** (1989) 5, 159-160. [[PubMed](#)] [IF=6,701]
- P10. Characterization of an OSCP epitope (Oligomycin sensitivity conferring protein) exposed at the surface of the mitochondrial ATPase-ATP synthase complex.  
Godinot C, Colorio S, Cretin F, Incauragarat B, Deléage G & B. Roux  
**Biochimie** (1989) 71, 917-929. [[PubMed](#)] [IF = 3.707]
- P11. Duck hepatitis B virus can tolerate insertion, deletion and partial frameshift mutation in the distal Pre S region.  
Li JS, Cova L, Buckland R, Lambert V, Deléage G & C. Trepo  
**J. Virol.** (1989) 63, 4965-4968. [[PubMed](#)] [IF = 5.225]
- P12. Mapping of a conserved neutralizing epitope on the duck hepatitis B virus pre-S protein.  
Lambert V, Fernholz D, Sprengel R, Fourel I, Deléage G, Wildner G, Peyret C, Trepo C, Cova L & H. Will  
**J. Virol.** (1989) 64, 1290-1297. [[PubMed](#)] [IF = 5.225]
- P13. Interaction between  $\alpha$  and  $\beta$  subunits of F1-ATPase from pig heart mitochondria. Circular dichroism and intrinsic fluorescence of purified or reconstituted  $\alpha\beta$  complex.  
Penin F, Deléage G, Gagliardi D, Roux B & DC. Gautheron  
**Biochemistry** (1990) 29, 9358-9364. [[PubMed](#)] [IF = 3.922]
- P14. Do synapsin I and Microtubule-associated proteins bind to a common site on polymerized tubulin?  
Aubert-Foucher E, Deléage G & B. Font  
**Biochem. Int.** (1990) 22, 821-827 [[PubMed](#)]
- P15. Intrinsic Tryptophan fluorescence of *Schizosaccharomyces pombe* mitochondrial F1-ATPase. A powerful probe for phosphate and nucleotide interactions.  
Divita G, Di Pietro A, Deléage G, Roux B & DC. Gautheron  
**Biochemistry** (1991) 30, 3256-3262 [[PubMed](#)] [IF = 3.922]
- P16. ANTHEPROT: An interactive graphic software for analyzing protein structures from sequences.  
Geourjon C, Deléage G & B. Roux  
**J. Mol. Graph.** (1991) 9, 188-190 [[PubMed](#)] [IF = 2.929]
- P17. Interactive and graphic coupling between multiple alignments, secondary structure predictions and motif/pattern scanning into proteins.  
Geourjon C & G. Deléage  
**Comp. Appl. Biosc.** (1993) 9, 87-91 [[PubMed](#)] [IF=6,701]
- P18. An interactive graphic program for calculating the secondary structures content of proteins from circular dichroism spectrum.  
Deléage G & C. Geourjon  
**Comp. Appl. Biosc.** (1993) 9, 197-199 [[PubMed](#)] [IF=6,701]
- P19. *FVT-1*, A novel human transcription unit affected by variant translocation t(2;18)(p11;q21) of follicular lymphoma.  
Rimokh R, Gadoux M, Bertheas MF, Berger F, Garoscio M, Deléage G, Germain D & JP. Magaud  
**Blood** (1993) 81, 136-142 [[PubMed](#)] [IF = 10.12]
- P20. SOPM: a self-optimised method for protein secondary structure prediction.  
Geourjon C & G. Deléage  
**Protein Engineering** (1994) 7, 157-164 [[PubMed](#)] [IF = 2.065]
- P21. Common topology within N-terminal domains of collagens.  
Moradi-Ameli M, Deléage G, Geourjon C & M. van der Rest  
**Matrix Biology** (1994) 14, 233-239. [[PubMed](#)]
- P22. Modifications in the binding domain of avian retrovirus envelope protein to redirect the host range of retroviral vectors.

- Valsesia-Wittmann S, Drynda A, Deléage G, Aumailley M, Heard JM, Danos O, Verdier G & FL.Cosset  
**J. Virol.** (1994) 68, 4609-4619. [[PubMed](#)] [IF = 5.225]
- P23. Cloning and sequence analysis of a polygalacturonase-encoding gene from the phytopathogenic fungus *Sclerotinia sclerotiorum*.  
 Reymond P, Deléage G, Rascle C & M. Fevre  
**Gene** (1994) 146, 233-237. [[PubMed](#)] [IF = 2.754]
- P24. Dimerization kinetics of HIV-1 and HIV-2 reverse transcriptase. A two step process.  
 Divita G, Rittinger K, Geourjon C, Deléage G & RS. Goody  
**J. Mol. Biol.** (1995) 245, 508-521. [[PubMed](#)] [IF = 5.239]
- P25. ANTHEPROT : A 3D module coupled to protein sequence analysis methods.  
 Geourjon C & G. Deléage  
**J. Mol. Graph** (1995) 13, 209-212. [[PubMed](#)] [IF = 2.929]
- P26. SOPMA: Significant improvement in protein secondary structure prediction by consensus prediction from multiple alignments.  
 Geourjon C & G. Deléage  
**Comp. Appl. Biosc.** (1995) 11, 681-684. [[PubMed](#)] [IF=6,701]
- P27. Surf, the four-cysteine motif of the amino-terminal propeptide of a sea urchin fibrillar collagen, is encoded by several genes  
 Exposito JY, Boute N, Deléage G & R. Garrone  
**Eur. J. Biochem.** (1995) 234, 59-65. [[PubMed](#)] [IF = 3.001]
- P28. ANTHEPROT : A software to display and analyze 3D NMR structures.  
 Deléage G & C. Geourjon  
**J. Trace and Microprobe Techniques**, (1995) 13, 337-338.
- P29. Recombinant N-terminal nucleotide-binding domain from mouse P-glycoprotein: overexpression, purification and role of cysteine -430.  
 Dayan G, Baubichon-Cortay H, Jault JM, Cortay JC, Deléage G & Di Pietro A.  
**J. Biol. Chem.** (1996) 271, 11652-11658. [[PubMed](#)] [IF = 6.482]
- P30. Isolation and characterization of Urbain, a 20-hydroxyecdysone-inducible gene expressed during morphogenesis of *Bombyx Mori* wing imaginal discs.  
 Besson MT, Chareyre P, Deléage G, Demont J, Quennedey B, Courent A, Fourche J & G. Bosquet  
**Roux's Arch. Dev. Biol.** (1996) 205, 333-343.
- P31. Definition of a consensus DNA-binding site for the *E.Coli* pleiotropic regulatory protein, FruR  
 Negre D, Bonod-Bidaud C, Geourjon C, Deléage G, Cozzzone AJ, Cortay JC.  
**Molecular Microbiology** (1996) 21, 257-266. [[PubMed](#)] [IF = 5.563]
- P32. Structure and organization of the *Bombyx Mori* sericin 1 gene and of the four sericins 1 deduced from the sequence of the SER 1B cDNA.  
 Garel A, Deléage G & JC. Prudhomme  
**Insect Biochem. Molec. Biol.** (1997) 27, 469-477. [[PubMed](#)]
- P33. Determination of the tertiary structure of DNA binding domain from *E. coli* FruR protein by NMR.  
 Penin F, Geourjon C, Montserret R, Bockmann A, Lesage A, Yang YS, Bonod-Bidaud C, Cortay JC, Negre D, Cozzzone AJ and G. Deléage  
**J. Mol. Biol.** (1997) 270, 496-510. [[PubMed](#)] [IF = 5.239]
- P34. Protein structure prediction. Implications for the biologist.  
 Deléage G, Blanchet C & C.Geourjon  
**Biochimie** (1997) 79, 681-686. [[PubMed](#)] [IF = 3.707]
- P35. Characterization of a bacterial gene encoding an autophosphorylating protein tyrosine kinase.  
 Grangeasse C, Doublet P, Vaganay E, Vincent C, Deléage G, Duclos B & AJ.Cozzzone

- Gene** (1997) 204, 259-265. [[PubMed](#)] [IF = 2.754]
- P36. Identification and characterization of a heparin binding site within the NC1 domain of chicken collagen XIV.  
Giry-Lozinguet C, Aubert-Foucher E, Penin F, **Deléage G**, Dublet B & M. van der Rest  
**Matrix Biology** (1998) 17, 145-149. [[PubMed](#)] [IF = 3.323]
- P37. Structure of P-Glycoprotein analyzed by circular dichroism and prediction from its sequence.  
Dong M, Ladaviere L, Penin F, **Deléage G** & LG. Baggetto  
**Biochim. Biophys. Acta** (1998) 1371, 317-334. [[PubMed](#)] [IF = 4.431]
- P38. Anti-free Prostate Specific Antigen monoclonal antibody epitopes defined by mimotopes and molecular modeling.  
Michel S, **Deléage G**, Charrier JP, Passagot J, Battail-Poirot N, Sibai G, Jolivet M & C.Jolivet-Reynaud  
**Clinical Chemistry** (1999) 45, 638 - 650. [[PubMed](#)] [IF = 5.538]
- P39. Improved Performance in Protein Secondary Structure Prediction by Inhomogeneous Score Combination  
Guermeur Y, Geourjon C, Gallinari P & **G. Deléage**  
**Bioinformatics** (1999) 15, 413-421. [[PubMed](#)] [IF=6,701] 
- P40. Structural Analysis of the Heparin-Binding site of the NC1 domain of Collagen XIV by CD and NMR  
Montserret R, Aubert-Foucher E, McLeish MJ, Hill JM, Ficheux D, Jaquinod M, van der Rest M, **Deléage G** & F.Penin  
**Biochemistry** (1999) 20, 6479-6488. [[PubMed](#)] [IF = 3.922]
- P41. Efficient Retargeting of Adeno-Associated Virus Type 2 (AAV2) by Genetic Modifications of the VP3 Viral Capsid Protein  
Girod A, Ried M, Wobus C, Lahm H, Leike K, Kleinschmidt J, **Deléage G** & M.Hallek  
**Nature Medicine** (1999) 5, 1052 - 1056. [[PubMed](#)] [IF = 30.55]
- P42. Efficient Retargeting of Adeno-Associated Virus Type 2 (AAV2) by Genetic Modifications of the VP3 Viral Capsid Protein  
Girod A, Ried M, Wobus C, Lahm H, Leike K, Kleinschmidt J, **Deléage G** & M.Hallek  
**Nature Medicine** (1999) 5, 1438. [[PubMed](#)] [IF = 30.55]
- P43. NPS@ : Network Protein Sequence Analysis  
Combet C, Blanchet C, Geourjon C & **G Deléage**  
**TIBS** (2000) 25, 147-150. [[PubMed](#)] [IF = 14.273] 
- P44. MPSA: integrated system for protein sequence analysis  
Blanchet C, Combet C, Geourjon C & **G. Deléage**  
**Bioinformatics** (2000) 16, 286-287. [[PubMed](#)] [IF=6,701]
- P45. Evidence for distinct complement regulatory and measles virus binding sites on CD46 SCR2.  
Christiansen D, **Deléage G** & D. Gerlier  
**Eur. J. Immunol.**, (2000), 12, 3457-3462. [[PubMed](#)] [IF = 4.536]
- P46. *AF15q14*, a novel partner gene fused to the *MLL* gene in an acute myeloid leukaemia with a t(11;15)(q23;q14)  
Hayette S, Tigaud I, Vanier A, Martel S, Corbo L, Charrin C, Beillard E, **Deléage G**, Magaud JP & R Rimokh  
**Oncogene** (2000) 19, 4446-4450. [[PubMed](#)] [IF = 6.495]
- P47. [Protéines en 3D.](#)  
**Deléage G.** & Geourjon C. (2000) *Biofutur*, 206, 66-71
- P48. Analysis of Prostate Specific Antigen and alpha 1 chymotrypsin Interaction by Using Anti Peptide Monoclonal Antibodies.  
Michel S, Charrier JP, **Deléage G**, Lacoux X, Battail-Poirot N, Sibai G, Jolivet M & Jolivet-Reynaud C





- J Urol.** (2001) 165, 301-306. [[PubMed](#)]
- P49. ANTHEPROT : An integrated protein sequence analysis software with client/server capabilities  
Deléage, G., Combet, C., Blanchet, C. & Geourjon, C.  
**Comput. Bio. Med.** (2001) 31, 259-267. [[PubMed](#)]
- P50. Identification of related proteins with weak sequence identity using secondary structure information.  
Geourjon C, Combet C, Blanchet C & G. Deléage  
**Protein Science** (2001) 10, 788-797. [[PubMed](#)] [IF = 3.787]
- P51. Conservation of the conformation and positive charges of hepatitis C virus E2 envelope glycoprotein hypervariable region 1 (HVR1). Points to a role in cell attachment.  
Penin F, Combet C., Germanidis G, Frainais PO, Deléage G. & J.M. Pawlotsky  
**J. Virology**, (2001) 12, 5703-5710. [[PubMed](#)] [IF = 5.225]
- P52. A common mechanism for transducing energy in ABC transporters and helicase super-families.  
Geourjon C, Orelle C, Steinfels E, Blanchet C, Deléage G, di Pietro A & J.M. Jault  
**TIBS**, (2001) 26, 539-544. [[PubMed](#)] [IF = 14.273]
- P53. Involvement of the Prostate-specific antigen C-terminal end in a conformational epitope : characterization by proteolytic degradation of monoclonal antibody-bound antigen and mass spectrometry.  
Michel, S, Forest E, Petillot Y, Deléage G, Heuze N, Courty Y, Gervasi G, Jolivet M & C. Jolivet-Reynaud  
**J. Mol. Recognition** (2001) 14, 406-413. [[PubMed](#)]
- P54. Geno3D: Automatic comparative molecular modelling of protein  
Combet C., Jambon M., Deléage G. & C. Geourjon  
**Bioinformatics** (2002) 18, 213-214. [[PubMed](#)] [IF=5.09] 
- P55. HCVDB : Base de données de séquences du virus de l'hépatite C et outils bioinformatiques d'analyse  
Combet C., Penin F., Geourjon C. & G. Deléage  
**Medecine/Sciences** (2002) 5, 639.
- P56. Molecular modeling of the anti-apoptotic NR-13 protein: evidence for crucial electrostatic interactions between Bcl-2 homology domains BH3 and BH4  
Lalle P., Aouacheria A., Dumont-Miscopein A., Jambon M., Venet S., Bobichon H., Colas P., Deléage G., Geourjon C. & G. Gillet  
**Biochemical Journal**, (2002) 368, 213-221. [[PubMed](#)] [IF = 4.101]
- P57. Detection of unrelated proteins in multiple sequence alignments using predicted secondary structures.  
Errami M., Geourjon C. & G. Deléage  
**Bioinformatics** (2003) 19, 506-512. [[PubMed](#)] [IF=5.09]
- P58. A new bioinformatic approach to detect common 3D sites in protein structures  
Jambon M., Imbert A., Deléage G. & C. Geourjon  
**Proteins** (2003) 52, 137-145. [[PubMed](#)] [IF = 4.313]
- P59. Procollagen C-Proteinase Enhancer, a CUB and NTR Domain-Containing Glycoprotein, has a Rod-like Structure  
Bernocco S, Steiglitz BM, Svergun D, Ruggiero F, Ricard-Blum S, Ebel C, Geourjon C, Deléage G, Font B, Eichenberger D, Greenspan DS & D.J.S. Hulmes  
**J.Biol. Chem.** (2003) 278, 7199-205. [[PubMed](#)] [IF = 6.482]
- P60. Conservation of amino acids into multiple alignments involved in pairwise interactions in three-dimensional protein structures  
Errami M, Geourjon C & G. Deléage  
**J. Bioinform Comput Biol** (2003)1, 505-520. [[PubMed](#)]
- P61. Integrated databanks access and sequence/structure analysis services at the PBIL  
Perrière G, Combet C, Penel S, Blanchet C, Thioulouse J, Geourjon C, Grassot J, Charavay C, Gouy M, Duret L & G.Deléage

