

HERCULES

Higher European research course for users of large experimental systems

2010

NEUTRON AND SYNCHROTRON RADIATION FOR PHYSICS AND CHEMISTRY OF CONDENSED MATTER



Photo: ESRF, P. Gähler

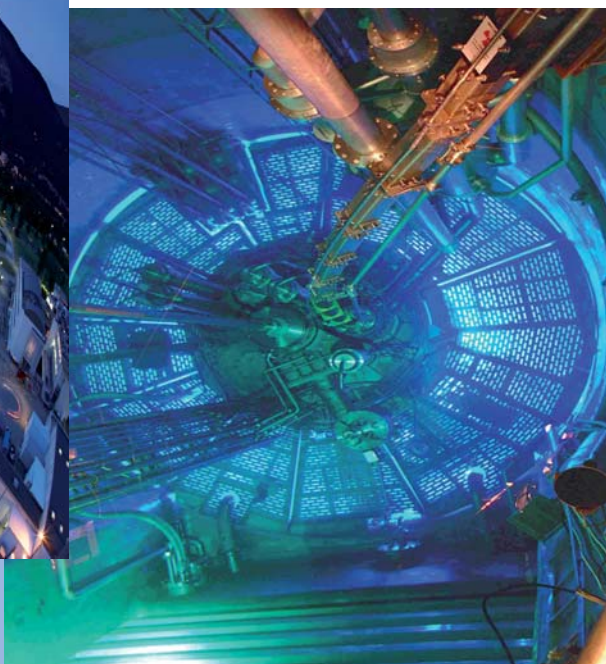


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20th Session - Grenoble, France :
February 21st - March 27th 2010

HERCULES XX symposium: March 25th and 26th

20

FIRST CIRCULAR



ORGANIZED / SPONSORED BY



Rhône-Alpes



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with the support of :

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- **Grenoble INP**

**ESRF, ILL, SOLEIL,
LLB, CNRS, CEA**

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SCOPE

This **five week course** is designed to provide training for PhD students, postdoctoral and senior scientists from European and non-European universities and laboratories in the field of **Neutron and Synchrotron Radiation for condensed matter studies** (Biology, Chemistry, Physics, Materials Science, Geosciences, Industrial applications).

It includes lectures, practicals and tutorials, visits of Large Facilities and a poster session (each participant will present a poster about her/his thesis or research topic).

This year a 2 days symposium will be organized at the end of the session for celebrating the 20th anniversary of the HERCULES programme.

Part I **BASIC METHODS AND INSTRUMENTS, is common to all participants**
(Common Part - 1,5 weeks)

Part II **is divided into two parallel specialized sessions (3,5 weeks)**

or **▪ Session A PHYSICS AND CHEMISTRY OF CONDENSED MATTER**
▪ Session B BIOMOLECULAR STRUCTURE AND DYNAMICS

The course is held in **Grenoble at the Polygone Scientifique Louis Néel**, where are located the Institut Laue-Langevin (ILL), the European Synchrotron Radiation Facility (ESRF), the European Molecular Biology Laboratory (EMBL) and the IBS (Institut de Biologie Structurale)

Practicals take place in these and other Grenoble laboratories.

A SPECIAL ONE WEEK PROGRAMME in the Paris area (March 14-21),
including lectures and practicals, will take place:

- either at **SOLEIL, Saint-Aubin (St-A)**, available for session A and session B participants, dedicated to a complementary synchrotron radiation programme including : free electron lasers, soft X-rays, ultraviolet and infrared radiation and their new fields of applications

- or at the **Laboratoire Léon Brillouin (LLB), CEA Saclay**, available for session A participants and a few session B participants (upon request): experimental reinforced neutron programme.

Important: on March 16th all participants will follow a common programme of lectures organized at SOLEIL, Saint-Aubin.

Part-time participants will attend only the lectures in Grenoble.

The language of the course is **English**.

ON LINE APPLICATION:

<http://hercules.grenoble.cnrs.fr>

WILL OPEN FROM SEPTEMBER 11TH TO OCTOBER 19TH, 2009

Applications are accepted from:

- **Students** enrolled in a doctoral programme of a European university.
- **Postdoctoral and senior scientists** from European public and industrial laboratories.
- The course is also open to **non-European doctoral students and postdoctoral scientists**.
- **The number of participants is limited.**

Selection is based on the advice of the Scientific Advisory and Organizing Committees.

