



2nd Meeting 2016

24-27 May, 2016. Madrid, Spain.

2nd CIRCULAR

Tuesday 24th May

DIOMUNE/CBM-CSIC

<http://bit.ly/1WmIQfe>

DIOMUNE/CBM-CSIC is located outside Madrid, at the Cantoblanco Universidad Autónoma de Madrid campus. **We strongly suggest to use the private bus at Aparthotel Muralto.**

9:00 hrs. Private bus towards DIOMUNE

MEETING POINT: Aparthotel Muralto: C/ Buen Suceso, 3, 28008-Madrid.

<http://www.muralto.es/en/location/>

10:00-11:15 hrs. “The Fight against Scientific Misconduct: Research Integrity and Good Scientific Practices”.

Prof. Pilar Goya (IQM-CSIC)

11:15-11:45 hrs. Coffee break

11:45-13:00 hrs. **Course 4 (I): Presentation and writing skills.**

Prof. Juan Mareque (CIC-biomaGUNE)

13:00-14:15 hrs. Lunch

14:15-15:15 hrs. Visit to Animalarium (DIOMUNE)

15:15-17:00 hrs. **Course 6 (I): Entrepreneurship and Company Management.** “From science to market “.

Dr. Miguel Ángel Llamas (DIOMUNE)

17:15 hrs. **Private bus** to Aparthotel Muralto.

19:00 hrs. **Networking & cultural activity.** Madrid city tour (MEETING POINT: fountain at Plaza de España).

<http://bit.ly/1Ty2puv>

20:30 hrs. End of the city tour at Plaza Mayor and tapas dinner.

<http://bit.ly/24GGIQv>

Wednesday 25th May
ICTAN-CSIC
<http://bit.ly/1Sympwx>

8:45-10:30 hrs. **Workshop 1. Ligand/protein interactions, the bottom-up approach.**
Modern NMR methods in molecular recognition.

Prof. Jesús Jiménez-Barbero (CIC-bioGUNE) & Prof. Alba Silipo (UNINA).

Introduction. The ligand based approach. Relaxation and dynamics. NOE. TrNOESY.
STD. WaterLOGSY.

10:30-11:00 hrs. Coffee break

11:00-12:45 hrs. **Workshop 1.**

Innovative microscopy techniques for receptor imaging and tracking in vivo and in tissues.

Dr. Wolfgang Hübner (UNIBI).

Nanoscopy techniques for the observation of cellular components.

12:45-14:00 hrs. Lunch

14:00-15:00 hrs. **Course 5 (I): “Pharmaceutical Quality System: EU GMPs requirements”.**

Dr. Ligorati (GMP Consultant)

15:00-16:00 hrs. **Workshop 1.**

Molecular modelling in supramolecular chemistry (CSIC).

Prof. Sonsoles Martín-Santamaría (CIB-CSIC).

Basis: Quantum Mechanics. Geometry optimization. Calculation of properties and transition states. NBO.

16:00-16:30 hrs. Coffee break

16:30-17:30 hrs. **Workshop 1.**

Modern NMR methods in molecular recognition.

Prof. Jesús Jiménez-Barbero (CIC-bioGUNE) & Prof. Alba Silipo (UNINA).

Diffusion. Other nuclei: ¹⁹F. Other methods. Some examples.

17:30-18:30 hrs. **Workshop 1.**

Molecular modelling in supramolecular chemistry (CSIC).

Prof. Sonsoles Martín-Santamaría (CIB-CSIC).

Basis: Molecular Mechanics. Force fields. Molecular dynamics simulations. QM/MM.

Thursday 26th May

CIB-CSIC, Room 377 (3rd Floor)

<http://bit.ly/238J7WV>

8:45-10:30 hrs. **Workshop 1. Ligand/protein interactions, the bottom-up approach.**
Innovative microscopy techniques for receptor imaging and tracking in vivo and in tissues.

Dr. Wolfgang Hübner (UNIBI).

Hands-on with Stochastic optical reconstruction microscopy on TLR4 expressing Liver Sinusoidal Endothelial Cells.

ICTAN-CSIC

<http://bit.ly/1Sympwx>

10:30-11:00 hrs. Coffee break

11:00-11:50 hrs. **Workshop 1.**

Modern NMR methods in molecular recognition.

Prof. Jesús Jiménez-Barbero (CIC-bioGUNE) & Prof. Alba Silipo (UNINA).

The receptor based approach. HSQC: SAR by NMR. Other variations. FBBD: Shapes. Some examples. Combining ligand- and receptor-based approaches. Some examples.

11:55-12:45 hrs. **Workshop 1.**

Molecular modelling in supramolecular chemistry (CSIC).

Prof. Sonsoles Martín-Santamaría (CIB-CSIC).

Molecular recognition: ligand/receptor and protein/protein interactions. Docking. Virtual screening.

12:45-14:00 hrs. Lunch

CIB-CSIC

<http://bit.ly/238J7WV>

14:00-15:10 hrs. **Visit to CIB-CSIC facilities (NMR, EM, X-Ray)**

- Route A (ESRs 1-6). 14:00-14:20-NMR. 14:25-14:45-EM. 14:50-15:10-X-Ray.

- Route B (ESRs 7-13). 14:00-14:20-EM. 14:25-14:45-X-Ray. 14:50-15:10-NMR.

ICTAN-CSIC

<http://bit.ly/1Sympwx>

15:15-16:45 hrs. **ESRs presentations* (10 + 5 min) ESR 1-6**

16:45-17:15 hrs. Coffee break

17:15-19:00 hrs. **ESRs presentations* (10 + 5 min) ESR 7-13**

***Guide lines for ESR presentation:** personal introduction (3 min, country of origin, graduate & master studies, etc.) + TOLLerant project (7 min, objectives & results).