- Nucl. Acids Res.** (2003) *31*, 3393-3399. [[PubMed](#)] [IF=6,575]
- P62.** Identification of antigenic regions of duck hepatitis B virus core protein with antibodies elicited by DNA immunization and chronic infection  
Thermet A, Robaczewska M, Rollier C, Hantz O, Trepo C, **Deléage G** & L.Cova  
**J. Virology** (2004) *78*, 1945-1953. [[PubMed](#)] [IF = 5.225]
- P63.** Characterization of mimotopes mimicking an immunodominant conformational epitope on the hepatitis C virus NS3 helicase  
Jolivet-Reynaud C, Adida A, Michel S, **Deléage G**, Parahnos-Baccala G, Gonin V, Battail-Poirot N, Lacoux X & D. Rolland  
**J. Med. Virol.** (2004) *72*, 385-395. [[PubMed](#)] [IF = 2.371]
- P64.** HCVDB: Hepatitis C Virus sequences DataBase.  
Combet C, Penin F, Geourjon C & **G. Deléage**  
**Applied Bioinformatics** (2004) *3*, 237-240 [[PubMed](#)]
- P65.** GENEFARM, structural and functional annotation of Arabidopsis gene and protein families by a network of experts.  
Aubourg S, Brunaud V, Bruyère C, Cock M, Cooke R, Cottet A, Couloux A, Déhais P, **Deléage G**, Duclert A, Echeverria M, Eschbach A, Falconet D, Filippi G, Gaspin C, Geourjon C, Grienberger JM, Houlné G, Jamet E, Lechauve F, Leleu O, Leroy P, Mache R, Meyer C, Nedjari H, Negrutiu I, Orsini V, Peyretailade E, Pommier C, Raes J, Risler JL, Rivière S, Rombauts S, Rouzé P, Schneider M, Schwob P, Small I, Soumayet-Kampetenga G, Stankovski D, Toffano C, Tognolli M, Caboche M & A. Lecharny.  
**Nucl. Acids Res.** (2005) *33*, 641-646. [[PubMed](#)] [IF=7,552]
- P66.** Consensus proposals for the nomenclature of HCV genetic variants: creation of unified system for name assignment and database access.  
Simmonds P, Bukh J, Combet C, **Deléage G**, Enomoto N, Feinstone S, Halfon P, Inchauspe G, Kuiken C, Mizokami M, Murphy D, Okamoto H, Penin, F., Pawlowsky JM, Thiel HJ, Sablon E, Stuyver L, Viazov S, Weiner A, Widell A  
**Hepatology** (2005) *42*, 962-73 [[PubMed](#)] [IF =10.416] 
- P67.** The SuMo server: 3D search for functional sites.  
Jambon M, Andrieu, O, Combet C, **Deléage, G**, Delfaud F & C. Geourjon  
**Bioinformatics** (2005) *21*, 3929-3930 [[PubMed](#)] [IF=5.09]
- P68.** Selective Recognition of Enzymatically Active Prostate-specific Antigen (PSA) by anti-PSA Monoclonal Antibodies.  
Michel S, Collomb-Clerc E, Geourjon C, Charrier J-P, Passagot J, Courty Y, **Deléage G** & C. Jolivet-Reynaud  
**J. Mol. Recognition.** (2005) *18*, 225-235 [[PubMed](#)] [IF =IF =3,712]
- P69.** NMR Structure and Molecular Dynamics of the In-plane Membrane Anchor Domain of Nonstructural Protein 5A from Bovine Viral Diarrhea Virus.  
Sapay N, Montserret R, Chipot C, Brass V, Moradpour D, **Deléage G** & F. Penin  
**Biochemistry** (2006) *45*, 2221-2233 [[PubMed](#)] [IF = 3.922]
- P70.** Hepatitis C databases, principles and utility to researchers.  
Kuiken C, **Deléage G**, Yusim K, Penin F, Charavay C, Tao N, Crisan D, Grando D, Dalwani A, Geourjon C, Agrawal A & C. Combet  
**Hepatology** (2006) *43*, 1157-1165 [[PubMed](#)] [IF =9,792]
- P71.** Characterization of prostate-specific antigen binding peptides selected by phage display technology  
Ferrieu-Weisbuch, C., Michel, S., Collomb-Clerc, E., Pothion, C., **Deléage, G.** and Jolivet-Reynaud, C.  
**J Mol Recognit** (2006) *19*, 10-20 [[PubMed](#)] [IF =3,712]
- P72.** Prediction of amphipathic in-plane membrane anchors in monotopic proteins using a SVM classifier.  
Sapay, N. Guermeur, Y. & **Deléage, G.**  
**BMC Bioinformatics** (2006) *7*, 255 [[PubMed](#)] [IF=5,42]

- P73.** A comprehensive system for consistent numbering of HCV sequences, proteins and epitopes  
Kuiken C, Combet C, Bukh J, **Deléage, G**, Mizokami M, Richardson R, Sablon E, Yusim K, Pawlowsky JM, Simmonds P, and the Los Alamos HIV database group.  
**Hepatology** (2006) 44, 1355-1361 [[PubMed](#)] [IF = 9,792]
- P74.** MAGOS: Multiple AliGnement and mOdelling Server  
Garnier, N., Friedrich, A, Bolze, R., Bettler, E., Geourjon, C. Thompson, JD, **Deléage, G.** and Poch, O.  
**Bioinformatics** (2006) 22, 2164-2165 [[PubMed](#)] [IF=5,019]
- P75.** GPS@ Bioinformatics Portal: from Network to EGEE Grid  
Blanchet, C., Lefort, V., Combet, C. & **Deléage, G.**  
**Stud Health Technol Inform** (2006) 120 : 187-193 [[PubMed](#)]
- P76** Secured Distributed Service to manage Biological Data on EGEE grid  
Blanchet, C., Mollon, R. & **Deléage, G.**  
**Stud Health Technol Inform** (2006) 120 : 142-152 [[PubMed](#)]
- P77** Insights into Early Extracellular Matrix Evolution: Spongin Short Chain Collagen-related Proteins are Homologous to Basement Membrane Type IV Collagens and Form a Novel Family Widely Distributed in Invertebrates  
Aouacheria, A, Geourjon, C, Aghajari, N, Navratil, V, **Deléage, G**, Lethias, C & Exposito, JY  
**Mol Biol Evol** (2006) 23, 2288-2302 [[PubMed](#)] [IF=6.355]
- P78.** euHCVdb: The European Hepatitis C Virus database  
Combet C, Garnier N, Charavay C, Grando D, Crisan D, Lopez J, Dehne-Garcia A, Geourjon C, Bettler E, Hulo C, Le Mercier P, Bartenschlager R, Diepolder H, Moradpour D, Pawlowsky JM, Rice C, Trépo C, Penin F, **Deléage G**  
**Nucl. Acids Res.** (2007) 35, 363-366 [[PubMed](#)] [IF=7.552]
- P79.** Conserved Determinants for Membrane Association of Nonstructural Protein 5A from Hepatitis C Virus and Related Viruses  
Brass, V, Pal, S, Sapay, N., **Deléage G**, Blum, HE, Penin F. & Moradpour, D.  
**J. Virol** (2007) 81, 2745-57 [[PubMed](#)] [IF = 5.178]
- P80.** Blast sampling for structural and functional analyses  
Friedrich A, Ripp R, Garnier N, Bettler E, **Deléage G**, Poch O & Moulinier, L  
**BMC Bioinformatics** (2007) 8, 62 [[PubMed](#)] [IF=4.96]
- P81.** HNRNP A2/B1 as antinuclear antibodies target: Epitope mapping and differential reactivity in autoimmune hepatitis and connective tissue diseases.  
Huguet S, Combet C, Ballot E, Johanet C, **Deléage G**, Samuel D, Duclos-Vallee JC  
**Journal of Hepatology** (2008) 48, S323
- P82.** MSX-3D : A tool to validate 3D protein models using mass spectrometry  
Heymann, M, Paramelle D, Subra G, Forest E, Martinez J, Geourjon C & **G Deléage**  
**Bioinformatics** (2008) 24 2782-2783 [[PubMed](#)] [IF=5.019]
- P83.** Identification of the wzc/cpsd/etk/ptk bacterial protein-tyrosin kinases  
Jadeau F, Béchet E, Cozzone AJ, **Deléage G**, Grangeasse C & C Combet  
**Bioinformatics** (2008) 24, 2427-2430 [[PubMed](#)] [IF=5.019]
- P84.** Mutation in the melanocortin 1 receptor (MC1-R) is associated with amber colour in the Norwegian Forest Cat (NFC)  
M. Peterschmitt, F. Grain, B. Arnaud, **G. Deléage** & V. Lambert  
**Animal genetics** (2009) 40, 547-552 [[PubMed](#)] [IF=2.64]
- P85.** PDB\_REDO: automated re-refinement of X-ray structure models in the PDB  
Joosten RP, Salzemann J, Blanchet C, Bloch V, Breton V, Da Costa AL, **Deléage G**, Dairena M, Fabretti R, Fettahi G, Flegel V, Kasam V, Pagni M, Reichstadt M, Sonnahammer ACB, Sockinger H, Vriend G

- J Applied Crystallography** (2009) 42, 376–384 [[PubMed](#)] [IF=3.629]
- P86. The euHCVdb suite of *in silico* tools for investigating the structural impact of mutations in Hepatitis C virus protein.  
Combet C, Bettler E, Terreux R, Garnier N & G. Deléage  
**Infectious Disorders Drug Targets** (2009) 9, 272-278 [[PubMed](#)]
- P87. SM2PH-db: an interactive system for the integrated analysis of phenotypical consequences of missense variations in proteins involved in human monogenic diseases.  
Friedrich A, Garnier G, Nguyen H, Albou LP, Bettler E, Deléage G, Moras D, Toursel T, Moulinier L & Poch O  
**Human Mutation** (2010) 31,127-135.[[PubMed](#)] [IF=7.033]
- P88. ViralORFeome: an integrated database to generate a versatile collection of viral ORFs  
Pellet J, Tafforeau, L, Lucas Hourani M, Navratil V, Meyniel L, Achaz G, Guironnet-Paquet, A, Aublin-Gex A, Caignard G, Cassonnet P, Chaboud A, Chantier T, Deloire A, Demeret C, LeBreton M, Neveu G, Jacotot L, Vaglio P, Delmotte S, Gautier C, Combet C, Deléage G, Favre M, Tanguy F, Jacob Y, André P, Lotteau V, Rabourdin-Combe C & Vidalain PO  
**Nucl. Acids Res.** (2010) 38, 371-378 [[PubMed](#)] [IF=7.552]
- P89. New applications of SUMO software for drug design  
Chemelle JA, Bettler E, Deléage G, Terreux R  
**Abstracts of Papers of the American Chemical Society** (2011), 242, 664
- P90. ByKdb: The Bacterial protein tyrosine Kinase database  
Jadeau F, Grangeasse C, Shi L, Mijakovic I, Deléage G & Combet C  
**Nucl. Acids Res.** (2012) 40, 321-324 [[PubMed](#)] [IF=8.026]
- P91. ❖ An interactive 3D viewer of molecules compatible with the suite of ANTHEPROT programs.  
G. Deléage  
**Journal of Biophysical Chemistry** (2012) 3, 35-38 [[Lien](#)]
- P92. HBVdb : a knowledge database for Hepatitis B Virus.  
J Hayer, F Jadeau, G Deléage, A Kay, F Zoulim & C Combet  
**Nucl. Acids Res** (2013) 41, 366-370 [[PubMed](#)] [IF=8.026]
- P93. Ultra-deep pyrosequencing and molecular modeling identify key structural features of hepatitis B virus RNase H, a putative target for antiviral intervention.  
Hayer J, Rodriguez C, Germanidis G, Deléage G, Zoulim F, Pawlotsky JM & Combet C  
**J. Virol.** (2014) 88, 574-582 [[PubMed](#)][IF=5.402]
- P94. BCL2DB: database of BCL-2 family members and BH3-only proteins.  
Rech de Laval V, Deléage G, Aouacheria A & Combet C  
**Database** (2014) bau013 [[PubMed](#)][IF=4.20]
- P95. Thyroglobulin Represents a Novel Molecular Architecture Designed for Vertebrates.  
Holzer G, Morishita Y, Fini JB, Lorin T, Gillet B, Hughes S, Tohme M, Deléage G, Demeneix B, Arvan P & Laudet V (2016). **J. Biol Chem.**[[PubMed](#)] [IF=4.4573]
- P96. ALIGNSEC: viewing protein secondary structure prediction within large multiple sequence alignment.  
Deléage G (2017). **Bioinformatics** [[PubMed](#)] [IF=7.27]

Publication list on the web : <https://www.gdeleage.fr/prof/publis.php>

-  Highly cited papers in the field (source ISI)
-  Publication cover

### IV.3. BOOKS CHAPTERS AND REVUES

- L 1. Proton translocation coupled to ATP synthesis and ATP hydrolysis in the mitochondrial ATPase-ATPsynthase.  
Godinot C, **Deléage G**, Penin F, Archinard P. & Gautheron D.C.  
in " H<sup>+</sup>-ATPase (ATPsynthase) : Structure, Function, Biogenesis of the Fo F1 complex of coupling membranes" (1984) (S. Papa, K. Altendorf, L. Ernster and L. Packer , Eds) pp. 281-282, ISCU press.
- L 2. Role of some components of the pig heart mitochondrial ATPase-ATPsynthase on proton flux, ATP hydrolysis and ATP synthesis in the reconstituted system.  
Penin F, **Deléage G**. & Godinot C.  
Eur. Bioenerg. Conf, short rep. (1984) 3, 349-350
- L 3. Functional and regulatory aspects of F1-FO ATPsynthase in reconstituted systems  
Gautheron D.C, Di Pietro A., **Deléage G**., Godinot C., Fellous G., Moradi-Améli M. & Penin F.  
Eur. Bioenerg. Conf., short rep. (1984) 3, 99-100
- L 4. Functional role of OSCP in ATPase and ATPsynthase activities.  
Gautheron D.C., Godinot C., **Deléage G**., Archinard P. & Penin F.  
in "Achievements and Perspectives of Mitochondrial Research"(1985) Vol. I , pp. 279-288, Elsevier Science Publishers, Amsterdam.
- L 5. ATP synthesis, proton fluxes and oligomycin-sensitivity in reconstituted mitochondrial FO-F1 complex. Role of OSCP.  
Penin F., Godinot C, **Deléage G**. & Gautheron D.C.  
Eur. Bioenerg. Conf, short rep. (1986) 4, 268
- L 6. Use of class prediction to improve protein secondary structure prediction. Joint prediction with methods based on sequence homology.  
**Deléage G**. & Roux B  
in "Prediction of protein structure and the principles of protein conformation" (1989), Chapitre sur invitation (G.D. Fasman, Ed.) *Chapter 13*, pp. 587-597, Plenum Press.
- L 7. Interaction between  $\delta$  and  $\epsilon$  subunits in  $\delta\epsilon$  complex from pig heart mitochondrial F1-ATPase.  
Penin F, **Deléage G**, Gagliardi D, Roux B & Gautheron D.C.  
Eur. Bioenerg. Conf, short rep. (1990) 6, 60.
- L 8. Intensive sequence comparisons to predict protein secondary structure. Integration into a software package: ANTHEPROT.  
**Deléage G**. & Geourjon C. (1995)  
Hawaiï International Conference on System Computers. IEEE press, 5, 292-301
- L 9. Bioinformatique structurale des protéines ou un enjeu pour l'après génome.  
**Deléage G**. & Geourjon C. (2003) *Revue Janvier 2003 du Palais de la Découverte*
- L 10. Des protéines au bout de la souris.  
**Deléage G** Interview sur la bioinformatique structurale  
**La recherche** 393, (2006) Supplément sur le calcul haute performance, 73-74
- L 11. Web Services Interface to Run Protein Sequence Tools on Grid, Testcase of Protein Sequence Alignment  
Blanchet, C, Combet, C. Daric, V & **Deléage G**  
**Biological and Medical Data Analysis** ISBN 978-3-540-68063-5  
(2006) 4345, 240-249

- L 12. SuMo method: a tool for protein function inference based on 3D structures.  
Chemelle JA, Bettler E, Combet C, Terreux R, Geourjon C & G. Deléage  
**Identification of Ligand binding site and protein-protein interaction area** Roterman-Konieczna, Irena (Ed.), Springer, ISBN 978-94-007-5284-9 (2013) 8, 1-23
- L 13. Bioinformatique des protéines  
G. Deléage & M. Gouy  
Editions Dunod (2013) Collection Sciences sup.  
ISBN 978-2-10-058751-3

