ISBIO2015

Report for Instruct

Ana Luísa Carvalho & Eurico Cabrita

INTEGRATIVE STRUCTURAL BIOLOGY TOOLS FOR THE STUDY OF PROTEIN-LIGAND INTERACTIONS

Integrative Structural Biology tools for the study of protein-ligand interactions

Venue: The course was held at the Chemistry Department of Faculdade de Ciências e Tecnologia (FCT-Universidade Nova de Lisboa), hosted by the Associate Laboratory REQUIMTE and Research Unit UCIBIO.

Date: From the 13th to the 19th of July 2015

Website: http://eventos.fct.unl.pt/isbio

Aim of the course: The second edition of this course was stimulated by the high number of applicants of its first edition (October 6-12, 2014) and built on the experience gained by the tutors and the extremely positive feedback of the participants, namely that the course would have an impact in their research.

Therefore, our main objective was not only to continue to illustrate but also to reinforce the added value of a structural biology approach to the study of protein-ligand interactions. In this edition this was achieved by introducing new core methodologies; EPR and Molecular Modeling, combined with the 4 of the first edition, X-ray Crystallography, NMR, Carbohydrate Microarrays and ITC. These methods were explored from a hands-on perspective, giving emphasis to their limitations and complementarities.
Besides the hands-on training there were theory lectures where the main theoretical aspects of each technique were explained always with an emphasis on the complementarities with the other techniques.

Outcome:
The seven days course was composed of theory lectures and practical sessions. These included hands-on training on various instruments and applications. The total number of participants was 18. Of these, 16 were PhD students, 1 Post-doctoral and 1 Graduate student, currently performing research work in Portugal (6), Germany (3), Israel (1), Switzerland (1), Sweden (1), Brazil (1), Finland (1), United Kingdom (1), Poland (1), Belgium (1) and Denmark (1).

During the 7-day course, all activities run according to scheduled, including lessons and social events. All participants were allowed to orally present their research work.

A Google Drive was prepared to make available all the course documentation to the participants:
https://drive.google.com/folderview?id=0B4UcDeYn0xOrYWZlS0FkOW54QjA&usp=sharing
Participants were asked to fill in a questionnaire reporting their view of the course (https://drive.google.com/open?id=0B4UcDeYn0xOrQkFOdHVXeENpSnc).

Generally, comments were very positive and enthusiastic.
Reading the comments, the organizers believe that the participants received an important overview of different biophysical methods available to study protein-ligand interactions, spanning from calorimetric techniques to spectroscopic and structural methods, associated to the valuable information provided by the array technology. Participants were generally familiar with one or more of these methods but had not before addressed these studies from an integrated structural biology perspective and we believe that this has been achieved with the course.

Course Organisers:

Title, Name, Organisation, Contact Details, Country
Assistant Researcher, Ana Luísa Carvalho, UCIBIO-REQUIMTE-FCT-UNL, almc@fct.unl.pt, Portugal
Assistant Professor, Eurico Cabrita, UCIBIO-REQUIMTE-FCT-UNL, ejc@fct.unl.pt, Portugal

The course theory and practical lessons were held by members of the different research groups from UCIBIO (http://eventos.fct.unl.pt/isbio/pages/course-tutors).

List of Invited Speakers:

Name	**Country**	**E-mail**	**Institute**
Fraser MacMillan	United Kingdom	fraser.macmillan@uea.ac.uk	University of East Anglia
Celso Reis	Portugal	celsor@ipatimup.pt	IPATIMUP & i3S

List of Participants:

Family name	***Name***	***email***	***Institution***	***Current activity***
Barber-Zucker	Shiran	shiranbarber@gmail.com	Ben-Gurion University of the Negev, Israel	PhD student
Diniz	Ana	a.diniz@campus.fct.unl.pt	UCIBIO-REQUIMTE, FCT-UNL, Portugal	PhD student
Franco Pinheiro	Pedro	pedro.pinheiro@ist.utl.pt	Instituto Superior Técnico, Portugal	Research grantee
Fuchs	Simon	simon.fuchs@biochemie.uni-freiburg.de	Universität Freiburg, Germany	PhD student
Gmeiner	Christoph	christoph.gmeiner@phys.chem.ethz.ch	ETH Zürich, Switzerland	PhD student
Gomes	Ana Sara	anasarag4@gmail.com	UCIBIO-REQUIMTE, ICBAS-UP, Portugal	PhD student
Gomes	Sara	up200802730@icbas.up.pt	UCIBIO-REQUIMTE, ICBAS-UP, Portugal	PhD student
Kesgin-Schäfer	Stephanie	stephanie.kesgin-schaefer@chemie.uni-hamburg.de	University Hamburg, Germany	PhD student
Leitão	André	andre.leitao87@gmail.com	Faculty of Veterinary Medicine, UL, Portugal	PhD student
Martínez	Markel	markel.martinez@dbb.su.se	Stockholm University, Sweden	PhD student