- **Participants are expected to attend the whole course:**

Common Part (Part I) + one of the specialized sessions (Part II, session A or session B), *except for industrial scientists* for whom flexible timetables composed of weekly units can be devised.

You will have to specify whether you choose session A or session B, if session A: preference for the one week programme at SOLEIL, Saint-Aubin or LLB, Saclay and if session B: special request for the LLB, Saclay programme (4-5 participants only)

20th ANNIVERSARY OF THE HERCULES PROGRAMME

Organisers : José Baruchel and Jean-René Regnard

- **A HERCULES symposium of two days, HERCULES XX**, will aim to bring together the past HERCULES participants and the 2010 participants and to promote scientific exchange between them at the occasion of the 20th session of the course. During these 2 days, **Thursday March 25th and Friday March 26th 2010**, the scientific programme will be composed of lectures on the breakthroughs and the future prospects of the neutron and SR Science. The selected lectures will be both given by European experts and by recognized past HERCULES participants.
- **A poster session** will foster the scientific and informal exchange among all the HERCULES participants, the HERCULES staff and the scientists of the relevant Grenoble Community. The scientific fields covered by the poster session will be broader and will reflect the multidisciplinary audience of the HERCULES course.
- **Representatives of our partners and sponsors** will be invited to celebrate this event and hopefully to probe a positive feedback from the dynamic HERCULES community still working in the field.
- **A special item** will be devoted to the HERCULES XX symposium **on the HERCULES website**.
- **A pre-inscription form will be addressed** via an e-mailing to all the electronically registered past participants.
- **Accommodation** will be proposed **at negotiated rates** in selected hotels near the "Polygone Scientifique Louis Néel". Reduced registration fees will be quoted for the HERCULES participants.

Please disseminate as far as possible this information to your colleagues who have attended the HERCULES annual sessions.

REGISTRATION FEES

➤ REGISTRATION FEES

▪ **Students and postdoctoral scientists**

↳ From laboratories located in European countries	<i>contribution of 900 euros</i>
↳ From laboratories located outside Europe	1 900 euros

▪ **Senior scientists** (permanent position) 4 000 euros

▪ **Industrial scientists** 1 000 euros per week or 4 000 euros for the whole course

➤ ACCOMMODATION COST

Covers:

- hotel for the whole period of the course, including breakfast
- lunches during the five weeks and the meals during the HERCULES XX symposium (dinner and weekend meals are not covered)
- group travel from Grenoble to Paris and back for week 14-21 March

▪ **Students and postdoctoral scientists**

↳ From laboratories located in European countries	<i>contribution of 750 euros</i>
↳ From laboratories located outside Europe	1 400 euros

▪ **Senior scientists** 1 400 euros

▪ **Grenoble participants**

↳ contribution to the Paris area programme and the HERCULES XX programme 350 euros

⇒ Financial support for scientists in France through "Formation Permanente" organizations: CEA, ESRF, ILL... consult your local institute,
CNRS: let us informed if you are a permanent CNRS scientist or BDI-CNRS

⇒ Requests for part-time attendance at the course may be considered under exceptional circumstances.

IMPORTANT:

Contrarily to the previous years, we are not able to provide any special fellowship for less favoured countries, due to the end of our Marie-Curie contract with the European Commission.

PROGRAMME

COMMON LECTURES

BASIC METHODS AND INSTRUMENTS (27 h)

- | | | |
|----|--|--|
| 1. | Diffraction, refraction and absorption of X-rays and neutrons | W. Kuhs |
| 2. | Recent developments in structural biology
The role of Large Facilities | E. Pebay-Peyroula |
| 3. | Synchrotron radiation,
- production: different sources and their characteristics
- X-ray optics
- detectors | D. Attwood
R. Barrett
H.Graafsma |
| 4. | Neutrons: scattering and instrumentation | H. Schober |
| 5. | Neutron and X-ray diffraction by crystals: kinematical approximation
- Experimental diffraction methods | W.Kuhs |
| 6. | Diffuse scattering | J. Doucet |
| 7. | Small angle scattering | M. Müller |
| 8. | X-ray absorption spectroscopy: fundamentals and simple model of EXAFS | S. Pascarelli |
| 9. | Imaging techniques | J. Baruchel |