#### IV.4. COMMUNICATIONS POSTER OR TALKS (\*) AT MEETINGS

- C1. Comparative studies of proton translocation, ATP hydrolysis, ATP synthesis in the mitochondrial ATPase-ATP synthase complex.  
Deléage G, Penin F & Godinot C  
15<sup>th</sup> FEBS Meeting, (1983) short rep. TU 194 bis, Bruxelles, Belgique.
- C2. The F1-ATPase, isolated or integrated in the ATPase-ATP synthase.  
Gautheron D.C, Di Pietro A, Fellous G, Moradi-Améli M, Archinard P, Deléage G, Penin F & Godinot C  
15<sup>th</sup> FEBS Meeting (1983), conférence sur invitation, Bruxelles, Belgique.
- C3. Electric birefringence of mitochondrial F1-ATPase.  
Deléage G, Marion C, Roux B & Godinot C  
Réunion annuelle de la société française de biophysique (1985) Autrans p7.
- C4. Stoechiométrie, topographie et fonction de l'OSCP dans le complexe ATPase-ATP synthase des mitochondries.  
Penin F, Archinard P, Deléage G, Moradi-Améli M & Godinot C  
Congrès de la société de Chimie Biologique (1985) Besançon
- C5. Etude de l'interaction entre l'ATPase mitochondriale (F1) de coeur de porc et l'inhibiteur protéique naturel (IF1) par biréfringence électrique.  
Deléage G, Penin F, Godinot C & Roux B  
Réunion annuelle de la société française de biophysique. (1986) Otrrott p.26
- C6. The "double prediction method" : An algorithm for improving the accuracy of secondary structure prediction of proteins from class prediction.  
Deléage G & Roux B  
Protein Engineering' 87 Conference. (1987) Oxford, U. K. 1, (3) N°55, p. 240
- C7. Marquage de la tubuline du cerveau de porc à l'aide d'une sonde fluorescente hydrophobe, le N-cyclohexyl N'(4-diméthylaminonaphtyl) carbodiimide (NCD-4).  
Suchère A, Deléage G & Roux B  
14<sup>ème</sup> Forum de la Société de Chimie Biologique, (Villeurbanne) 1-4 Sept. 1987, p.72
- C8.\* Prédiction de la structure secondaire des protéines.  
Deléage G  
14<sup>ème</sup> Forum de la Société de Chimie Biologique, (Villeurbanne) 1-4 Sept. 1987
- C9. Homology in primary and secondary structure between  $\alpha$  and  $\delta$  subunits of mitochondrial F1-ATPase and proteins of known structure.  
Deléage G & Roux B  
14<sup>th</sup> International Congress of Biochemistry (10-15 juillet 1988) Prague, Tchécoslovaquie.
- C10. ANTHEPROT: Un logiciel destiné à l'analyse des séquences de protéine.  
Deléage G, Clerc F.F, Roux B & Gautheron DC

Rencontres Biologie Moléculaire et Informatique (8 et 9 juin 1989) Paris

- C11.** Fluorescence intrinsèque de l'ATPase-F1 mitochondriale de la levure *Schizosaccharomyces pombe*. Modifications en présence de nucléotides.  
Divita G, Di Pietro A, Gautheron DC, Deléage G & Roux B  
Forum des jeunes chercheurs (1989), Sophia-Antipolis.
- C12.** Spectroscopic studies of the interaction between subunits in F1-ATPase from pig heart mitochondria.  
Penin F, Deléage G, Gagliardi D, Roux B & Gautheron DC  
10<sup>th</sup> international congress of Biophysics (1990) Vancouver-Canada
- C13.** Interaction between  $\delta$  and  $\epsilon$  subunits in  $\delta\epsilon$  complex from pig heart mitochondrial F1-ATPase  
Penin F, Deléage G, Gagliardi D, Roux B & Gautheron DC  
6<sup>th</sup> European Bioenergetics Conference, Noordwijkerhout, Hollande, Août 1990.
- C14.** Utilisation des méthodes informatiques pour la recherche de motifs structuraux, signatures de fonctions biologiques dans les protéines.  
Geourjon C, Deléage G & Roux B  
SYNBIO, Techniques Avancées pour les Sciences de la Vie (17-19 Octobre 1990) Lyon-Villeurbanne
- C15.** Utilisation du dichroïsme circulaire et de la fluorescence intrinsèque pour étudier l'interaction entre 2 protéines.  
Deléage G, Penin F, Gagliardi D, Roux B & Gautheron DC  
SYNBIO, Techniques Avancées pour les Sciences de la Vie (17-19 Octobre 1990) Lyon-Villeurbanne
- C16.\*** ANTHEPROT: Un programme graphique interactif pour l'analyse de la structure des protéines à partir de leurs séquences.  
Geourjon C, Deléage G & Roux B  
Rencontres Biologie Moléculaire et Informatique (16-18 avril 1991) Paris
- C17.** Recherche de motifs et de zones conservées dans les protéines.  
Geourjon C & Deléage G  
19<sup>ème</sup> Forum des Jeunes Chercheurs, 7-10 Juillet 1992, Université de Caen.
- C18.** Modifications in the binding domain of envelope proteins to redirect ALV host-ranges.  
Valésia-Wittman S, Drynda A, Deléage G, Aumailley M, Heard JM, Damos O, Verdier G & Cosset FL  
Cold Spring Harbor May 1993 New-York Retrovirus.
- C19.** Etude structurale du répresseur bactérien *FruR* : modélisation moléculaire et RMN du domaine d'interaction avec l'ADN (hpf 60).  
Penin F, Montserret R, Deléage G, Geourjon C, Cortay J.C, Bonnot C, Nègre D, Fenet B & Cozzone AJ  
5<sup>ème</sup> Journée grenobloise de RMN, 23 juin 1993, Université J. Fourier
- C20.** Etude structurale du répresseur bactérien *FruR* : RMN du domaine d'interaction avec l'ADN (hpf60).  
Penin F, Fillon A, Montserret R, Deléage G, Geourjon C, Cortay J.C, Bonnot C, Nègre D, Fenet B & Cozzone AJ  
5<sup>ème</sup> groupe Thématique Magnétisme Nucléaire et Biologie, 5-8 oct.1993, Toulouse
- C21.** Domaines nucléotidiques de la Glycoprotéine-P responsable du transport de drogues anti-tumorales : production par génie génétique et propriétés.  
Di Pietro A, Cortay H, Dayan G, Penin F, Geourjon C, Deléage G & Baggetto L  
5<sup>ème</sup> Réunion du groupe Thématique de Bioénergétique, 11-13 octobre 1993, Marseille, Presqu'île de Giens.
- C22.** Un nouveau concept dans la prédiction des structures secondaires des protéines : auto-optimisation des paramètres de prédiction.  
Geourjon C & Deléage G  
Congrès d'automne de la Société Française de Biochimie et Biologie Moléculaire, 7-9 décembre 1993, Villepinte Paris-Nord.

- C23. Topologie commune aux domaines non-collagéniques de différents types de collagènes.  
Moradi-Améli M, Deléage G, Geourjon C & van der Rest M  
Réunion annuelle de la Société Française du Tissu Conjonctif, 25-26 Mars 1994, Toulouse
- C24.\* Applications d'ANTHEPROT à la modélisation moléculaire sous contraintes RMN.  
Réunion des utilisateurs de la Société Oxford Molecular 21-22 avril 1994, Dijon  
Deléage G & Geourjon C
- C25. Logiciel ANTHEPROT : de la séquence à la structure tridimensionnelle des protéines  
Geourjon C, Penin F & Deléage G  
Forum LABO CNIT Paris La Défense, 27-30 Avril 1994.
- C26. Etude RMN de la région N-terminale de la protéine Core du virus de l'hépatite C.  
Ladavière L, Jolivet M, Deléage G & Penin F  
Vlème Journée Grenobloise de RMN, 22 Juin 1994, Grenoble.
- C27. Un nouveau concept dans la prédiction des structures secondaires des protéines : autooptimisation des paramètres de prédiction.  
Geourjon C & Deléage G  
21<sup>ème</sup> Forum des Jeunes Chercheurs, 5-8 juillet 1994, Université de Reims
- C28. Logiciel ANTHEPROT : Visualisation et analyse 3D des structures RMN.  
Geourjon C, Penin F & Deléage G  
13<sup>o</sup> Colloque annuel de la Société Française de Biophysique "Imagerie des systèmes macromoléculaires"  
8-12 septembre 1994, Annecy
- C29.\* Connexion graphique interactive entre alignements multiples, prédictions de structures secondaires, recherches de sites et motifs dans les banques de séquences et de structures.  
Deléage G & Geourjon C  
Groupe de travail du GDR CNRS "Recherche de motif dans les protéines", 15-16 Septembre 1994, Lille
- C30. Analyse de séquences, prédictions de structures, et modélisation moléculaire de protéines  
Congrès IMABIO, 20-22 septembre 1994, La Grande-Motte  
Deléage G & Geourjon C
- C31.\* Intensive sequences comparisons to predict protein secondary structures. Integration into a software package : ANTHEPROT  
Deléage G & Geourjon C  
Hawaii International Conference on System Sciences - 28, January 3-6 1995, HAWAII
- C32. Domaines protéiques de fixation à l'ADN: de l'analyse de séquence à la structure tridimensionnelle (3D) par RMN  
Penin F, Geourjon C & Deléage G  
9<sup>ème</sup> réunion peptides et protéines, Aussois, 8-13 janvier 1995
- C33. Tridimensional structure of *E. coli* fructose repressor DNA-binding domain by NMR  
Penin F, Geourjon C, Montserret R, Yang Y.S, Cortay JC & Deléage G  
First European Symposium of the Protein Society, Davos, Suisse (28 mai-1<sup>er</sup> juin 1995)
- C34. Protein domain design and molecular modelling using the ANTHEPROT package. Applications to NMR studies  
Geourjon C, Yang YS, Gagliardi D, Penin F & Deléage G  
First European Symposium of the Protein Society, Davos, Suisse (28 mai-1<sup>er</sup> juin 1995)
- C35. Structural analysis of the immunodominant antigenic domain of the hepatitis C virus nucleocapsid by NMR.  
Penin F, Ladavière L, Dalbon P, Deléage G Jolivet M  
14<sup>th</sup> International Positive Strand RNA Virus Symposium Utrecht, Pays-Bas (25-30 mai 1995)



- C36. Structure 3D par RMN du domaine de fixation à l'ADN du régulateur bactérien FruR.  
Geourjon C, Penin F, Monserret R, Bonod C, Cortay J.C, Nègre D, Ladavière L, Cozzone AJ & Deléage G  
22ème Forum des Jeunes Chercheurs, 4-7 Juillet 1995, Université de Grenoble
- C37. A consensus DNA operator for the FruR regulator of *E. coli*  
Nègre D, Bonod-Bidaud C, Oudot C, Geourjon C, Deléage G, Cozzone AJ & Cortay JC  
23rd Meeting of the Federation of the European Biochemical Societies (FEBS), Bâle, Suisse Août 1995
- C38. Protein domains design using the ANTHEPROT package. Applications to NMR studies.  
Geourjon C, Yang Y.S, Gagliardi D, Penin F & Deléage G  
Perspectives on protein engineering: "from folds to functions"  
5th International conference 2-6 mars 1996, Montpellier, France
- C39. Conception de domaines protéiques grâce au programme ANTHEPROT. Applications aux études RMN du domaine d'interaction avec l'ADN du facteur de choc thermique.  
Deléage G, Geourjon C, Yang Y.S, Gagliardi D, Ladavière L, Montserret R, Blanchet C & Penin F  
Congrès IMABIO, Strasbourg, 16-17 décembre 1996
- C40. Analyse de la structure secondaire de la glycoprotéine-P par dichroïsme circulaire et prédiction à partir de la séquence.  
Dong M, Ladavière L, Deléage G, Penin F & Baggetto LG  
XVI ème Forum de cancérologie (Paris, 17-19 juin 1996)
- C41. Editeur d'alignements multiples de protéines couplées à des prédictions de structure secondaire.  
Blanchet C, Geourjon C & Deléage G  
23ème forum des Jeunes Chercheurs, 2-5 Juillet 1996, Université de Poitiers
- C42. Identification of an heparin binding site within overexpressed NC1 domain of chicken collagen XIV  
Giry-Lozingue C, Aubert-Foucher E, Penin F, Deléage G, Dublet B & van der Rest M  
Xvth FECTS Meeting, Munich, 4 - 9 Août 1996
- C43.\* Prédiction de structures secondaires de protéines.  
Deléage G  
IXèmes Entretiens Jacques Cartier  
Conférence sur invitation (Montréal, 1-4 octobre 1996)
- C44. Prédiction de structure secondaire, un outil pour l'étude des relations structure-fonction des protéines.  
Geourjon C, Blanchet C & Deléage G  
15ème congrès annuel de la Société Française de Biophysique, St-Malo, 22-25 septembre 1996
- C45. Purification, functional and structural studies of P-glycoprotein from different resistant cancer cell lines.  
Baggetto L.G, Dong M, Tenin C, Ladavière L, Deléage G & Penin F  
Predictive Oncology & Therapy conference, 3rd International Symposium, Impact of Cancer Biotechnology, Diagnostic & Pronostic Indicators  
Nice (26-28 octobre 1996)
- C46. Prédiction de structure secondaire des protéines : Applications et perspectives.  
Geourjon C, Blanchet C, Combet C & Deléage G  
Réunion du Groupe de Graphisme Moléculaire, 21-23 Mai 1997, Dourdan
- C47. PSA : Logiciel multi-plateforme d'analyse de séquences.  
Blanchet C, Geourjon C, Deléage G  
24ème Forum des Jeunes Chercheurs de la SFBBM, 8-11 Juillet 1997, Corté
- C48. Protein structure prediction and molecular biocomputing. Applications to protein "Domain design"  
Deléage G, Blanchet C, Combet C, Penin F & Geourjon C  
2nd European Biophysics Congress, 13-17 July 1997, Orléans
- C49. Délimitation de domaines protéiques à l'aide du programme ANTHEPROT. Applications pour l'étude

- structurale du domaine d'interaction avec l'ADN du facteur de choc thermique (HSF) de maïs par RMN.  
Deléage G, Yang YS, Geourjon C, Montserret R, Blanchet C, Penin F  
Journées Lyonnaise de Biologie, 20-21 Janvier 1998, ENS - Lyon Gerland
- C50. MPSA: A software for Multiple protein sequence analysis.  
Blanchet C, Geourjon C & Deléage G  
Computational chemistry and the living world, 20-24 avril 1998, Chambéry
- C51. Structural analogy modeling of proteins.  
Combet C, Deléage G & Geourjon C  
"Computational chemistry and the living world", 20-24 avril 1998, Chambéry
- C52. Etude structurale d'un peptide issu de la partie C-terminale du domaine NC1 du collagène XIV de poulet.  
Montserret R, Aubert-Foucher E, Geourjon C, Deléage G, Penin F  
Rencontres Rhône-Alpes de RMN, 25 juin 1998, Villeurbanne
- C53. NPS@/mpsa : Outils clients – serveurs d'analyse de séquences de protéines  
Blanchet C, Geourjon C & Deléage G  
"9<sup>èmes</sup> rencontres régionales de la recherche ", 3 novembre 1998, Lyon
- C54. Système intégré d'analyse de séquences biologiques.  
Blanchet C, Combet C, Geourjon C & Deléage G  
9<sup>ème</sup> Rencontres Régionales de la Recherche, Palais des Congrès de Lyon, 3 novembre 1998
- C55. Le pôle Bioinformatique Lyonnais  
Perriere G, Blanchet C, Duret L, Geourjon C, Thioulouse J, Gouy MC & Deléage G.  
"Journées Biologiques de Lyon", 21-22 janvier 1999, Lyon
- C56. The Bioinformatic Pole of Lyon  
Perriere G, Blanchet C, Duret L, Geourjon C, Thioulouse J, Combet C, Gouy MC & Deléage G  
The Third Annual Conference on Research in Computational Molecular Biology (RECOMB 99) 11-14 avril 1999, Lyon
- C57. Protein sequence analysis software with Web facilities.  
Blanchet C, Geourjon C & Deléage G  
The Third Annual Conference on Research in Computational Molecular Biology (RECOMB 99) 11-14 avril 1999, Lyon
- C58. Etude de la forme libre du PSA par des approches immunologiques, biochimiques et par la modélisation moléculaire.  
Michel, S, Deléage G, Piga N, Jolivet M & Jolivet-Reynaud C  
XI<sup>èmes</sup> journées du Groupe de Graphisme et Modélisation Moléculaire, Dardilly 10-12 Mai 1999
- C59. MPSA : Ressources bio-informatiques et réseaux pour l'analyse de séquences de protéines.  
Blanchet C, Combet C, Geourjon C & Deléage G  
XI<sup>èmes</sup> journées du Groupe de Graphisme et Modélisation Moléculaire, Dardilly 10-12 Mai 1999
- C60. Relations structure-fonction du 2<sup>ème</sup> domaine nucléotidique de la glycoprotéine P impliquée dans la chimiorésistance des cellules cancéreuses : apport de la modélisation moléculaire.  
Geourjon C, Steinfels E, Deléage G, di Pietro A, & Jault, JM  
XI<sup>èmes</sup> journées du Groupe de Graphisme et Modélisation Moléculaire, Dardilly 10-12 Mai 1999
- C61.\* Outils client-serveurs d'analyse de séquences de protéines  
IV colloque des partenaires du CEA "Le CEA et ses partenaires dans le monde du calcul scientifique : expériences et perspectives", Université Joseph Fourier, Grenoble Novembre 1999  
Invitation de Martin Fields  
Deléage G
- C62. Conformational conservation of the hypervariable Region 1 (HVR1) of hepatitis C virus E2 envelope glycoprotein.