Montefusco Pereira	Carlos Victor	cmontefusco@gmail.com	University of Barcelona, Spain	PhD student
Muleta	Abdi Worku	amuleta@btk.fi	University of Turku, Finland	PhD student
Mullen	Anna	a.mullen@uea.ac.uk	University of East Anglia, United Kingdom	Graduate student
Otręba	Marta	marta.otreba@chem.uni.wroc.pl	University of Wroclaw, Poland	PhD student
Ramou	Ioanna	ioanna.ramou@ugent.be	Ghent University, Belgium	PhD student
Santos	Marino	mf.santos@campus.fct.unl.pt	UCIBIO-REQUIMTE, FCT-UNL, Portugal	PhD student
Soerensen	Marlene Uglebjerg	marlene.soerensen@mbg.au.dk	Aarhus University, Denmark	PhD student
Tavares Macedo	Joana	joana.tavares-macedo@uni-tuebingen.de	University of Tuebingen, Germany	PhD student

Course Program:

ISBio2015 Training Course, Caparica, Portugal

	13th July Monday - Day 1		*14th July Tuesday - Day 2*		*15th July Wednesday - Day 3*		*16th July Thursday - Day 4*	
9:00-10:30	Registration, knowing the participants and other introductory remarks Lecture: Carbohydrate microarrays and ligand discovery *2.17D*		Lecture: - ITC and protein-ligand interactions - Case studies *2.17D*		Lecture: NMR and protein-ligand interactions *2.17D*		Hands-On: Training session on NMR (the ligand viewpoint) (Group 1) *NMR Lab (1st floor)*	Hands-On: Training session on NMR (the ligand viewpoint) (Group 2) *2.04*
10:30-11:00	*Coffee break (2.17D, 2nd floor)*							
11:00-13:00	Hands-On: Training session on Microarray screening analysis (Group 1) *Lab 6.25*	Hands-On: Training session on fluorescence imaging (Group 2) *Lab 4.15*	Hands-On: Training session on ITC (sample preparation, starting the experiment) / Planning the experiment (Group 1) *Lab ITC (6th floor)*	Hands-On: ITC data analysis (Group 2) *2.04*	Hands-On: Training session on NMR (sample preparation, acquisition and basic processing) (Group 1) *NMR Lab (1st floor)*	Hands-On: Training session on NMR (sample preparation, acquisition and basic processing) (Group 2) *2.04*	Hands-On: Training session on NMR (the protein viewpoint) (Group 1) *NMR Lab (1st floor)*	Hands-On: Training session on NMR (the protein viewpoint) (Group 2) *2.04*
13:00-14:30	*Lunch break (Ágora room, next to FCT Library building)*							
14:30-15:30	Invited lecture (Prof. Celso Reis, IPATIMUP, Portugal) *2.17D*		Hands-On: ITC data analysis (Group 1) *2.04*	Hands-On: Training session on ITC (sample preparation, starting the experiment) / Planning the experiment (Group 2) *Lab ITC (6th floor)*	Lecture: NMR and protein-ligand interactions *2.17D*		Lecture: Molecular Modeling *2.17D*	
15:30-16:00	*Coffee break (2.17D, 2nd floor)*							
16:00-18:30	Hands-On: Training session on fluorescence imaging (Group 1) *Lab 4.15*	Hands-On: Training session on Microarray screening analysis (Group 2) *Lab 6.25*	*(this period is allocated to work on students' own samples, if any)*		*Social program (Lisbon walking tour)*		Hands-On: Molecular Modeling *2.04*	
	Hands-On: Training session on microarray data analysis and identification of ligands *2.04*							
18:30-19:00	"Integrative" discussions of each day subjects, including poster presentations from the course participants *2.17D*		"Integrative" discussions of each day subjects, including poster presentations from the course participants *2.17D*				"Integrative" discussions of each day subjects, including poster presentations from the course participants *2.17D*	
					Social dinner from 7:30pm (Lisbon, Põe-te Na Bicha)			

	17th July Friday - Day 5	18th July Saturday - Day 6		19th July Sunday - Day 7
9:00-10:30	Invited lecture - EPR (Prof. Fraser MacMillan, Univ East Anglia, UK) 2.2	Lecture: X-ray Crystallography and protein-ligand interactions (X-ray sources, diffraction and data analysis) 2.17D		Lecture: X-ray Crystallography and protein-ligand interactions (the phase problem, 3D structure solution) Lecture: Model and ligand building, refinement and validation) 2.17D
10:30-11:00	*Coffee break (room 2.17L, 2nd floor)*	*Coffee break (room 217D, 2nd floor)*		
11:00-13:00	Hands-On: EPR 2.04	Hands-On: Cryo-preservation of protein crystals and X-ray diffraction (Group 1) *1.12 (X-ray Lab)*	Hands-On: Indexing, integration and scaling of X-ray diffraction data (Group 2) 2.04	Hands-On: Structure solution by MR methods; structure analysis, validation and representation 2.04
		Hands-On: Indexing, integration and scaling of X-ray diffraction data (Group 1) 2.04	Hands-On: Cryo-preservation of protein crystals and X-ray diffraction (Group 2) *1.12 (X-ray Lab)*	Closing remarks, lunch and departure
13:00-14:30	*Lunch break (Ágora room, next to FCT Library building)*	*Lunch break (restaurant Campus.Come)*		
14:30-15:30	Lecture: X-ray Crystallography and protein-ligand interactions (crystallization, symmetry and spacegroups) 2.2	Invited lecture (Prof. Maria João Romão, UCIBIO, Portugal) 2.17D		
15:30-16:00	*Coffee break (room 2.17L, 2nd floor)*	*Social program (free afternoon)*		
16:00-18:30	Hands-On: Crystallization of protein-ligand complexes *Lab 6.23*			
18:30-19:00	"Integrative" discussions of each day subjects, including poster presentations from the course participants 2.2			

