Location/venue (French Jura Mountains, close to Switzerland border)

Hôtel Club Le Risoux – 39220 Bois d'Amont – France
From main cities, TGV and flights to Geneva, Lausanne or Besançon (Vallorbe)

Dates

From Monday, December 11, 2006 (welcome reception at 11h30, start at 14h) –Thursday, December 14, 2006 (13h00)

Registration, residence and accommodation fees

INRA staff (including PhD students and postgraduate researchers): pedagogical, accommodation and residence fees are supported by the corresponding INRA departments; transport charges are paid by the research units.
Others (non invited persons, send us a purchase order) Participation to pedagogical, accommodation and residence fees are: 150€ for staff from non-INRA research units; 200 € for staff from Universities and other academic Institutions; 600 € for attendants from Private Sector.

Organization Committee

Fanny Guyomarch (fanny.guyomarch@rennes.inra.fr), Anne Tromelin (anne.tromelin@dijon.inra.fr), Cécile Tournu-Sammartino (tournu@nantes.inra.fr), Olivier Vitrac (olivier.vitrac@reims.inra.fr)

Registration

Please fill the registration form and include a short presentation of your research programs and concerns with respect to the proposed themes of the school.

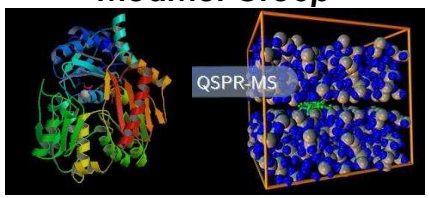
Send your registration by e-mail or Fax to:
nathalie.frelat@paris.inra.fr
Tel: +33 (0)1 42 75 90 33 - Fax: +33 (0)1 42 75 94 31

INRA

DEPARTMENT OF
SCIENCE AND PROCESS ENGINEERING
OF AGRICULTURAL PRODUCTS

PERSONNEL TRAINING
FormaSciences

ModMol Group



WINTER SCHOOL (3RD EDITION) IN

« Molecular and supramolecular modelling

Methods / Applications / Projects »

DECEMBER 11 – 14, 2006

HAUT-JURA (39)

Context

Molecular and supramomolecular modelling gathers different concepts, tools and methods to understand and to explore the assembly and the interactions between the components of the matter. In our department, Science and Process Engineering of Agricultural Products (CEPIA), these methods are primarily used to understand the interactions between the main components of the living matter (proteins, polysaccharides, lipids…) in their original environment (e.g. cell) or under their conditions of use (in reactor, in finished materials, in food…). With technological or cognitive ends, other applications are also considered: sensory perception of food (flavor, astringency), membrane separation techniques, food safety…

This modelling approach from molecular to supra-molecular levels presents rich and varied potentialities with regard to the scales of studies and the objectives, which are continued at INRA. To encourage an interdisciplinary construction of research programs, our department CEPIA set up in 2004 the transverse group MODMOL. It has already organized 2 research schools in 2004 and 2005 with the aim of bringing closer the following complementary disciplines: biology, physico-chemistry and condensed matter physic. To take part continuously in the development of this community, this third session focuses particularly on the partnerships with the specialists in molecular/supra-molecular modelling and on the support for the application to National and European research calls.

Objectives

Our objectives for the participants are :

- to acquire the basic knowledge, which facilitates the dialogue between specialists in molecular modelling and its users ;
- to share common tools and methods and to identify technical and practical needs;
- to identify people resources and to facilitate the emergence of future collaborations; to analyze collectively the existing disciplines and available competences within our department CEPIA, within and outside INRA;
- to exchange around projects under construction and to identify collectively the scientific questions, where molecular modelling could offer pertinent answers.

Participants

This school is initiated by the department CEPIA of INRA and is widely open to any researcher (permanent researcher, engineers, PhD students) interested in Molecular Modelling at atomistic scale or at mesoscopic scale.
Attendants will be selected on the basis of their research program.

Provisional Program

1. Introduction to molecular and supramolecular modelling, theoretical backgrounds → to acquire basic knowledge, to share similar concepts and vocabulary (the list of participants will be detailed in October)

- introduction to molecular mechanics "all atoms"
- introduction to coarse grained modelling: how to gather efficiently atoms ?
- extensions to multiscale computations and modelling at mesoscopic scale
- Dynamics and conformation searches of large molecular assemblies
- Principles of modelling of proteins by homologies

2. Molecular and supramolecular modelling in practice → to understand the approach and to identify the specificities and the technical requirements (the list of participants will be detailed in October)

This sequence is based on the illustrations of the experience of several researchers including "biologists" and "modellers" with a cross-representation of expectations, constraints, questions related to molecular modelling.

* Modelling of polysaccharides and cell wall constituents
* Practical application of mesoscopic modelling
* Modelling of the self-assembly of caseins
* Modelling of the structure and mechanical properties of Elastin
* Integration of spectroscopic data in molecular modelling approaches
* An example of need: approaches, questions, constraints *(F.Guyomarch)*

Round Table: discussion between biologists, physico-chemists and physicists with experience in modeling or not (why? which assumptions and approaches? how to integrate bio-physical data?, etc.)

3. Interactive sequences

Workshop 1: On the basis of presented lectures and experiences (theoretical and technical), the objective is to identify and to improve the current offer in specific training, shared databases, computational facilities and methods. The collected priorities will be used to set up actions in 2007.

Workshop 2: On the basis of three existing research programs (molecular interactions involved in astringency perception – modelling of low structured proteins and their interactions – modelling of transport properties in dense membrane of reverse osmosis), the objective is to illustrate and suggest specific supports for the definition and application of research programs: pertinent research questions, main limitations, possible collaborations…

4. Synthesis and perspectives

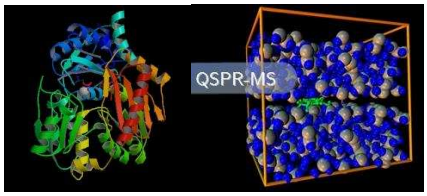
This final sequence will summarize the needs and proposals. Finally, a time schedule will be discussed for future actions.

INRA
Institut National de la Recherche Agronomique

FORMASCIENCES

DEPARTMENT of Science and Process Engineering of Agricultural Products

ModMol Group



WINTER SCHOOL

MOLECULAR AND SUPRA-MOLECULAR MODELLING

METHODS / APPLICATIONS / PROJECTS

11 – 14 DECEMBRE 2006
HAUT-JURA (39) - FRANCE

PRE-REGISTRATION FORM[1]

To send before October 2, 2006 by e-mail or fax :

nathalie.frelat@paris.inra.fr
Tél. : +33.(0)1.42.75.90.33 – Fax : +33.(0)1.42.75.94.31

Surname : .....
First name : .....

Institution : .....
Fonction : .....
Département : .....
Unit : .....

Professional adress : .....
.....

Tel. : .....
Fax : .....
Email : .....

☞ …/…

[1] *Since the number of places is limited, the organization will select the participants on the basis of the information provided in this form.*

Describe in few lines your topics and perspectives of research in the field of molecular modelling.

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-

Which are your concerns, questions and expectations with respect to this School? (e.g. training, methods, exchanges, collaborations…)

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On which topic or scientific questions – *either cognitive or methodological* – would you like to work more particularly during workshops? -

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Do you wish to exchange on your future research project or on your research project in progress? If so, specify the set of themes and the objects of debate which you would wish to address during the school.

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Other suggestions

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