- Penin F, Combet C, Germanidis G, Frainais PO, [Deléage G](#) & Pawlotsky JM  
10<sup>th</sup> International symposium on viral hepatitis and liver disease  
9-13 avril 1999 Atlanta
- C63.** Efficient retargeting of AAV2 by genetic modification of the viral capsid protein  
Girod A, Ried M, Wobus C, Kleinschmidt J, [Deléage G](#), Hallek M  
European Journal Of Cancer 35: 71 (1999)
- C64.** Efficient retargeting of adeno-associated virus type 2 (AAV2) by genetic modification of the viral capsid protein.  
Girod A, Ried MU, [Deléage G](#) & Hallek M  
Blood 94 , 2722, Nov. 1999
- C65.** Conservation conformationnelle de la région hypervariable 1 (HVR1) de la glycoprotéine d'enveloppe E2 du virus de l'hépatite C (VHC).  
Penin F, Combet C, Germanidis G, Frainais PO, [Deléage G](#) & Pawlotsky JM  
II Journées francophones de virologie 6-7 avril 2000. Paris
- C66.** NPS@ : Un serveur Web intégré d'analyse de séquence protéique.  
Combet C, Blanchet C, Geourjon C & [Deléage G](#)  
Journées Ouvertes Biologie et Informatique Mathématiques (JOBIM 2000), 3-5 mai 2000, Montpellier
- C67.\*** HCVDB: Banque de séquences du virus de l'hépatite C  
[Deléage G](#) & Combet C  
3 mars (2000) Colloque national du réseau national hépatites
- C68.** Conformational conservation and basic character of the hypervariable region 1(HVR1) of hepatitis C virus (HCV) E2 envelope glycoprotein. Clues for HVR1 biological role.  
Penin F, Combet C, Germanidis G, Frainais PO, [Deléage G](#) & Pawlotsky JM  
7<sup>th</sup> International hepatitis C virus & related diseases (Molecular virology and pathogenesis) 3-7 décembre 2000
- C69.\*** NPS@ : Serveur Web intégré d'analyse de séquences protéiques Colloque TAS (Traitement et Analyse de Séquences) » (IMPG) Evry 23-24 novembre 2000  
[Deléage G](#)
- C70.** Geno3D un serveur Web automatique de modélisation moléculaire.  
Combet C, Jambon M, [Deléage G](#) & Geourjon C  
XII<sup>e</sup> Rencontre du Groupe de Graphisme et Modélisation Moléculaire, Nimes, 9-11 mai 2001
- C71.** SuMo : une méthode de comparaison des propriétés de surface des protéines.  
Jambon M, Combet C, [Deléage G](#) & Geourjon C  
XII<sup>e</sup> Rencontre du Groupe de Graphisme et Modélisation Moléculaire, Nimes, 9-11 mai 2001
- C72.** Development of the SuMo method to detect 3D sites in proteins  
Jambon M, Errami M, [Deléage G](#) & Geourjon C  
Summer school on the following topic : The prediction and mechanism of protein folding from topology to intermediate states, Cargese, 20-26 mai 2001
- C73.** SuMo : une méthode de détection de similitudes structurales et fonctionnelles à la surface des protéines.  
Jambon M, Errami M, [Deléage G](#) & Geourjon C  
Journées Ouvertes Biologie et Informatique Mathématiques (JOBIM 2001), 30 mai - 1 juin 2001, Toulouse
- C74.** HCVDB : the hepatitis C virus sequence database.  
Combet C, Penin F, Geourjon C & [Deléage G](#)  
Journées Ouvertes Biologie et Informatique Mathématiques (JOBIM 2001), 30 mai - 1 juin 2001, Toulouse

- C75.\* HCVDB: Hepatitis C Virus Database  
Combet, C, Penin, F, Geourjon C & Deléage G  
8<sup>th</sup> International Symposium on Hepatitis C Virus and Related Viruses, 2-5 septembre 2001, Paris
- C76. DNA immunization for identification and localization of antigenic regions on duck hepatitis B virus core protein.  
Thermet A, Robaczewska M, Charollois C, Rollier C, Kay A, Cagnon N, Geourjon C, Deléage G, Trepo C & Cova L *Hepatology*, 34, 601 Octobre 2001
- C77. Electrostatic interactions between Bcl-2 homology domains BH3 and BH4 are essential for Nr-13 anti death activity  
Lalle P, Geourjon C, Dumont-Miscopein A, Aoucheria A, Jambon M, Venet S, Deléage G and Gillet G  
Apoptosis and Cancer : Basic mechanisms and therapeutic opportunities in the post-genomic era  
13-17 Février 2002, Hawaii
- C78. SuMo : a software that detects 3D sites shared by protein structures.  
Jambon M, Imberty A, Deléage G & Geourjon C  
Journées Ouvertes Biologie et Informatique Mathématiques (JOBIM 2002), 10-12 juin 2002, Saint Malo
- C79. Detection of non-related proteins in low identity multiple sequence alignments.  
Errami M, Geourjon C & Deléage G  
Journées Ouvertes Biologie et Informatique Mathématiques (JOBIM 2002), 10-12 juin 2002, Saint Malo
- C80.\* HCVDB: European Hepatitis C Virus Database  
Deléage G, Combet C, Penin F & Geourjon C  
HepCVax kick-off meeting, 15 octobre 2002, Leiden, Pays-Bas
- C81. Modélisation moléculaire à bas taux d'identité, analyse qualitative et implémentation dans le serveur Geno3D  
Geourjon C, Combet C & Deléage G  
Réunion IMPG : Protéomique structurale, protéomique fonctionnelle et Bioinformatique  
20-23 janvier 2003 Marseille, France
- C82.\* Bioinformatics: from sequence to structure/function relationships  
Deléage G  
First French-Cuba symposium on bioinformatics, 1-8 février 2003, La Havane (CUBA)
- C83. The GENEFARM project : structural and functional annotation of Arabidopsis gene and protein families by a network of experts  
Filippi G, Brunaud V, Cock M, Cooke R, Déhais P, Deléage G, Echeverria M, Falconet D, Gaspin C, Geourjon C, Grienenberger JM, Houlne G, Lecharny A, Leroy P, Mache R, Meyer C, Negrutiu N, Risler JL, Samson D, Schneider M, Small I, Toffano C, Caboche M, Rouzé P & Aubourg S  
Séminaire Genoplante 2003, 18-20 mars 2003, Poitiers
- C84. Modélisation moléculaire à bas taux d'identité : analyse qualitative à grande échelle via le serveur Geno3D.  
Geourjon C, Misserey S, Combet C & Deléage G  
XIII<sup>ème</sup> Rencontre du Groupe de Graphisme et Modélisation Moléculaire, 5-7 mai 2003, Cabourg
- C85. SuMo: un outil d'annotation fonctionnelle de protéines à parti deds structures.  
Jambon M, Deléage G & Geourjon C  
XIII<sup>ème</sup> Rencontre du Groupe de Graphisme et Modélisation Moléculaire, 5-7 mai 2003, Cabourg
- C86. Development of a European sequence database dedicated to HCV  
Dorkeld F, Combet C, Penin F & Deléage G  
HepCVax cluster year 1 meeting, 10-12 septembre 2003 Bari, Italie
- C87. \*Bio-informatique: des données génomiques et post-génomiques aux connaissances biologiques  
Deléage G  
Séminaire INRIA l'NTECH

23 octobre 2003, Lyon, *Invitation de François Rechenmann*

- C88.** Etude bioinformatique et structurale de peptides amphipathiques d'insertion membranaire.  
Sapay N, Montserret R, Penin F & **Deléage G** (P108)  
Congrès Annuel de la Société Française de Biochimie et Biologie Moléculaire, POSTGENOMIQUE : De la protéine aux molécules bioactives. 4-5 Novembre 2003, Lyon, France.
- C89.** EuHCVdb : une banque de donnée dédiée à l'étude du génome du virus de l'hépatite C.  
Dorkeld F, Combet C, Penin F & **Deléage G** (P41)  
Congrès Annuel de la Société Française de Biochimie et Biologie Moléculaire, POSTGENOMIQUE : De la protéine aux molécules bioactives. 4-5 Novembre 2003, Lyon, France.
- C90.** Genefarm: Structural and fonctionnal annotation of Arabidospis gene and protein families by a network of experts.  
Aubourg S, Brunaud V, Bruyère C, Cock M, Cooke R, Cottet A, Couloux A, Déhais P, **Deléage G**, Duclert A, Echeverria M, Eschbach A, Falconet D, Filippi G, Gaspin C, Geourjon C, Grienenberger JM, Houlné G, Jamet E, Lechauve F, Leleu O, Leroy P, Mache R, Meyer C, Nedjari H, Negrutiu I, Orsini V, Peyretailade E, Pommier C, Raes J, Risler JL, Rivière S, Rombauts S, Rouzé P, Schneider M, Schwob P, Small I, Soumayet-Kampetenga G, Stankovski D, Toffano C, Tognolli M, Caboche M & Lecharny A  
PlantGEMs, September 23-25, 2004, Lyon
- C91.** Structural analysis of membrane association domain of nonstructural protein 5A from HCV related viruses.  
Sapay N, Montserret R, Brass V, Pal Z, Moradpour D, **Deléage G** & Penin F  
Peptide-membrane interactions. October 9-12, 2004, Namur, Belgium.
- C92.** Eu-HCVDB: Europea Hepatitis C virus Database  
Combet C, Dorkeld F, Penin F & **Deléage G**  
11<sup>th</sup> International Symposium on Hepatitis C Virus and Related Viruses, 3-7 octobre 2004, Heidelberg
- C93.** Determination of proteins 3D structure at low resolution by mass spectroscopy and structural bioinformatics  
Misserey S, Lascoux D, Sidaner F, Hubert A, Cravello L, Müller M, Galinier A, **Deléage G**, Forest E & Geourjon C  
Proteomics : New insights and prospects, November 8-9, 2004, Lyon
- C94.** Demonstration of the First Prototype of RUGBI, Design and Deployment of a Grid for Bioinformatics  
C Blanchet, V. Breton, **G Deléage**, N. Démésy, F. Hernandez, N. Jacq, S. Langlois, A. Lecluse, Y. Legré, D. Linglin, J.F. Musso, R. Nougarede, H. PrévotEAU, S. Reynaud, J.P. Roebuck  
*HealthGRID 7-9 avril 2005, Oxford : Royaume-Uni*
- C95.** Structural analysis of membrane association domain of nonstructural protein 5A from HCV related viruses  
Sapay N, Montserret R, Brass V, Pal Z, Chipot C, Moradpour D, **Deléage G** & Penin F  
XIIIème Rencontre du Groupe de Graphisme et Modélisation Moléculaire, 2-4 mai 2005, Iles des Embiez
- C96.** Détermination à basse résolution de la structure 3D de protéines par spectrométrie de masse.  
Misserey S, Lascoux D, Sidaner F, Hubert A, Cravello L, Müller M, Galinier A, **Deléage G**, Forest E & Geourjon C  
XIIIème Rencontre du Groupe de Graphisme et Modélisation Moléculaire, 2-4 mai 2005, Iles des Embiez
- C97.** Core extraction based neural network model for proteins fold recognition  
Benabdeslem K, **Deléage G** & Geourjon C  
6 au 8 juillet 2005, JOBIM, 2005, Communication courte
- C98.** Prediction of in-plane amphipathic membrane segment based on a SVM method  
Sapay N, Guermeur Y & **Deléage G**  
6 au 8 juillet 2005, JOBIM, 2005, Communication longue
- C99.** The European Hepatitis C Virus database

- Charavay C, Crisan D, Grando D, Geourjon C, Penin F, **Deléage G** & Combet C.  
6 au 8 juillet 2005, JOBIM, 2005, Communication longue
- C100.** Méthodes de filtrage des résultats des recherches BLAST pour l'obtention d'alignements multiples dédiés à l'analyse structurale  
Friedrich A, Moulinier L, Ripp R, Garnier N, Bettler E, **Deléage G** & Poch O  
6 au 8 juillet 2005 JOBIM, Lyon, Communication longue
- C101.** Structure des protéines et cross-link intra-moléculaire : limites et perspectives  
Lascoux D, Geourjon C, Subra G, Martinez J, **Deléage G** & Forest E  
1er Symposium de Chimie et Biologie analytiques : De la molécule au protéome, SFSM, 26-29 septembre 2005, Montpellier
- C102.** A neural network system based on structural alignment and clustering for proteins fold recognition  
Benabdeslem K, **Deléage G** & Geourjon C  
ECCB'2005, September 28th – October 1st 2005, Madrid, Espagne
- C103.** A comprehensive system for consistent numbering of HCV sequences, proteins and epitopes  
Kuiken C, Bukh J, Combet C, **Deléage G**, Mizokami M, Richardson R, Sablon E, Yusim K, Pawlotsky JM, Simmonds P and the HIV database group.  
12<sup>th</sup> International Symposium on Hepatitis C Virus and Related Viruses, October 2-6, 2005, Montreal (2005)
- C104.** Consensus proposals for the unified system of nomenclature of hepatitis C virus genotypes.  
Simmonds P, Bukh J, Combet C, **Deléage G**, Enomoto N, Feinstone S, Halfon P, Inchauspé G, Kuiken C, Maertens G, Mizokami M, Murphy D, Okamoto H, Pawlotsky JM, Penin F, Sablon E, Shin-I T, Stuyver LJ, Thiel HJ, Viazov S, Weiner AJ & Widell A  
12<sup>th</sup> International Symposium on Hepatitis C & Related Viruses. October 2-6, 2005, Montreal, Canada.
- C105.** Extraction de coeurs structuraux et réseaux de neurones pour la reconnaissance des repliements de protéines.  
Guermeur Y, Benabdelsem K, Brehelin L, Capponi C, Coste F, Darcy Y, **Deléage G**, Denis F, Gascuel O, Geourjon C, Gibrat JF, Jacquemin I, Magnan C, Marin A, Martin J, Nicolas J, Ralaivola.  
Journées des ACI STIC, 21,22 et 23 Novembre 2005 Bordeaux
- C106.** International Consensus Proposals for the Nomenclature and Numbering of HCV: Creation of a Unified System for Assignment and Database Access.  
Kuiken C, Bukh J, Combet C, **Deléage G**, Enomoto N, Feinstone S, Halfon P, Inchauspe G, Maertens G, Mizokami M, Murphy DG, Okamoto H, Pawlotsky JM, Penin F, Richardson R, Sablon E, Shin-I T, Stuyver LJ, Thiel HJ, Viazov S, Weiner AJ, Widell A, Yusim K & Simmonds P  
HepDart meeting  
11-15 décembre 2005, Big Island , Hawaï
- C107.** Alignement structural et classification hiérarchique pour l'extraction des cœurs structuraux  
Benabdeslem K, **Deléage G** et C Geourjon  
Extraction et gestion des Connaissances : EGC 2006  
Lille, Janvier 2006
- C108.** MS2PH-db: a new database to analyse proteins implicated in human genetic diseases  
Friedrich A, Garnier N, Nguyen H, Bettler E, **Deléage G**, Poch O & Moulinier L  
5 au 7 juillet 2006, JOBIM 2006, Bordeaux, Communication longue
- C109.** MAGOS: Multiple AliGnment and mOdelling Server  
Garnier N, Friedrich A, Nguyen H, Bettler E, Moulinier L, Geourjon C, **Deléage G** & Poch O  
5 au 7 juillet 2006 JOBIM 2006, Bordeaux, Communication longue
- C110.** euHCVdb: on the road to euHCVdb-3D  
Charavay C, Crisan D, Grando D, Lopez J, Garnier N, Geourjon C, Bettler E, Penin F, **Deléage G** & Combet C  
VIRGIL Innotech meeting, 14 avril 2006, Amsterdam, Netherlands