“REFRESHER” LECTURES (9.5 h)

- | | | |
|-----|------------------------------------|-----------------|
| 11. | Crystallography | B. Grenier |
| 12. | Magnetism | D. Givord |
| 13. | Introduction to spectroscopy | G. Margaritondo |
| 14. | Fourier Transform : basic concepts | C. Knupp |
| 15. | Quantum Mechanics | E. Belorizky |

PRESENTATION OF ILL AND ESRF

- | | |
|---|-------------|
| - Introduction to SR and ESRF, with emphasis on materials science | F. Sette |
| - Introduction to Neutron Science and ILL | A. Harrison |

SESSION A: PHYSICS AND CHEMISTRY OF CONDENSED MATTER

LECTURES (45 h/50 h)

I-

A'1. Neutron sources, optics and detectors (Saclay) A. Menelle/F. Ott

II- Interaction of radiation with matter: elastic case

A2.	Dynamical theory	T. Baumbach
A3.	Self-organised nano-structures in the light of synchrotron radiation	T.H. Metzger
A4.	Tomography and topography	J. Baruchel
A5.	Coherent imaging	P. Cloetens
A6.	Neutron and X-ray reflectometry	O. Seeck
A7.	Single crystal structure analysis	G. Heger
A8.	Magnetic scattering: X-rays and neutrons	C. Vettier
A9.	Powder diffraction	J. Rodriguez-Carvajal
A'10.	Polarized X-rays (Saint-Aubin)	M. Altarelli
A11.	Polarized neutrons	R. Stewart

III- Interaction of radiation with matter: inelastic case

A 12.	X-ray photon correlation spectroscopy	G. Grübel
A 13.	X-ray absorption spectroscopy : theoretical basis	J.Vogel
A 14.	X-ray absorption spectroscopies: the monoelectronic approach	Y. Joly
A'15.	Circular dichroism in XAS and its application (Saint-Aubin)	F. Baudelet
A'16.	Magnetic dichroism with photoelectron spectroscopy (Saint-Aubin)	F. Sirotti
A'17.	Soft X-rays magnetic dichroism (Saint-Aubin)	M. Sacchi
A18.	X-ray photoemission electron microscopy	C.M. Schneider
A19.	Neutron triple axis spectroscopy	R. Currat
A20.	Neutron time of flight spectroscopy	S. Bennington
A21.	Neutron spin echo spectroscopy	P. Fouquet
A22.	Neutron back-scattering spectroscopy	B. Frick
A23.	Diffraction anomalous fine structure	V. Favre-Nicolin
A24.	Inelastic X-ray scattering	M. Krisch
A25.	X-ray and UV photoemission spectroscopy	D. Malterre

IV- Special topics and selected examples of applications

A26.	Soft X-rays and VUV: specific optics and applications	D. Attwood
A'27.	Free electron lasers and ultra fast X-ray science (Saclay & St-Aubin)	M. Altarelli
A'28.	Synchrotron infrared emission and spectroscopic applications (Saclay & St-Aubin)	P. Dumas
A'29.	Solving surface problems using SR techniques (Saclay & St-Aubin)	A.Taleb / G. Renaud
A30.	Magnetic layers and multilayers	H. Zabel
A31.	Liquid and amorphous materials	A. Barnes
A32.	Soft condensed matter	A. Rennie

PRACTICALS Session A

All **full time participants** will carry out seven practicals in the Grenoble laboratories, European Facilities, and at SOLEIL, Saint-Aubin or Laboratoire Léon Brillouin, Saclay, from the following provisional list.

Applicants will have to state their preference in relation to the one week programme* proposed at SOLEIL or LLB in their application. However, as a quota of participants is required in each location, the organizers, on the basis of the scientific information provided by the applicants, could modify this choice.