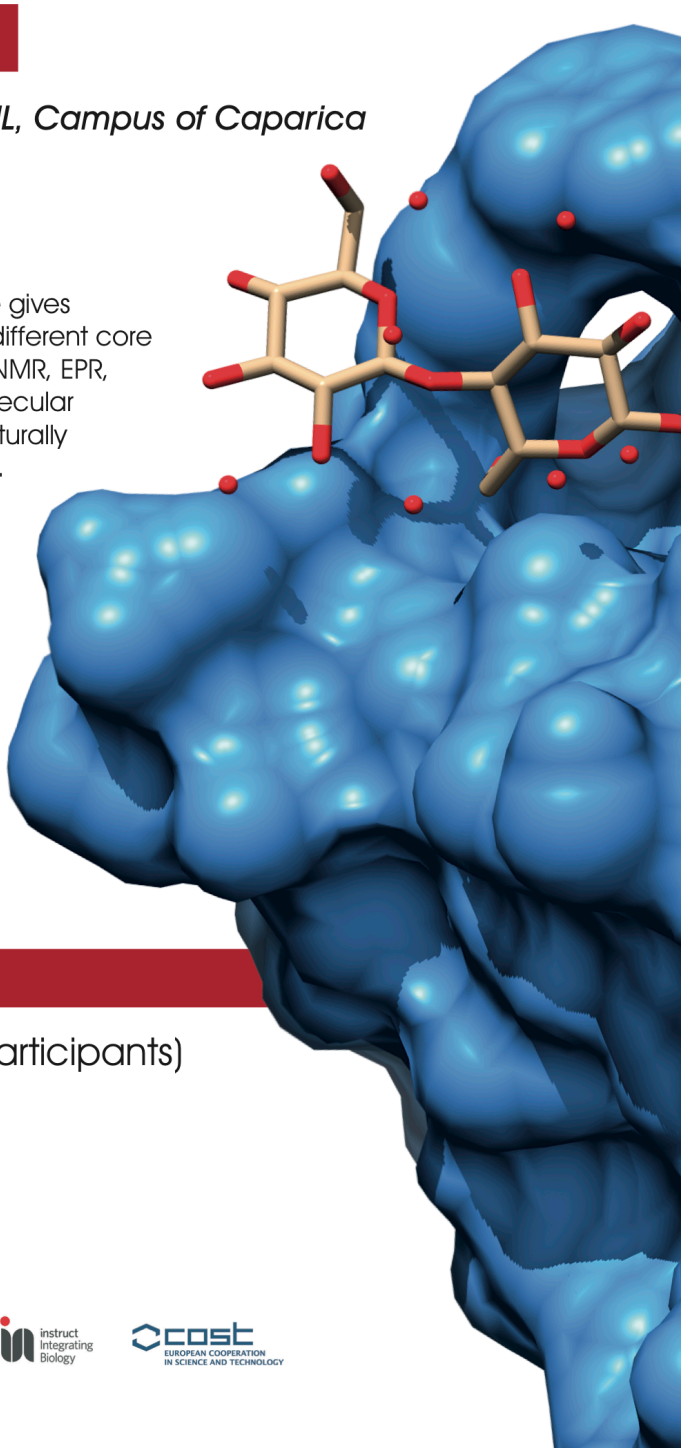
instruct Integrating Biology

Poster or other material advertising the course:

Integrative Structural Biology tools
for the study of protein-ligand interactions

13th to 19th July 2015

Chemistry Department, FCT-UNL, Campus of Caparica



This INSTRUCT-supported Training Course gives a hands-on perspective on the use of different core methodologies (X-ray Crystallography, NMR, EPR, Carbohydrate Microarrays, ITC and Molecular Modeling), in a combined way, to structurally characterise protein-ligand interactions.

Besides the hands-on training there will be theory lectures where the main theoretical aspects of each technique will be explained always with an emphasis on the complementarity with the other techniques.

Application deadline:

15th of June (limited to 18 participants)

http://eventos.fct.unl.pt/isbio

FCT Faculdade de Ciências e Tecnologia Universidade Nova de Lisboa

UCIBIO @ REQUIMTE

PTNMR

instruct Integrating Biology

cost European Cooperation in Science and Technology

Group Photo:


ISBIO 2015
Integrative Structural Biology tools for the study of protein-ligand interactions
Chemistry Department, UCIBIO-FCT-UNL, Caparica, Portugal
July 13-19, 2015
Organizers: Ana Luísa Carvalho & Eurico Cabrita