- C111.** Building an Encrypted File system on the EGEE grid: Application to Protein Sequence Analysis  
Mollon R, Blanchet C & **Deléage G**  
20-22 avril 2006 ARES Conference (2006) Proceedings 965-971, Vienne, Autriche
- C112.** Integrating Bioinformatics Resources on the EGEE Grid Platform  
Blanchet C, Combet C & **Deléage G**  
Sixth IEEE International Symposium on Cluster Computing and the Grid Workshops (CCGRIDW\06)  
18 mai 2006 Singapour
- C113.\*** 2D and 3D prediction of protein structure from sequences.  
**Deléage G**  
3rd Indo-French Bioinformatics Meeting (IFBM 2006)  
June 12-15, 2006, Bangalore, India
- C114.\*** Structural bioinformatics.  
**Deléage G**  
1<sup>st</sup> Meeting of the GDRE - RA Comparative  
June 27-28, 2006, Lyon, France
- C115.** The international HCV databases: an update on their collaborative effort.  
Kuiken C., Mizokami M., **Deléage G**, Yusim K., Penin F., Shin-I T., Charavay C., Tao N., Crisan D., Grando D., Dalwani A., Geourjon C., Agrawal A. and Combet C  
13th International Meeting on Hepatitis C Virus and Related Viruses, 27-31 2006 August st Cairns, Australia.
- C116.** Grid deployment of legacy bioinformatics applications with transparent data access  
Blanchet C, Mollon R, Thain D & **G. Deléage**  
7 th IEEE/ACM International Conference on GRID Computing  
28-29 septembre 2006, Barcelone
- C117.** A comprehensive system for consistent numbering of HCV sequences, proteins and epitopes  
Kuiken C, Combet C, Bukh J, **Deléage G**, Mizokami M, Richardson R, Sablon E, Yusim K, Pawlotsky JM, & Simmonds P  
57th Annual Meeting of the American-Association-for-the-Study-of-Liver-Diseases  
Boston, MA, OCT 27-31, 2006
- C118.** Web Services Interface to Run Protein Sequence Tools on Grid, Testcase of Protein Sequence Alignment  
Blanchet C, Combet C, Daric V & **Deléage G**  
7th International Symposium on Biological & Medical Data Analysis (ISBMDA2006)  
Décembre 2006, Grèce
- C119.** euHCVdb3D: A 3D model database and bioinformatic tools to help analyzing viral resistance to drugs  
Garnier N, Bettler E, Geourjon C, Penin F, **Deléage G** and Combet C  
3rd year VIRGIL meeting  
22-23 mai 2007 Lyon, France
- C120.** Modeome3D: un système distribue de création et de gestion de modèles 3D de protéines.  
Garnier, N, Combet, C, Geourjon C, **Deléage G** and Bettler E  
Journées Ouvertes Biologie et Informatique Mathématiques (JOBIM 2007)  
10-12 Juin 2007 Marseille, France
- C121.** euHCVdb: the European Hepatitis C Virus Database.  
Combet C, Garnier N, Charavay C, Grando C, Crisan D, Lopez J, Dehne-Garcia A, Geourjon C, Bettler E, Hulo C, Le Mercier P, Bartenschlager R, Diepolder H, Moradpour D, Pawlotsky J.M, Rice C.M, Treppe C, Penin F, **Deléage G**  
Christophe Mérieux Conference: Trends in Virology, 25-26 Juin 2007, Veyrier du Lac
- C122.** euHCVdb: the European Hepatitis C Virus Database

- Combet C, Garnier N, Charavay C, Grando C, Crisan D, Lopez J, Dehne-Garcia A, Geourjon C, Bettler E, Hulo C, Le Mercier P, Bartenschlager R, Diepolder H, Moradpour D, Pawlowsky JM, Rice CM, Trepo C, Penin F & [Deléage G](#)  
HCV classification and nomenclature group 2<sup>nd</sup> meeting  
11 septembre 2007 Glasgow, Scotland, UK
- C123.** ViralORFeome: a database for the management of viralORF collection and virus-host interactome  
Navratil V, Pellet J, Achaz G, Vidalain PO, Jacob Y, Jacotot L, Vaclio P, [Deléage G](#), Combet C, Tafforeau L, de Chasse B, Gautier C, Tangy F, Chaboud A, The Infection Mapping Project I-MAP, P. André, V. Lotteau and C. Rabourdin-Combe  
7th ORFeome meeting, 24-26 oct 2007, Boston, USA
- C124.** euHCVdb: the EUropean Hepatitis C Virus DataBase.  
Combet C, Garnier N, Charavay C, Crisan D, Grando D, Lopez J, Dehne-Garcia A, Dorkeld F, Geourjon C, Bettler E, Penin F & [Deléage G](#)  
Conference Hepatitis B & C Virus Resistance to Antiviral Therapies Paris  
February 14-16th 2008 Paris, France.
- C125.** ViralORFeome : une base de données dédiée à la gestion d'une collection d'ORF virales et de l'interactome virus-hôte  
Pellet J, Navratil V, Meyniel L, Achaz G, Vidalain PO, Tafforeau L, Aublin-Gex A, Guironnet-Paquet A, Le Breton M, Lucas-Hourani M, Caignard G, Chantier T, Faria BF, Hiet MS, Pradezynski F, Chaboud A, Davoust-Nataf N, De Chasse B, Mangeot PE, Jacotot L, Vaglio P, [Deléage G](#), Combet C, Delmotte S, Gautier C, Tangy F, Jacob Y, André P, Lotteau V, Rabourdin-Combe C  
Xes Journées Francophones de Virologie, 27-28 mars 2008, Institut Pasteur, Paris, France.
- C126.** HnRNP A2/B1 as antinuclear antibodies target: epitope mapping and differential reactivity in autoimmune hepatitis and connective tissue diseases.  
Huguet S, Combet C, Ballot E, Johanet C, [Deléage G](#), Samuel D & J Duclos-Vallée  
43rd Annual Meeting of the European Association for the Study of the Liver (EASL)  
April 23-27th 2008 Milan, Italy
- C127.** MSX-3D : A tool to validate 3D protein models using mass spectrometry  
Heymann, M, Paramelle D, Subra G, Forest E, Martinez J, Geourjon C and [Deléage G](#)  
JOBIM, 31 juin-02 Juillet 2008, Lille
- C128.** HCV NS3-4A protease variants and mutants analyses by molecular simulation.  
Terreux R, Barbotte L, Chatron M, Charre C, Penin F, [Deléage G](#), Pawlowsky JM & Combet C  
15th International Symposium on Hepatitis C Virus and Related Viruses  
5-9 octobre 2008 San Antonio USA
- C129.** hnRNP A2/B1 as antinuclear antibodies target : Epitope mapping and differential reactivity in autoimmune hepatitis and connective tissue diseases.  
Ballot E, Combet C, Huguet S, Johanet C, [Deléage G](#), Samuel D, Duclos Vallee JC  
EASL Monothematic Conference Immune Mediated Liver Injury,  
December 4-6 2008 Hamburg
- C130.\*** Méthodes d'analyse de séquences et de structures 3D de protéines et leur intégration au sein de Webiciels.  
Conférence plénière invitée. JOBIM 9 -11 Juin 2009 Nantes  
[Deléage G](#)
- C131.** CaBioMinDB, a relational database for the proteins of CaCO<sub>3</sub> mineralized tissues: further application to the shell proteins of the freshwater mussel *Unio pictorum*  
Ramos-Silva P, Marin F, [Deléage G](#), Combet C, Luquet G,  
7th International Symposium on Networks in Bioinformatics (ISNB 2010), Amsterdam, The Netherlands, 22nd-23rd April 2010.
- C132.** CaBioMinDB, a relational database for the proteins of CaCO<sub>3</sub> mineralized tissues: further application to the shell proteins of the freshwater mussel *Unio pictorum*



- Ramos-Silva P, Combet C, **Deléage G**, Luquet G, Marin F  
12èmes Journées Françaises de Biologie des Tissus Minéralisés (12èmes JFBTM), St-Etienne, France, 9th-11th June 2010.
- C133.** Characterization of the Bcl-2 family using structure-aided HMM framework  
Aouacheria A, Rech de Laval V, **Deléage G** & Combet C  
JOBIM 7-9 septembre 2010 Montpellier
- C134.** BYKdb: a database of bacterial tyrosine kinases.  
Jadeau F, Grangeasse C, **Deléage G** & Combet C  
JOBIM 7-9 septembre 2010 Montpellier
- C135.** HBVdb: A knowledge database for the Hepatitis B Virus.  
Hayer J, Jadeau F, **Deléage G** & Combet C  
JOBIM 7-9 septembre 2010 Montpellier
- C136.** Bioinformatics Public web interfaces on grid  
Michon A., Blanchet C., Bettler E., Combet C., Penin F. & **Deléage G**  
Poster EGEE2009, 21-25/09/2009, Barcelone
- C137.** HBVdb: a Knowledge Database for the Hepatitis B Virus.  
Hayer J, Jadeau F, **Deléage G**, Combet C  
International Meeting on Molecular Biology of Hepatitis B Viruses  
October 9-13<sup>th</sup> 2010 Taipei, Taiwan.
- C138.** Characterization of the Bcl-2 family using structure-aided HMM Framework.  
Aouacheria A, Rech de Laval V, **Deléage G**, Combet C  
Groupement De Recherche Européen - Arc Rhône Alpin ? Comparative Genomics(GDRE - RA)  
November 16-17th 2010 Barcelone, Espagne
- C139.** HBVdb: une base de connaissances du virus de l'hépatite B. C130.  
Hayer J, Jadeau F, **Deléage G**, Combet C  
11ème Réunion du réseau national hépatites de l'ANRS, 27-28 janvier 2011 Paris
- C140.** Automated identification of Bcl-2 homologues using structure-aided HMM Framework.  
Rech de Laval V, Combet C, **Deléage G**, Aouacheria  
Cell Signal-omics, January 26-28th 2011 Luxembourg
- C141.** New applications of SUMO software for drug design.  
Chemelle JA, Bettler E, **Deléage G**, Terreux R  
242nd National Meeting of the American-Chemical-Society (ACS)  
28Th september 2011 Denver, USA
- C142.** Molecular modeling of the Hepatitis B Virus polymerase reverse transcriptase and ribonuclease H domains.  
Hayer J, Durantel D, **Deléage G**, Zoulim F & Combet C  
Intl meeting on Molecular Biology of HBV viruses  
9-12 octobre 2011, Orlando, USA
- C143.** HBVdb: Applications to structural and functional analysis of HBV Polymerase  
Hayer J, Jadeau F, Kay A, Durantel D, **Deléage G**, Zoulim F & Combet C  
26-27 Janvier 2012, Paris
- C144.** HBVdb: A knowledge database for the Hepatitis B Virus.  
Hayer J, Jadeau F, **Deléage G**, Kay A, Zoulim F, Combet C  
Molecular Biology of Hepatitis B Viruses  
September 22-25th 2012, Oxford, United Kingdom
- C145.** 123 STRUCTURE OF THE HEPATITIS B VIRUS RNase H, A TARGET FOR NEW ANTIVIRAL DRUG DEVELOPMENT, UNRAVELED BY ULTRA-DEEP PYROSEQUENCING AND MOLECULAR MODELING

J Hayer, C Rodriguez, G Germanidis, **Deléage G**, F Zoulim, JM Pawlotsky, C Combet  
48th Annual meeting of the European Association for the Study of the Liver  
24-28 April 2013 Amsterdam, The Netherlands

- C146.** The BCL-2family database (BCL2DB): a mixed bag for a family of four.  
Rech de Laval V, **Deléage G**, Aouacheria A & C Combet  
JOBIM 2013, Toulouse 1-4 Juillet 2013, Toulouse, France

La liste est aussi disponible sur Internet à l'URL : <https://www.gdeleage.fr/prof/publis.php>

#### IV.5. PARTICIPATION TO THESIS AND HDR JURYS

- J1.\*** ANTHEPROT: Un logiciel d'analyse de séquences et de structures tri-dimensionnelles de protéines. Application à la détermination de structure sous contraintes RMN.  
**Christophe GEOURJON** (1<sup>er</sup> juin 1994) Directeur de thèse : **Deléage G**.
- J2.°** Combinaison de classifieurs statistiques. Application à la prédiction de la structure secondaire des protéines.  
**Yann GUERMEUR** (10 décembre 1997) Directeur de thèse : P. Gallinari. Université de Paris 6
- J3.°** Conception et développement de systèmes d'aide à la compréhension de données biologiques et moléculaires  
**Fabien CAMPAGNE** (28 septembre 1998) Directeur de thèse : B. Maigret. Université de Nancy 1
- J4.°** Modélisation moléculaire par homologie des protéines:ses applications en Biologie et en Bioinformatique  
**Jean-Luc PELLEQUER** (22 Janvier 1999) HDR. Université des Sciences de Luminy (Marseille II)
- J5.\*** Logiciel MPSA et ressources bio-informatiques client-serveur Web dédiés à l'analyse de séquences de protéine.  
**Christophe BLANCHET** (31 Mai 1999) Directeur de thèse : **Deléage G**.
- J6.°** Analyse et prédiction des contacts entre les chaînes latérales des protéines  
**Marie-Hélène MUCHIELLI-GIORGI** (8 Juin 1999) Directeur de thèse : S. Hazout. Université Paris 7
- J7.°** Prédiction de la structure secondaire des protéines par analyse spectrale de la séquence d'hydrophobicité  
**Patrick ROMANET** (17 Septembre 1999) Directeur de thèse : Y. Dupont, Université J. Fourier Grenoble
- J8.°** Contribution à l'étude structurale de protéines impliquées dans la transcription/réparation de l'ADN  
**Valérie LAMOUR** (13 Décembre 1999) Directeur de thèse : J-C Thierry, Université Pasteur, Strasbourg
- J9.°** Etude par modélisation moléculaire d'un polymère à usage thérapeutique; le poly(méthylidène malonate 2.1.2), structure tridimensionnelle, propriétés moléculaires et influence de la solvataion.  
**Eric VANGREVELINGHE** (29 Février 2000) Directeur de thèse: L. Morin-Allory, Orléans
- J10.** Cartographie épitopique du PSA (Prostate Specific Antigen) : Caractérisation d'épitopes spécifiquement reconnus par des anticorps monoclonaux discriminant une hyperplasie bénigne d'un cancer de la prostate.  
**Sandrine MICHEL** (10 Avril 2000) Directeur de thèse : C. Jolivet-Reynaud, Université Lyon 1, Villeurbanne
- J11.** Habilitation à diriger des recherches.  
**Gilles LABESSE** (6 septembre 2000) Université Montpellier I,
- J12.°** Oligosaccharides et xénotransplantation : Etude et production par voie biotechnologique du xénoantigène Gal $\beta$ Gal. Modélisation moléculaire de l' $\beta$ 3-galactosyltransférase.  
**Emmanuel BETLLER** (25 octobre 2000) Directeurs de thèse : Roberto Geremia et Anne Imberty, CERMAV