Synchrotron Radiation practicals at ESRF, Grenoble

- EXAFS-XANES
- Circular magnetic dichroism in X-ray absorption
- Small angle X-ray scattering
- X-ray microscopy
- Energy dispersive X-ray spectroscopy
- Surface diffraction
- High pressure diffraction and/or spectroscopy
- High energy X-ray diffraction
- Micro-diffraction
- X-Ray powder diffraction
- Magnetic structure from neutron powder diffraction
- DAFS and anomalous scattering
- X-Ray topography
- X-Ray photon correlation spectroscopy

Synchrotron Radiation practicals at SOLEIL, Saint-Aubin

- Wavefront analysors and adaptative optics
- Chemical analysis of polymer films
- VUV ultra-high resolution absorption spectroscopy in the gas phase with a Fourier-Transform spectrometer
- Magnetic dichroism with photoelectron spectroscopy
- Optical study of material in the far infrared range
- Characterization of optic components for synchrotron radiation
- XAS under pressure
- Diffraction and EXAFS characterization
- Coupling VUV and Raman spectroscopies with X-ray spectroscopies
- High resolution ARPES
- Coherent diffraction
- X-Ray detector

Experimental demonstrations at ILL Grenoble

The ILL will not be in operation during the HERCULES 2010 session but a detailed tour of selected instruments and work on actual data with the instrument scientist will be organized. The instruments that can be visited include

- In situ time-resolved neutron powder diffraction
- Time of Flight inelastic neutron scattering
- Neutron Spin Echo
- Magnetic diffuse scattering with polarisation analysis
- Powder neutron diffraction
- Single-crystal magnetic diffraction
- Introduction to the neutron backscattering Technique
- Three Axis Inelastic neutron scattering
- Neutron Reflectometry
- Small Angle Scattering

Neutron practicals at LLB, Saclay

The LLB will be in operation, then providing the opportunity to perform experiments with neutrons beams.

- Neutron reflectometry
- Small angle neutron scattering
- Neutron scattering from liquids and amorphous materials
- Neutron powder diffraction
- Neutron single crystal diffraction
- Polarized neutron scattering
- Inelastic scattering, triple axis spectrometry
- Quasielastic scattering, TOF (time-of-flight) spectrometry
- Material science, stress & strain, texture

Laboratory practicals at Grenoble (CEA, CNRS, ESRF)

- Laue diffraction
- X-ray powder diffraction
- 2D single crystal diffraction
- Small angle X-ray scattering
- STM surface analysis and nanostructure

TUTORIALS

All **full time participants** will carry out at least four tutorials from the following provisional list. One of these tutorials will involve analysis of data collected during the practicals.

TUTORIALS

- X-ray topography
- Single crystal diffractometry
- Neutron and synchrotron powder diffraction data analysis
- Application of EXAFS data analysis in materials science
- XANES data analysis
- Anomalous scattering and DAFS on Q-dots systems
- Powder Diffraction
- Resonant X-ray magnetic scattering
- Circular magnetic dichroism in X-ray absorption
- Magnetization density studies by polarized neutrons
- Magnetic structure determination
- Quasi-elastic scattering
- Numerical modeling of molecular dynamics
- Small angle X-ray and neutron scattering
- Reflectometry
- Amorphous materials and liquids (structure factor determination)
- Surfaces, grazing incidence diffraction
- Diffuse scattering analysis
- Tomography reconstruction
- Coherent scattering
- Synchrotron beamline optics

Each student (within a small group) will be assigned a set of practicals and tutorials from the above list to match her/his background as closely as possible. If, however, **one or two** special requests are made for a given practical or tutorial, every effort will be made to satisfy this demand within the resources available.

See "Special request for practical/tutorial" when applying

NB: Full time participants are required to attend the entire practical and tutorial programme assigned to them.

SESSION B: BIOMOLECULAR STRUCTURE AND DYNAMICS

LECTURES (43 h)

I- Introduction

B1. Challenges in structural molecular biology A. Leslie

II- Protein crystallography

B2. Basics of protein crystallography, data collection, data reduction, phasing M.Roe
B3. Neutron crystallography M. Blakeley

III- Protein dynamics

B4. Introduction to the dynamics of macromolecules G. Zaccaï
B5. Protein dynamics by neutron scattering G. Zaccaï
B6. Kinetic protein crystallography D. Bourgeois
B7. Disorder and diffuse X-ray scattering D. Moss

IV- Diffusion and diffraction on larger scale biological systems

B'8. Small angle X-ray scattering on solutions (St-Aubin) P. Vachette
B9. Small angle neutron scattering G. Zaccaï
B10. Fibre and muscle diffraction C. Knupp

V- Spectroscopy

B11. Local order by X-ray absorption spectroscopy L. Murphy
B12. Time-resolved fluorescence and circular dichroism studies with SR G. Jones
B'13. Synchrotron infrared emission and spectroscopic applications (Saclay & St-Aubin) P. Dumas