20:15 hrs. **MEETING DINNER.**

Círculo de Bellas Artes. C/ Alcalá, 42. 28014 Madrid (“Banco de España” Tube Station).

<http://bit.ly/1ObpBSU>

20:15 hrs. Vine & Soft drinks at Azotea (rooftop) of “Círculo de Bellas Artes”

<http://www.circulobellasartes.com/azotea/>

21:00 hrs. Meeting Dinner. Restaurant “La Pecera” of “Círculo de Bellas Artes”

<http://www.lapeceradelcirculo.com/>

The **Círculo de Bellas Artes (CBA)** is a private, non-profit, cultural organization that was founded in 1880. Its building is located in the “castiza” Alcalá Street. The CBA is a major multidisciplinary centre with one of the most active cultural programmes in Madrid. It has exhibition rooms, a cinema, a theatre, concert halls, lecture halls, artists’ workshops, a library, a cafeteria, a shop and many other facilities. Every day it puts on activities to do with the visual arts, music, film, the stage, literature, science, philosophy and poetry.

The building which houses the Círculo de Bellas Artes was designed by the architect Antonio Palacios and constructed in 1926. It is an emblematic building and from its rooftop you can enjoy some of the best views of Spain’s capital city.

More information about the “Círculo de Bellas Artes”:

<http://www.circulobellasartes.com/>

https://en.wikipedia.org/wiki/C%C3%ADrculo_de_Bellas_Artes

Friday 27th May

CIB-CSIC

<http://bit.ly/238J7WV>

9:00-10:30 hrs. **Workshop 1. Ligand/protein interactions, the bottom-up approach.**

Hands-on tutorial on molecular modelling: docking of IAXO-102 into TLR4/MD-2 (CSIC).

Prof. Sonsoles Martín-Santamaría (CIB-CSIC).

Demonstrators: Jean-Marc Billod, Joan Guzmán-Caldentey, Alessandra Lacetera and Florent Cochet.

10:30-11:45 hrs. ESRs meeting/IPs meeting.

(In parallel rooms including coffee break)

11:45-13:15 hrs. SB meeting.

13:15-13:30 hrs. Closing.

VENUES:

24th May 2016

9:00 hrs. Private bus towards DIOMUNE

(MEETING POINT: Aparthotel Muralto: C/ Buen Suceso, 3, 28008-Madrid).

<http://www.muralto.es/en/location/>

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DIOMUNE Laboratories at CBM-CSIC. <http://www.cbm.uam.es/joomla-rl/index.php/en/>

Google Map: <http://bit.ly/1MOuHmU>



VENUES:

25th-27th May 2016

ICTAN-CSIC (neighbour building to CIB-CSIC)

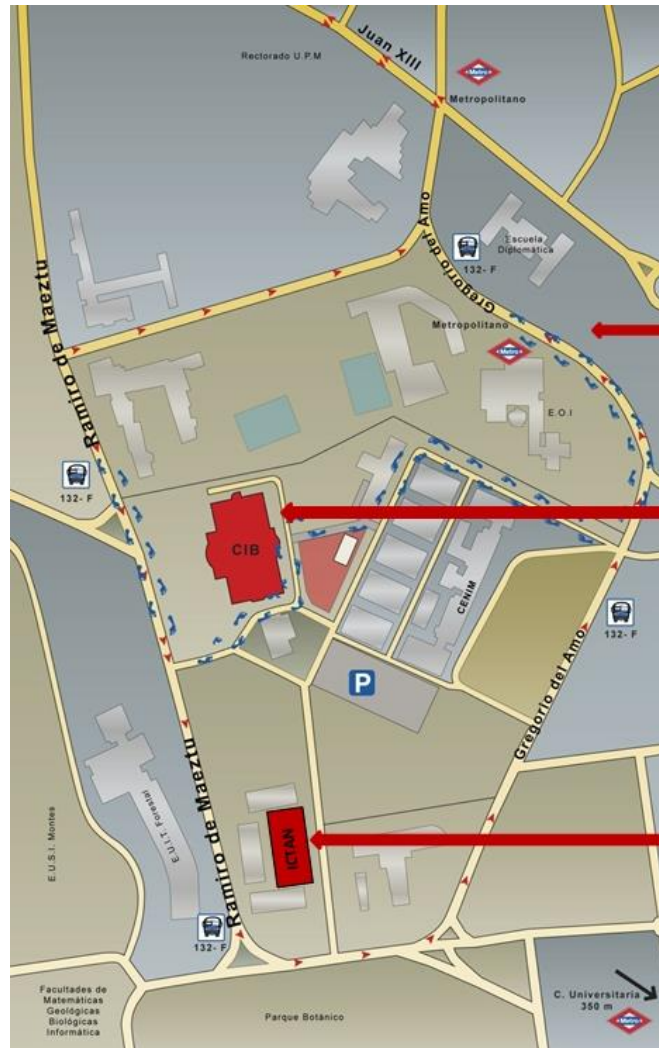
<http://www.ictan.csic.es/en/>

Google Map: <http://bit.ly/1Sympwx>

CIB-CSIC (visit, Hands-on tutorials and SB meeting)

<http://www.chemphysbiol.org/contact/>

Google Map: <http://bit.ly/238J7WV>



Metro Line 6
Station "Metropolitano"
EXIT: Gregorio del Amo

CIB
CIB research facilities
(visit on Thu 26th May)
<http://bit.ly/238J7WV>

VENUE
ICTAN (Institute of Food
Science, Technology &
Nutrition)
<http://bit.ly/1Sympwx>