Université Joseph Fourier, Grenoble

- J13.** Bioinformatique structurale.  
**Christophe GEURJON** (11 décembre 2000) IBCP-Université Claude Bernard Lyon1 HDR
- J14.°** Ingénierie des acides nucléiques sur ordinateur par un algorithme novateur permettant l'optimisation de la séquence des bases.  
**Ingrid LAFONTAINE** Directeur de thèse : R. Lavery IBPC Université Paris 7, 22 janvier 2001
- J15.°** Nouvelles stratégies d'analyse et de prédictions des structures tridimensionnelles des protéines  
**Alexandre de BREVERN.** Directeur de thèse : S. Hazout Université Paris 7, 6 Février 2001
- J16.** Prédiction du repliement peptidique grâce aux invariants structuraux de protéines homologues.  
**Marc LAMARINE.** Directeur de thèse : J. Chomillier Université Paris 6, 20 mars 2001
- J17.\*** HCVDB : Une base de données de séquences du virus de l'hépatite C interconnectée au Webiciel NPS@d'outils bioinformatiques d'analyse de séquences et de structures.  
**Christophe COMBET** Directeur de thèse : **Deléage G.** (5 Juin 2001)
- J18.°** Analyse standardisée IMGT des relations séquences-structure des immunoglobulines et récepteurs T  
**Manuel RUIZ,** Directeur de thèse : M.P. Lefranc, Université Montpellier II, 30 novembre 2001
- J19.°** Développement d'une méthode de reconnaissance de repliements des protéines et application aux séquences "orphelines" issues du séquençage de *B. subtilis*"  
**Antoine MARIN,** Directeur de thèse : J-F Gibrat, Université de Versailles, 29 Janvier 2002
- J20.** Hétérogénéité génomique et étude des caractères structuraux de la protéine TAT des lentivirus des petits ruminants.  
Examineur du mémoire du diplôme de l'Ecole Pratique des Hautes Etudes.  
**Joëlle CHASTANG** 23 octobre 2002
- J21.\*** Analyse statistique des structures tridimensionnelles des protéines et validation de familles structurales à bas taux d'identité  
**Mounir ERRAMI,** Directeur de thèse : **Deléage G.** (20 novembre 2002)
- J22.** Habilitation à diriger des recherches  
**Jean-Michel JAULT** (24 octobre 2003)
- J23.°** Développements méthodologiques pour la modélisation des structures de protéines et la recherche in silico d'inhibiteurs : Application aux sérine/thréonine kinases de *Mycobacterium tuberculosis*  
**Vincent CATHERINOT** (2004) Directeur de thèse : G. Labesse Université Montpellier 16 décembre 2004
- J24.°** Comment lire la séquence de la double hélice ? Le développement et l'application d'un outil pour analyser quantitativement les interactions spécifiques entre protéine et ADN.  
**Guillaume PAILLARD** (2005), Directeur de thèse : Richard Lavery (31 janvier 2005)
- J25.°** Conception d'une base de données thématique sur les récepteurs nucléaires : Application à l'étude des relations séquence / structure / fonction des récepteurs nucléaires ECR et USP intervenant dans la mue et la métamorphose chez les insectes.  
**Souphatta SASORITH** (2005) Directeur de thèse : D. Moras Université Louis Pasteur Strasbourg (21 Février 2005)
- J26.** Caractérisation des changements de conformation de BmrA, un transporteur ABC de multiples drogues chez *Bacillus subtilis* : exploitation des modèles structuraux.  
**Olivier DALMAS** (2005) Directeur de thèse : A di Pietro UCBL (29 juin 2005)
- J27.°** Analyse et prédiction des structures tridimensionnelles locales des protéines.  
**Cristina BENROS** (2005) Directeur de thèse : S. Hazout Paris 7 (16 septembre 2005)
- J28.°** Prédiction de la structure locale des protéines par des modèles de Markov cachés

- Juliette MARTIN** (2005) Directeur de thèse : JF Gibrat (17 novembre 2005)
- J29.°** Etudes fonctionnelles et structurales d'un transporteur membranaire de multiples drogues et de deux saccharose isomérases bactériennes  
**Stéphanie RAVAUD** (2005) Directeur de thèse : R. Haser (9 décembre 2005)
- J30.\*** Les peptides d'ancrages à l'interface membranaire: analyses structurales par RMN et dynamique moléculaire et développement d'une méthode de prédiction bioinformatique.  
**Nicolas SAPAY** Directeurs de thèse : **G. Deléage** et F. Penin (11 janvier 2006)
- J31.°** Etude de la régulation transcriptionnelle des gènes de *Plasmodium falciparum* lors de la phase erythrocytaire par des méthodes bioinformatiques.  
**Charlotte BOSCHET** Directeur de thèse : C. Vaquero (26 Juin 2006)
- J32.** Etudes des interactions intra et inter moléculaires de BmrA, un transporteur ABC de multiples drogues chez *Bacillus subtilis*  
**Marie-Ange DO CAO**, 4 Juillet 2006 Directeur de thèse : A. di Pietro
- J33.°** Habilitation à diriger des recherches.  
**Alexandre de BREVERN** (2006) Bioinformatique structurale Université Paris 04 Octobre 2006
- J34.** Utilisation de séquences d'un alphabet structural et nouvelles perspectives pour la recherche et l'analyse des structures des protéines.  
**Manoj TYAGI** (2006) Université St Denis de la Réunion 29 septembre 2006
- J35.°** Habilitation à diriger des recherches.  
**Bernard OFFMANN** (2006) Bioinformatique structurale Université St Denis de la Réunion 30 septembre 2006
- J36.°** Analyse bioinformatique des sites d'interactions protéine-protéine et prédiction épitopique.  
**Violaine MOREAU** (2006) Université de Montpellier 17/11/2006 Directeurs de thèse : C. Granier et F. Molina
- J37.** Habilitation à diriger des recherches.  
**Nushin AGHAJARI** (2007) Université Claude Bernard Lyon 1. 2 mai 2007
- J38.** Modélisation des doamines C2 des protéines kinase C alpha, beta et epsilon, et conception d'inhibiteurs *in silico*  
**Méderic ROUAULT** (2007) Université de Lyon, 5 septembre 2007 Thèse d'exercice de Pharmacie
- J39.** Etude du phénotype odontoblastique: caractérisation de 2 nouvelles protéines  
**Florence CAROUELLE** (2007) Université de Lyon 26 octobre 2007 Directeur de thèse : F. Bleicher
- J40.** Habilitation à diriger des recherches.  
**Yves-Henri SANNEJOUAND** (2007) Université Claude Bernard Lyon 1. 05 November 2007
- J41.** Modélisation de complexes molécule bioactive/biopolymère  
**Raphael TERREUX** PHD defended at Université Claude Bernard Lyon 1 on 13 december 2007
- J42.** Surexpression hétérologue et purification du transporteur membranaire ABCG2: mécanisme d'interaction avec les substrats et des inhibiteurs spécifiques  
**Alexandre POZZA** PHD defended on 18-12-2007 Université Lyon1 Directeur de thèse : A Di Pietro
- J43.** Modélisation moléculaire de l'allergie immédiate aux bêta-lactamines  
Thèse d'exercice de Pharmacie defended on 19-12-2007 Université Claude Bernard Lyon1  
**Julie-Anne CHEMELLE** (2007) Université de Lyon, 19 décembre 2007
- J44.°** Evolution dirigée d'asparaginyI-ARNt-synthetases (AsnRS)  
**Anne LOPES** PHD defended on 30-01-2008 devant l'Ecole Polytechnique, Directeur de thèse : T. Simonson

- J45.\* Mise en place d'un environnement bioinformatique d'évaluation et de prédiction de l'impact de mutations sur le phénotype de pathologies humaines.  
**Nicolas GARNIER**, PHD defended on 10-10-2008, Université de Lyon, Directeur de thèse : [Deléage G](#)
- J46. Development of a method which predicts N-Terminal target peptides and study of protein sorting in eukaryote genomes  
**Bernhard GSCHLOESSL**, PHD defended on 17-12-2008, Université Pierre et Marie Curie Paris 6, Directeur de thèse : M. Cock
- J47.\* Développements bioinformatiques en protéomique : Modifications post-traductionnelles et modélisation moléculaire  
**Michael HEYMANN**, PHD defended on 09-01-2009, Université de Lyon, Directeur de thèse : [Deléage G](#)
- J48.° Vers la conception d'un nouvel outil de docking protéique interactif.  
**Matthieu CHAVENT**, PHD defended on 30-01-2009, Université de Nancy, Directeurs de thèse : B. Maigret et B. Levy
- J49.° Développement d'une nouvelle méthode performante de classification des surfaces protéiques d'interaction. Optimisations et extensions du logiciel MED-SuMo.  
**Olivia DOPPELT**, PHD defended on 30 Mars 2009, Université Paris 7, Directeur de thèse : Alexandre de Brevern
- J50.° Habilitation à diriger des recherches.  
**Raphaël GUERROIS**, HDR defended on 10 november 2009, Université Paris 6, 2009
- J51. Le transporteur ABCG2 : rôle d'une séquence spécifique et recherche d'inhibiteurs sélectifs  
**Sira MACALOU**, PHD defended on 11 december 2009, Université Lyon 1, Directeur de thèse : Attilio di Pietro
- J52.° Contributions des approches moléculaires *in silico* à la compréhension des liens structure/fonction des ARN.  
**Fabrice LECLERC** HDR defended on 16 december 2009, Université Henri Poincaré Nancy
- J53.° Construction et analyse de réseaux d'interactions extracellulaires.  
**Emilie CHAUTARD**, PHD defended on 21 september 2010, Université Lyon 1, Directeur de thèse: Sylvie Ricard-Blum
- J54. Caractérisation d'une nouvelle génération de détergents stabilisateurs des transporteurs abc en solution. Cristallisation de BmrA, transporteur ABC bactérien  
**Rima MATAR-MEHREB**, PHD defended on 16 december 2010, Université de Lyon, Directeur de Thèse: P. Falson
- J55. Réalisation d'ontologies de tâches et de domaine en bioinformatique et utilisation de la sémantique pour l'appariement semi-automatique de services web.  
**Nicolas LEBRETON**, PHD defended on 21 december 2010, Université de Rennes Directrice de thèse: A. Burguin
- J56. Recalage flexible de modèles moléculaires dans les reconstructions 3D de microscopie électronique.  
**Gaël GORET**, PHD defended on 26/09/2011, Université de Grenoble, Directeur : J. Navazza
- J57. Scalability of protein domain family inference pour l'appariement semi-automatique de services Web.  
**Clément REZVOY**, PHD defended on 28/09/2011, Université de Lyon 1, Directeur : D. Kahn
- J58. Coarse-grain modeling of proteins: mechanics, dynamics and function  
**Nicoletta CERES**, PHD defended on 16/03/2012, Université de Lyon 1, Directeur : R. Lavery
- J59. Aspects mécanistiques et énergétiques des interactions entre l'ADN et une molécule intercalante.  
**Mathieu WILHEM**, PHD defended on 13/07/2012, Université de Lyon 1, Directeur : R. Lavery

- J60.** Création d'un outil Internet d'évaluation des variants de signification clinique incertaine dans les gènes à haut risque de susceptibilité au cancer du sein BRCA1 et BRCA2.  
**Maxime VALLEE**, PHD defended on 10 october 2012, Université Lyon1, Directeur : S. Tav-tigian
- J61.°** Développement d'une infrastructure d'analyse multi-niveaux pour la découverte des relations entre génotype et phénotype dans les maladies génétiques humaines.  
**Luu TIEN-DAO**, PHD defended on 24/10/2012, Université de Strasbourg, Directeur : O. Poch
- J62.** Eradication ciblée des cellules cancéreuses chimiorésistantes par des activateurs du transporteur de drogues MRP1 : mécanismes moléculaires et cellulaires.  
**Doriane LORENDEAU**, PHD defended on 06/12/2102, Université Lyon1, Directeur : Hélène Cortay
- J63.°** Méthode de prédiction ab initio de la structure tertiaire des protéines dans l'espace des angles dièdres  
**Tristan BITARD-FEILDEL**, PHD defended on 21/12/2012, Université Paris 7, Directeur : JF Gibrat, A Vigneron
- J64.°** Evolutionary studies on structure and function of proteins (External reviewer)  
**Garima AGARWAL**, Indian Institute of Science, Bangalore, India. Directeur: N. Srinivasan
- J65.\*** Développement d'une base de connaissances du virus de l'hépatite B, HBVdb, pour l'étude de la résistance aux traitements. Intégration d'outils d'analyses de séquences et application à la modélisation moléculaire de la polymérase.  
**Juliette HAYER**, soutenue le 15/02/2013, Université Lyon1, Directeurs : G. Deléage & C. Combet.
- J66.** Rôle de la serine-thréonine kinase STKP dans la division et la morphogénèse du pneumocoque.  
**Aurore FLEURIE**, PHD defended on 2 october 2013, Université Lyon1, Directeur: C. Grangeasse
- J67.** Structural bioinformatics, Biomolecular Interactions & Drug Design : A case study on specific Protein-Protein and Protein-Ligand interactions systems  
External examiner PHD defended by **A. Gandhimathi** on 31-12-2013 Barathidasan University, India, Directeur R. Sowdhamini
- J68.** Modèles bio-informatiques pour les peptides non-ribosomiques et leurs synthetases  
HDR defended by **Maud PUPIN** on 03-12-2013 Université de Lille  
Directeur Hélène Touzet
- J69.\*** Analyse bioinformatique des protéines BCL-2 et développement de la base de connaissances dédiée, BCL2DB  
**Valentine RECH DE LAVAL**, PHD defended on 11/12/2013, Université Lyon1, Directeur: G. Deléage (encadrants A Aouacheria /C. Combet)
- J70.** Désordre intrinsèque et analyses de réseaux d'interactions extracellulaires : des protéines et polysaccharides aux interactions hôte-pathogène (*Leishmania*)  
**Franck PEYSSELON**, PHD defended on 12/12/2013 2013, Université Lyon1, Directeur: S. Ricard-Blum
- J71.** Bases de données biologiques spécialisées et outils bioinformatiques d'analyses intégrés des agents pathogènes inducteurs de cancer.  
**Christophe COMBET**, HDR defended on 03/07/2014, Université Lyon1
- J72.** De l'analyse des structures de protéines à leurs prédictions: cas général et cas particuliers  
**Jean-Christophe GELLY**, HDR defended on 04/09/2014, Université Paris 7 Diderot
- J73.** Etudes biochimiques et cellulaires de tyrosine-kinases bactériennes  
**Julien NOURIKYAN**, Thèse defended on 19-12-2014 devant l'Université Claude Bernard Lyon 1 Directeur C. Grangeasse
- J74.** Etude Structurale de l'hélicase répllicative et de l'activation du primosome de *Helicobacter pylori*.  
**Alexandre BAZIN**, PHD defended on 29-01-2015 devant l'Université Claude Bernard Lyon1  
Directeur L. Terradot

- J75. Deciphering the structure and function of Olfactory receptors in selected eukaryotic organisms using in silico modeling and docking approaches  
**K. HARINI**, External reviewer PHD soutenue le 31-12-2015 devant l'University Bharathidasan, Inde. Directeur R. Sowdhamini
- J76. Development of a wheat germ cell-free expression system for the production, the purification and the structural and functional characterization of eukaryotic membrane proteins.  
**Marie-Laure FOGERON**, Président 30 June 2015, Université Claude Bernard Lyon1, Directeur A. Bockmann
- J77. Du duel au pluriel: regards croisés sur les régulateurs de vie ou de mort cellulaire de la famille BCL-2.  
**Abdel AOUACHERIA**, HDR defended on 13 November 2015, Université Claude Bernard Lyon1
- J78. Régulation de la morphogénèse et de la division cellulaire du pneumocoque par phosphorylation : rôle de la sérine/thréonine protéine kinase STKP et des protéines DIVIVA, GPSB et MAPZ  
**Sylvie MANUSE**, PHD defended on 14 december 2015, Université Claude Bernard Lyon1, Directeur C. Grangeasse
- J79. Régulation de l'activité anti-apoptotique de la protéine BFL-1 : visées thérapeutiques.  
**Jérôme KUCHARCZAC**, HDR defended on 9 June 2016, Université Claude Bernard Lyon1