VI- Imaging

B'14. Soft X-ray microscopy and spectroscopy with zone plates (Saclay & St-A) C. Jacobsen
B'15. Medical imaging with synchrotron radiation (Saint-Aubin) G. Tromba
B16. Synchrotron radiation as a tool for cancer research G. Le Duc

VII- Special topics

B17. Soft X-rays and VUV: specific optics and applications D. Attwood
B'18. Free electron lasers and ultra fast X-ray science (Saclay & Saint-Aubin) M. Altarelli
B'19. Biology with 4th generation sources (Saclay & Saint-Aubin) C. Jacobsen
B20. The ribosome at high resolution: selected steps in protein biosynthesis A. Yonath
B21. Crystallography of viruses and very large macromolecules D. Stuart
B22. Analysis and visualisation of 3D X-ray data C. Buckley
B23. X-ray and neutron reflectivity in biophysics T. Salditt
B24. Biomolecular simulation: theory and application M. Field

PRACTICALS

Session B

All **full time participants** will carry out one experimental project on protein crystallography and eight practicals in the Grenoble laboratories, European Facilities, plus, SOLEIL, Saint-Aubin or Laboratoire Léon Brillouin, Saclay, from the following provisional list.

Synchrotron Radiation practicals at ESRF, Grenoble

- EXAFS on biological samples
- Small angle X-ray scattering in solution
- Crystallography: Multi-wavelength data collection (MAD method)
- Powder diffraction applied to structural biology
- Time-resolved Laue diffraction
- X-ray imaging with soft X-rays
- Medical applications of synchrotron radiation
- Grazing incidence diffraction – Systems in solution
- Microtomography applied to biological systems
- Spectroscopy on biological samples (Cryobench)

Synchrotron Radiation practicals at SOLEIL, Saint-Aubin

- Synchrotron radiation protein crystallography : introduction to data collection and structure determination
- Single cells and human tissues biochemical imaging
- VUV ultra-high resolution absorption spectroscopy in the gas phase with a Fourier-Transform spectrometer
- Synchrotron radiation protein crystallography : introduction to data collection and structure determination
- Coupling VUV and Raman spectroscopies with X-ray spectroscopy
- Small Angle X-ray Scattering of online purified protein solutions
- Biological study in the far infrared range

Experimental demonstrations at ILL Grenoble

The ILL will not be in operation during the HERCULES 2010 session but a detailed tour of selected instruments and work on actual data with the instrument scientist will be organized. The instruments that can be visited include:

- Lipids and Protein dynamics
- Laue diffraction
- Protein crystallography at low resolution
- Neutron reflectometry from lipid/protein interactions
- Small Angle Scattering from protein solutions

Neutron practicals at LLB, Saclay

The LLB will be in operation, then providing the opportunity to perform experiments with neutrons beams.

- Neutron reflectometry
- Small Angle Neutron Scattering
- Neutron scattering from liquids
- Quasielastic scattering, TOF (time-of-flight) spectrometry

Laboratory practicals at Grenoble (ESRF, IBS, EMBL)

- Cryocrystallography
- Model building
- Protein expression
- Protein deuteration
- Crystallogensis & automation in structural genomics
- Crystal handling under controlled (anaerobic) atmosphere

TUTORIALS

All **full time participants** will carry out at least six tutorials from the following provisional list. One of these tutorials (solving protein structure) will involve analysis of data collected during practicals.

COMMON TUTORIALS

- Protein crystallography
- Applications of synchrotron infrared microspectrometry
- Fundamental on neutron scattering

TUTORIALS

- Solving protein structures with the MAD method
- EXAFS data analysis in biology
- Small angle diffraction
- X-ray Absorption Near Edge Spectroscopy data analysis

Each student (within a small group) will be assigned a set of practicals and tutorials from the above list to match her/his background as closely as possible. If, however, a special request is made for a given practical or tutorial (especially for the experimental project) every effort will be made to satisfy this demand within the resources available.

See "Special request for practical/tutorial" when applying

NB: Full time participants are required to attend the entire practical and tutorial programme assigned to them.

TRAVEL

Grenoble can be reached easily:

- by **TGV train** from Paris, Lille or Lyon
- **by air via Lyon airport (St Exupéry)**, with regular shuttle connections to Grenoble,
- also via Geneva and Grenoble airport.

HERCULES organizes travel by coach or TGV train to Paris for the week 15-21 March.

ACCOMMODATION

Accommodation will be provided in hotels located in Grenoble, and the 'plateau de Saclay' in the Paris area (including breakfast), as well as lunches during the week on the various sites.

ENTERTAINMENT

Grenoble is the capital of the French Alps and the course takes place during the skiing season. Several ski resorts and scenic sites are easily accessible from Grenoble by public transport.

SUPPORTED BY:

▶ European Commission : Research Infrastructures

↳ European Light Sources Activities (ELISA)

↳ Integrated Infrastructure Initiative for Neutron Scattering and Muon Spectroscopy (NMI3)

▶ European Synchrotron Radiation Facility (ESRF)

▶ Institut Laue Langevin (ILL)

▶ Ministère de l'Enseignement Supérieur et de la Recherche - France

▶ Centre National de la Recherche Scientifique (CNRS):

↳ Formation Permanente

↳ Laboratoires du Polygone Scientifique de Grenoble

▶ Commissariat à l'Energie Atomique (CEA):

↳ Direction des Sciences de la Matière (DSM)

↳ Direction des Sciences du Vivant (DSV)

↳ CEA Grenoble : Institut Nanosciences et Cryogénie (INAC)

▶ SOLEIL

▶ Laboratoire Léon Brillouin (LLB)

▶ Région Rhône-Alpes

▶ Conseil Général de l'Isère

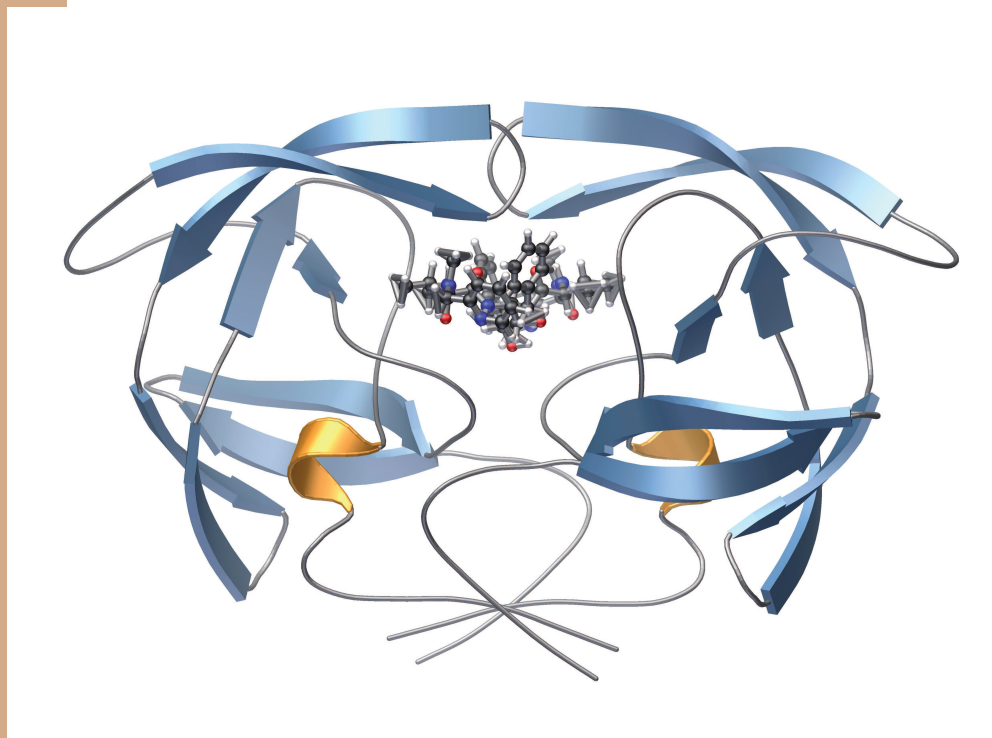
▶ METRO

▶ Ville de Grenoble

▶ UFR de Physique (Université Joseph Fourier)

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X Ray structure of HIV - 1 protease in situ product complex © J-L FERRER et al. FIP-BM30A-ESRF-Grenoble

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ON-LINE APPLICATION

<http://hercules.grenoble.cnrs.fr>
Open from September 11th to October 19th 2009