\* Thèses dirigées et/ou co-encadrées

° Thèses et HDR rapportées

The updated list is available at URL : <https://www.gdeleage.fr/prof/publis.php>

#### IV.6. RESEARCH CONTRACTS

- G1. Implantation du logiciel ANTHEPROT sur station IBM 6150  
 Activity report N°1988-107 with IBM France company.  
Deléage G, Geourjon C. & Roux B (1989)
- G2. Mise en place d'un appareil de dichroïsme linéaire et circulaire  
 (1994) Bonus Qualité Recherche BQR UCBL  
Deléage G, 120 000 FTTC
- G3. Incorporation des méthodes prédictives d'ANTHEPROT dans les produits d'Oxford Molecular.  
 Mise à disposition gratuite des produits d'Oxford Molecular depuis 1993
- G4. Prédiction de structures secondaires et bases de données de séquences.  
 Actions Concertées des Sciences du Vivant (ACC-SV13 bioinformatique)  
 (1995-1997) Deléage G. et M. Gouy (Total 450 kF TTC) (225 kF)
- G5. Obtention de vaccins destinés à prévenir les effets pathogènes associés à une infection rétrovirale.  
 P. F. Serres, Geourjon C, Deléage G. & C. Combet  
 Hippocampe SA (1997) patent 17/11/1997 under N° 97 14387
- G6. Pôle Bioinformatique Lyonnais (PBIL).  
Deléage G. & M.Gouy  
 Comité Informatique du CNRS (1997) 500 000 FHT
- G7. Structure function relationships between genes and functions  
 (1997-1999) Call "Programme GENOME du CNRS" grouping 6 french teams  
 150 000 FHT for IBCP Lyon (Deléage G. et M. Gouy)
- G8. Molecular Bioinformatics : a regional challenge  
 (1998) Programme EMERGENCE de la région Rhône-Alpes  
 644 000 TTC Pôle Bioinformatique Lyonnais Deléage G. (responsable du projet) et M. Gouy

- G9.** Development of a HCV database of sequence related to pathogenicity (1999) Programme Microbiologie du MENESR « Réseau National Hépatites » 100 000 FHT  
[G. Deléage](#) & [F. Penin](#)
- G10.** Pôle BioInformatique Lyonnais  
[M. Gouy](#) & [G. Deléage](#)  
Contrat de plan pluriformation de l'Université Claude Bernard Lyon 1 (1999-2003)
- G11.** PRABI :Le Pôle Rhône Alpin de BioInformatique  
Contrat de Plan Etat Région : (2000-2006) 21,7 MF (5MF pour IBCP)  
[C. Gautier](#), [G. Deléage](#) & [F. Rechenman](#)
- G12.** Secondary structure prediction, molecular modeling and interface with PRODOM domain database  
[G. Deléage](#), [D. Kahn](#), [P. Gouet](#)  
Multi-organisms call (INSERM, CNRS, INRA, MESR) 200 000F (2000)
- G13.** Development of a HCV database of sequence related to pathogenicity (2000) Programme Microbiologie du MENESR « Réseau National Hépatites » 90 000 FHT
- G14.** Pôle Bioinformatique Lyonnais (PBIL): setup of a molecular modeling web server and database of gene family.  
[G. Deléage](#) et [M. Gouy](#) (2001) Bonus Qualité Recherche. 120 000 F
- G15.** HepCVax-PARTIC : HCVDB European HCV sequence database.  
[G. Deléage](#) (responsable WP1.4) , [C. Combet](#), [C. Geourjon](#), [C. Blanchet](#), [F. Penin](#)  
Contract QLK2-CT-2002-01329  
Total amount of money : 3,5 M€ (Head of project: [W. Spaan](#))  
5<sup>th</sup> Framework program 01/09/2002-31-08-2005 285 916 € HT
- G16.** Development of a HCV database of sequence related to pathogenicity (2000) Microbiology program of French minister of research « Réseau National Hépatites » 50000 FHT
- G17.** Structure and spécificity of the CUB domain: interaction domain involved in invertebrate immunity response, development and tissue repair.  
[D. Hulmes](#), [J. Fontecilla](#), [G. Arlaud](#), [G. Deléage](#)  
(2001) CNRS call « Protéomique et Génie des Protéines » 50 000 FHT (Total 380kFHT)
- G18.** RUGBI : Realisation and Utilisation of a Grid for BioInformatics.  
(2003-01-08) 256 853 €  
[J-F. Musso](#), [C. Blanchet](#), [G. Deléage](#), [V. Breton](#), [D. Linglin](#), [F. Hernandez](#), [V. PrévotEAU](#)
- G19.** Genoplante II program.  
(2002) [S. Aubourg](#), [G. Deléage](#), [C. Geourjon](#) et al. 164 k€
- G20.** Pôle Bioinformatique Lyonnais (PBIL).  
[M. Gouy](#) & [G. Deléage](#)  
(2003) Service and platforms inter-EPST call 75 k€ (Total 150 k€)
- G21.** GENOTO3D.  
[Y. Guermeur](#), [C. Geourjon](#), *et al.*  
(2003) ACI Data Storage Call (Total 348 k€) 90k€ for LBR-IBCP- Lyon
- G22.** Pôle Bioinformatique Lyonnais  
[M. Gouy](#), [G. Deléage](#) et [J. Thioulouse](#)  
(2003) PPF 2003-2006 10 k€ / an
- G23.** viRgil : European vigilance network for the management of antiviral drug resistance.  
Network of excellence 503559 6<sup>e</sup> Framework Program (54 partners) Total amount of money 9 M€ on 4 years



(Head of project F. Zoulim) (135k€ for LBRS-IBCP) (2004-05-01-2008-04-30)

- G24. PBIL-Extension  
ACI IMPBio call (2003-2005): C.Combet, M.Gouy, V. Laudet *et al*  
35 k€ PBIL-IBCP (total 75k€)
- G25. Determination of 3D structure of proteins at low resolution by MS and molecular modeling.  
Emergency program call of Région Rhône-Alpes 1 thesis fellowship for 2006-2008 + 20 k€.
- G26. MS2PH from structural mutation to human phenotype..  
Décrypton call from AFM-IBM-CNRS 2005-2007 62k€ for IBCP 1 CDD (2 years)
- G27. Pôle Rhône Alpin de Bioinformatique  
Réseau National des Génopoles 2005 (35 k€ for the group)
- G28. InterVir3D: large scale modeling of viral proteomes and protein-protein interactions at 3D level.  
CPER Région call 2006 65 k€
- G29. Abondement OSEO-ANVAR. « Criblage et ciblage cellulaires et moléculaires de nouvelles molécules anti-cancéreuses : abolition de la chimiorésistance et inhibition de l'angiogénèse des cellules tumorales »  
50k€ Coordinateur : G. Deléage, F. Ruggiero, A Di Pietro
- G30. PRABI. Pôle Rhône-Alpin de Bioinformatique.  
Appel national IBISA 2009 355 k€ pour PRABI-Gerland (C. Gautier, C. Combet, G. Deléage)
- G31. Plateau de graphisme 4D à l'IBCP.  
Extension du bâtiment IBCP plan campus (Lyon Cité Campus 2,2 M€ Conseil Général)  
G. Deléage, C. Geourjon
- G32. ECOFECT projet Labex (6M€) Investissements d'avenir  
D. Pontier/FL Cosset

#### IV.7. PATENTS

- V1. ANTHEPROT: Un logiciel d'analyse de séquences protéiques.  
Brevet déposé à l'ANVAR sous le numéro 87-5451.00  
Deléage G. & Roux B (1988)
- V2. AAV structural protein, production and applications.  
Medigene patent DE 19827457 and MG-AAV/98-01-US  
Hallek M, Ried M, Deléage G. & Girod A. (1998)
- V3. Patent WO03104388  
Process for identifying similar 3D substructures onto 3D structures and its applications.  
M. Jambon, G. Deléage, C. Geourjon (2003)

#### IV.8. MEETINGS ORGANISATIONS

- O1. Participation to European BioEnergetics Conference Organisation,  
July 1982, Villeurbanne, Resp : D.C. Gautheron
- O2. Responsable de l'organisation de l'atelier technique "Apport de l'informatique à l'analyse des protéines et des gènes" et membre du comité de lecture. 14<sup>ème</sup> Forum des jeunes chercheurs, Société de Chimie Biologique, Septembre 1987, Villeurbanne, Responsable L. Baggetto
- O3. Organisateur avec C. Geourjon des 11<sup>èmes</sup> rencontres nationales du "Groupe de Graphisme et Modélisation Moléculaire GGMM", Congrès de Lyon (Dardilly), 10-12 mai 1999

- O4. Responsable d'un groupe thématique intitulé "Analyse systématique des structures tridimensionnelles et des interactions" dans le cadre de l'action nationale IMPG "Informatique, Mathématiques et Physique pour la génomique" et organisateur d'une journée nationale sur la bioinformatique structurale (5 novembre 1999).
- O5. Membre du comité de programme et présidence invitée d'une session à JOBIM Journées Ouvertes: Biologie, Informatique et Mathématiques (JOBIM) 3 - 4 -5 mai 2000
- O6. Organisateur d'une journée thématique nationale sur le thème : "La modélisation moléculaire de protéines à faible taux d'identité" dans le cadre du GDR CNRS 2193 "Modélisation et simulation en biologie structurale" à Lyon le 14 décembre 2000.
- O7. Membre du comité scientifique de la première conférence européenne HealthGRID organisée à Lyon les 16-17 Janvier 2003.
- O8. Membre du comité scientifique du congrès « Bioinformatic Approaches to Protein—Protein Interactions », 11-12 Décembre 2003, Ecole Polytechnique.
- O9. Membre du comité scientifique de la 2<sup>e</sup> conférence européenne HealthGRID organisée à Clermont-Ferrand les 29-30 Janvier 2004.
- O10. Membre du comité scientifique et du comité d'organisation du congrès JOBIM 2005 à Lyon (6-8 juillet 2005).
- O11. Membre du comité scientifique des 11<sup>e</sup> journées de Gerland « Systèmes complexes et Biologie » 11-12 décembre 2006, Lyon
- O12. Membre du comité de programme à JOBIM Journées Ouvertes: Biologie, Informatique et Mathématiques (JOBIM) mai 2011
- O13. Membre du comité de programme à JOBIM Journées Ouvertes: Biologie, Informatique et Mathématiques (JOBIM) Juillet 2012

#### IV.9. TV INTERVIEW

- T1. TV interview (20') in City Campus Télé Lyon Métropole "La BioInformatique" (9 décembre 1999)
- T2. Interview on CORNEA contract in JT 19/20 02/06/2009

#### IV.10. IMPLICATION IN SCHOOL

- I1. The DOT Plot module of NATHEPROT has been integrated into ANAGENE a second degree school teaching software  
Collaboration with « Centre National de Documentation Pédagogique » (Mr Bouys
- I2. Conference for national teaching responsables for school programs INRP Lyon.  
15 septembre 2006

#### IV.11. SEMINARS AND INVITED TALKS

- S1. Méthodes de prédiction de la structure secondaire des protéines. Applications à un modèle de protéine enveloppe de rétrovirus aviaire. Séminaire donné au Centre de Génétique Moléculaire. *Invitation of Pr. J. Godet*, le 14 décembre 1990.
- S2. Démonstration d'ANTHEPROT à Oxford. *Invitation of Dr Steve Gardner* (Oxford Molecular avril 1992)
- S3. ANTHEPROT: un programme graphique interactif pour l'analyse de la structure des protéines à partir

- des séquences. (prédiction de structures, hydrophobicité, antigénicité, alignements multiples et recherche de sites fonctionnels) Séminaire et démonstration Ecole polytechnique *Invitation of E. Guittet and R. Lahana*. (9 juin 1992)
- S4. Démonstration de modélisation moléculaire lors de l'inauguration de l'IBCP le 16 octobre 1992 en présence du Directeur Général du CNRS et du ministre de la Recherche et de l'Espace.
- S5. Prédiction de structures de protéines et modélisation moléculaire sous contraintes RMN. Applications. Cours de DEA de Biomembranes, option Biochimie, Biologie Moléculaire et Biotechnologies. IBMIG, Université de Poitiers. *Invitation of Pr. Y. Cenatiempo*, 27 Mai 1994.
- S6. ANTHEPROT: de l'analyse de séquence à la détermination de la structure 3D de domaines protéiques par RMN. *Séminaire sur l'invitation of Pr. M. Ptak*, 19 novembre 1994
- S7. Prédiction de structures de protéines. INRA Toulouse, le 18 octobre 1996 *Invitation of Dr D. Kahn*
- S8. Détermination du pourcentage de structure secondaire d'une protéine à partir du dichroïsme circulaire. 26-27 novembre 1996, Vannes *Invitation of P. Masson (Sociétés Archimex et Jasco)*
- S9. Analyse de séquences en amont et en aval de la détermination de structures de protéines. 7 novembre 1997, Institut de Biologie Structurale, Grenoble *Invitation of Dr O. Dideberg*
- S10. De l'analyse informatique de la séquence protéique à la structure 16 décembre 1997, Institut National des Sciences Appliquées, Lyon *Invitation of Pr. J. Robert-Bauduy*
- S11. La relation séquence-structure 2D et 3D dans les protéines 2 mars 1998, Schering-Plough, Dardilly *Invitation of Dr E. Bates*
- S12. Méthodes de déconvolution de spectres de dichroïsme circulaire en pourcentage de structure secondaire d'une protéine. Séminaire à l'Institut Pasteur (26 Février 1999), Paris. *Invitation of Dr. Alain Chaffotte*
- S13. Bioinformatique moléculaire et structurale intégrée. Applications biologiques. Séminaire à l'IGBMC (13 décembre 1999), Strasbourg. *Invitation of JC Thierry et D. Moras*
- S14. « Recherche de domaines protéiques fonctionnels et modélisation de structures protéiques ». Journée thématique «Les banques de données en biologie : pourquoi, comment ?» à l'Institut Albert Bonniot (3 octobre 2000), Grenoble. *Invitation of J.J Lawrence*
- S15. Méthodes de prédictions de structures secondaires de protéines. Méthodologies et applications. 26 janvier 2001, CEA Marcoule. *Invitation of E. Quémeneur*
- S16. Apports et perspectives des prédictions structurales dans l'étude des interactions moléculaires. 18 janvier 2002, Grenoble. Séminaires Interface Biologie Informatique et Modélisation (IBIM)
- S17. Méthodes de prédictions de structures protéiques. Méthodes et applications 24 avril 2003, Bordeaux. *Invitation of Antoine de Daruvar*
- S18. Principes et applications des méthodes de prédictions des structures protéiques 2 octobre 2003, Nancy. *Invitation of Guy Branlant*
- S19. Principes et applications des méthodes de prédictions des structures protéiques 30 septembre 2004, Nancy. *Invitation of Guy Branlant*
- S20. Prédiction de structures protéiques, comment et pourquoi faire ? 11 mars 2005 IFR 136, Tours. *Invitation of Thierry Moreau*
- S21. De l'utilité pour le biologiste de prédire et modéliser la structure des protéines ? 30 mars 2005 Journées CBS, Montpellier. *Invitation of Cyrille Sarrauste de Menthère*

- S22. Principes et applications des méthodes de prédictions des structures protéiques  
8 septembre 2005, Nancy. *Invitation of Guy Branlant*
- S23. Utilisation des structures secondaires pour inférer des homologues lointains.  
17 avril 2009, Journées EVOL3D Paris. *Invitation of Bernard Labedan*

#### IV.12. PARTICIPATIONS TO EXTERNAL TEACHING

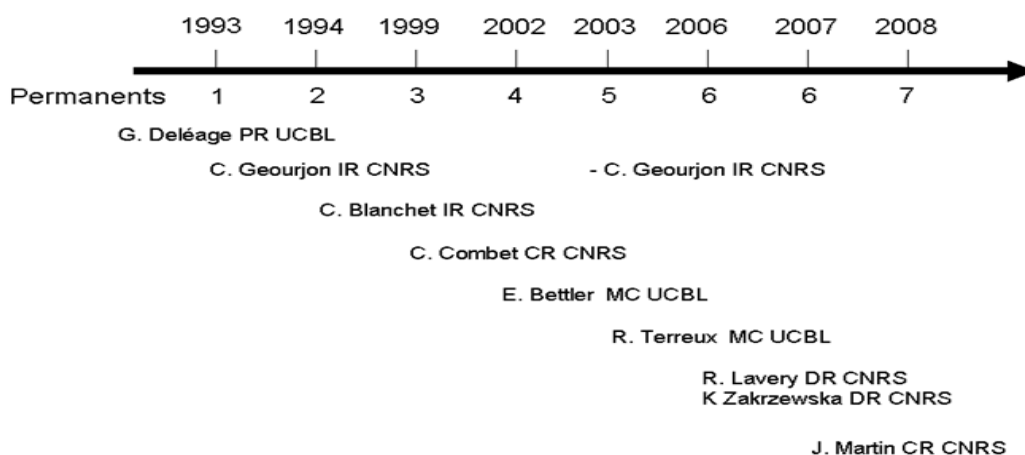
- F 1. Participation à la formation permanente du CNRS "Analyse statistique des séquences génétiques" Lyon (Organisation de la journée du 5 juillet 1989)
- F 2. Prediction of proteins structure and fundamentals of protein conformation. The state of the art. Dept. of Biochemistry. Université Nationale Autonome de Mexico. *3 jours de cours et formation pratique sur l'invitation du Pr. Mario Calcagno et du Dr Myriam Altamirano* 8-10 Juillet 1991
- F 3. RMN et Modélisation Moléculaire des protéines. Principes, exemples et applications. Co-organisation avec F. Penin d'une formation Interne du CNRS, Institut de Biologie et Chimie des Protéines du CNRS, Lyon, 24 Mai 1994.
- F 4. Organisateur de la formation permanente du CNRS "Réseau Internet en Biologie" Présentation et démonstrations, 26 janvier 1995.
- F 5. Organisateur d'une journée de formation EMBO : A practical approach to sequence analysis and molecular evolution (26-30 juin 1995) *Invitation de M. Gouy*
- F 6. Intervenant dans une formation permanente du CNRS sur l'analyse de séquences protéiques organisée par C. Geourjon le 14 septembre 1995
- F 7. Intervenant invité dans la formation aux journées thématiques "Bioinformatique" à l'Université de Rouen coorganisée par le CRIHAN (Centre Régional Informatique de Haute Normandie). (25-29 septembre 1995) *Invitation du Dr J. Alexandre*
- F 8. Cours portant sur les méthodes prédictives et biophysiques des protéines. Institut Mérieux *Invitation du Dr C. Valentin* (12 octobre 1993)
- F 9. Cours de formation « Les différents niveaux d'organisation des protéines » 15 septembre 1998 Société bioMérieux. *Invitation du Dr P. Dalbon*
- F 10. Cours de formation «Modélisation moléculaire des protéines» 17 novembre 1998 Société bioMérieux. *Invitation du Dr P. Dalbon*
- F 11. Intervenant invité dans la formation du CNRS aux journées thématiques "Bioinformatique" à l'Université de Rouen coorganisée par le CRIHAN (Centre Régional Informatique de Haute Normandie). (24 - 27 novembre 1998) *Invitation du Dr J. Alexandre*
- F 12. Intervenant invité dans le DESS de Bioinformatique de Rouen "Etude de Génomes, Outils Informatiques et Statistiques". (7 décembre 2000). *Invitation du Dr J. Alexandre*
- F 13. Conférencier dans l'atelier de formation INSERM 2001 organisé à Lyon le 11-12 Janvier 2001. Bio-Informatique : méthodes et pratiques pour l'analyse de l'information génomique. *Invitation de F. Rechenmann*
- F 14. La protéomique, un outil pour l'étude structurale et fonctionnelle des génomes. Ecole thématique INRA-CNRS Responsables : M. Rossignol et P. Jouin *Invitation du Dr. O. Gascuel* 8-12 octobre 2001
- F 15. Bioinformatique structurale des protéines Formation permanente du CNRS à l'IBCP. Responsable : C. Geourjon Lyon le 5 Juillet 2004.

### IV.13. GROUP COMPOSITION

Our group Bioinformatique:Structure et Interactions welcomed master graduate students from Lyon 1 university (resp :Pr. B. Roux, then V. Bulone, then S. Ricard-Blum). The team participates as a member of a European GDR-RA on comparative genomics (resp:C. Biemont) and has been evaluated as **A+** by independent AERES.

Name	Activity	Arrival-Leave	Function
DELÉAGE Gilbert	Bioinformatics	1993	Professor CE UCBL
BETTLER Emmanuel	Bioinformatics	2003	MC2-UCBL
BLANCHET Christophe	Bioinformatics	1999	IR1-CNRS
COMBET Christophe	Bioinformatics	2002	CR1-CNRS
GEOURJON Christophe	Bioinformatics	1994-2006	IR1-CNRS
<b>LIVERY Richard</b>	Molecular modeling	2007	DR1-CNRS
MARTIN Juliette	Bioinformatics	2008	CR2-CNRS
TERREUX Raphaël	Molecular modeling	2007	MC
ZAKRZEWSKA Krystina	Molecular modeling	2007-2012	DR2-CNRS

Progression of bioinformatics at IBCP



## V. TEACHING DUTIES

Since my nomination in 1984 and till in 2009, I made the totality of my teaching charge (in average 200H eqTD/year).

### V.1. MAIN COURSES (1985-1995)

- TD of Physico-chemistry in «Maîtrise de Biochimie» (B.P.M) on thermodynamics of solution and equilibrium of molecular association.
- Travaux dirigés de Biochimie structurale en Licence de Biochimie (B.S.M) on protein structure
- Travaux pratiques de Physico-chimie en Maîtrise de Biochimie (Fluorescence, diffusion de lumière et mesures de viscosité).
- Travaux pratiques de Biochimie Métabolique et Enzymologie (Localisation de l'activité glutamate dés-hydrogénase du foie de rat).

## V.2. COMPLEMENTARY TEACHING

- Cours magistraux et travaux dirigés dans l'U.V. d'Immunologie moléculaire.
- Travaux pratiques de Biochimie en DEUG Filière 4 2<sup>ème</sup> année

## V.3. NEW COURSES

- Adaptation de travaux pratiques sur la fluorescence en maîtrise de Biochimie: Etude par fluorescence de l'intercalation d'agents chimiques dans des molécules d'ADN.
- Montage de nouveaux travaux pratiques en fonction depuis octobre 1992 dans les U.V. de Biochimie Physico-chimique et Enzymologie et de Biosynthèse et Interactions des Macromolécules
- Analyse informatisée des séquences protéiques et initiation à la modélisation moléculaire.
- Cours dans l'option physico-chimie du DEA de biochimie: Méthodes d'analyse de la séquence des protéines.
- Cours de Modélisation Moléculaire dans l'U.V. de Biologie Structurale de l'Ecole Normale Supérieure de Lyon.
- Cours de Bioinformatique protéique à l'INSA de Lyon Filière Bioinformatique et Modélisation (BIM).
- Tutorat de stagiaires de L3 de l'ENS-Lyon et de l'INSA.

## V.4. SOFTWARE AND WEBSERVER FOR TEACHING PURPOSES

- **SIMULATION** : Software for simulated annealing simulation «sailor man algorithm» on 80 cities  
URL [http://pbil.ibcp.fr/~deleage/Cours/software/recuit\\_simule.exe](http://pbil.ibcp.fr/~deleage/Cours/software/recuit_simule.exe)
- **TITRATION**: Soft for titration curve calculation of proteins from sequence and PI calculation  
URL : [http://pbil.ibcp.fr/~deleage/Cours/software/Titration\\_Curve.exe](http://pbil.ibcp.fr/~deleage/Cours/software/Titration_Curve.exe)
- **ANTHEPROT 3D** : 3D molecular viewer (OpenGL)  
URL [http://pbil.ibcp.fr/~deleage/Cours/software/AntheProt\\_3D.exe](http://pbil.ibcp.fr/~deleage/Cours/software/AntheProt_3D.exe)
- **ANTHENUC** : [http://pbil.ibcp.fr/~deleage/Cours/software/ANTHE\\_NUC.exe](http://pbil.ibcp.fr/~deleage/Cours/software/ANTHE_NUC.exe)

## V.5. SUPERVISION OF STUDENTS

- E 1. « Etude d'une protéine par fluorescence intrinsèque: Facteur F1 du complexe ATPase-ATPsynthase. »  
N. Gedda  
(Biochemistry Master), February 1986.
- E 2. « Etude de la relation entre la classe structurale prédite des protéines avec le dichroïsme circulaire. »  
M. I. Moine  
(Biochemistry Master), February 1988.
- E 3. « Etude des effecteurs de la créatine kinase mitochondriale par fluorescence intrinsèque. »  
Geourjon C.  
(Biochemistry Master), February 1989
- E 4. « Alignements de séquences protéiques par programmation dynamique sur station de travail IBM Risc 6000 ». C. Aubin et I. Chabre

Computer science from Technology University Institute (Resp. Pr. Reboulet).

- E 5. Molecular modeling of *lac* operon repressor.  
G. Monard  
Structural Biology from ENSL (1-31 may 1993)
- E 6. Molecular modeling of BPTI under NMR restraints.  
F. Bard  
Structural Biology from ENSL (june 1993)
- E 7. Searching for consensus patterns in protein sequences  
C. Royet  
Grenoble DESS, 3 july - 25 september 1995
- E 8. Codon usage and secondary structure predictions  
J. Clevström, University Upsala Student (Sweden) 14 June – 30 july 1999
- E 9. Superimposition of protein 3D structures on the Web  
F. David, Lyon University, 2 july -10 August 2001
- E 10. Setup of a user licence system for ANTHEPROT software  
P. Cadet, Besançon University. 14 february 2005-29 July 2005

## V.6. PHD DIPLOMA RESPONSABILITIES

- R 1. G. Divita  
Structural and functional approaches of the mechanism of mitochondrial F1-ATPase-F1 from *Schizosaccharomyces pombe*  
Intermediate 1 year report DEA de Biochimie, Juin 1988  
Thesis defense : 15 october 1991
- R 2. C. Geourjon  
Methods to predict secondary structure of proteins Structural studies of mitochondrial F1 ATPase-F1.  
Intermediate 1 year report DEA de Biochimie, Juin 1990,  
Rhône-Alpes region fellowship  
Thesis defense : 1<sup>st</sup> june 1994  
Young researcher price of Lyon City 1995
- R 3. C. Lacombe (october 1993)  
Molecular modeling coarse.
- R 4. C. Blanchet  
« Etude de la stabilité de mutants d'hp $\beta$  par dichroïsme circulaire et modélisation moléculaire. »  
Intermediate 1 year report DEA de Biochimie, June 1995  
Thesis defense : 31 may 1999
- R 5. C. Combet  
Mise en place d'une banque de données cliniques et de séquences d'HCV  
Intermediate 1 year report DEA « d'analyse de séquences et de modélisation moléculaire » June 1997  
Thesis defense : 2001
- R 6. M. Errami  
Etude statistique des alignements multiples de séquences protéiques. Recherche d'une méthode de détection de mutations corrélées.  
Thesis defense : 2002
- R 7. N. Sapay  
« Les peptides d'ancrages à l'interface membranaire: analyses structurales par RMN et dynamique moléculaire et développement d'une méthode de prédiction bioinformatique. »

Intermediate 1 year report DEA « d'analyse de séquences et de modélisation moléculaire » (2002)  
co-direction with F. Penin  
Thesis defense : 31 may 2005

- R 8. N. Garnier (supervision by E. Bettler)  
« Développement d'une base de données de modèles 3D. »  
Thesis defense : October 2008
- R 9. M. Heymann (supervision by C. Geourjon)  
Développement d'une méthode de prédiction de structure 3D de protéine par couplage spectrométrie de masse et modélisation moléculaire  
Thesis defense : January 2009
- R 10. J.Hayer (encadrement par C. Combet)  
Thèse financée par une bourse fléchée du MESRT.  
Start : 01/10:2009
- R 11. V. Rech de Laval (encadrement par C. Combet/A Auouacheria)  
Thèse financée par une bourse Ligue.  
Start : 01/10:2009

## V.7. INVOLVEMENT IN THE STRUCTURATION OF LYON1 UNIVERSITY

In the context of new habilitation of diplomas in 1994, I setup a obligatory module (40H) of the master of Biochemistry diploma entitled: "Molecular modeling and biological sequence analysis" j'assume la responsabilité. The aim was to initiate the students with modern bioinformatics methods (biological databases, software usage and molecular modeling techniques) .At that time the purpose was not to make students programming. Since then, this has completely changed and I proposed a new module entitled "Graphics programming for biologists".

In the context of new habilitation of diplomas in 1998, a new module (UE) entitled « Bio-Informatics and Structural Biology » 125H was created in the master of Biochemistry. I assumed the responsibility of that module with Dr R. Haser, which covered biocrystallography, NMR and molecular modeling. In the new « LMD » program, I proposed a serie of programming modules (client/server and graphics) in Licence, of « molecular modeling and drug design» in professional Master and of "structural bioinformatics" in the research master in Biochemistry.

Besides, I am also co-chairman with D. Mouchiroud of M2 master module MIV entitled "Methods in Molecular Bioinformatics".

Today, the bioinformatics cursus is organised as follows:

At Claude Bernard Lyon 1 University:

Licence:

- UE IBIS "Introduction to structural Bioinformatics" (3 credits L2S4 resp: G. Deléage)
- UE "Graphics programming in Biochemistry" (3 crédits en L3 S5 resp: G. Deléage)

Master :

- UE "Structural Bioinformatics" (6 credits M1 resp: G. Deléage)
- UE "Molecular modeling and drug design" (M2 PRO resp: E. Bettler)
- UE "Methods in Molecular Bioinformatics" (UE M2, resp. D. Mouchiroud and G. Deléage)



Doctorat: Module of Bioinformatics shared by health ED

At "Ecole Normale supérieure de Lyon":

- UE "Statistics and computer science Applied to Biology" (3 credits L3 of master, resp. D. Mouchiroud and G. Deléage)

At "Institut National des Sciences Appliquées"(INSA) (60H):

- "Bioinformatique protéique" in INSA engineer school BIM "Bioinformatics and Modeling" 4<sup>th</sup> year (resp: G. Deléage)

**Table 1.** Teaching duties for the last 5 years

Module	2007	2008	2009	2010	2011	2012
Bioinformatique Structurale	36	35	35	35	35	35
Statistiques et Informatique Appliquées	18	6	9			
Mathématiques et Informatique du Vivant	6	-				
Bases de données 3D en biochimie					13	13
Informatique Graphique en Biochimie	22	26		34	34	34
Modélisation Moléculaire et Drug	5	5	5	5	5	6
Bioinformatique INSA	36	36	36	36	36	36
Introduction à la Bioinformatique	75	83	97	97	76	76
	<b>197</b>	<b>190</b>	<b>181*</b>	<b>207</b>	<b>199</b>	<b>200</b>

## V.8. SETUP OF BIOINFORMATICS MODULE AT "ECOLE NORMALE SUPERIEURE DE LYON"

In the context of Biology and Molecular and Cellular magister (BMC), I share the responsibility with D. Mouchiroud of the course "Statistics and computer science Applied to Biology" open in 1999-2000 and extended in the next contracts.

In addition, I was part of the team and participate in the jury of DEA "Analysis of Genomes and molecular modeling" under the supervision of Prof. S. Hazout (Diderot University, Paris 7).

I was also involved in the module 10 of Bioinformatics in "DEA de Génie Biologique et Médical" at doctoral school "Engineering for Health" in Grenoble.

I gave a course in bioinformatics (3H) in the Master in Computer Science from the University Joseph Fourier, Grenoble.

I am responsible for the Bioinformatics module protein at INSA Lyon in the engineering sector in Bioinformatics and Molecular Modeling. Finally, in 2001, a module with 3 transverse bioinformatics doctoral biological Lyon (E2M2, and EDISS BMIC) was set up and I was responsible for the EDISS doctoral school.