

## Open PHACTS 2nd Workshop

February 16<sup>th</sup> and 17<sup>th</sup>, 2015

Venues: Casa de Europa, Santiago de Compostela

CiMUS Research Center, Santiago de Compostela

(Limited seats available)

**February 16th, Monday. Venue: Casa de Europa** (Parque Vista Alegre, Rúa Salvadas s/n)

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### Reception and Welcome Coffee

08:30-09:00

Reception: Maribel Cadavid, Alba Iglesias, Sonia Lage, Oscar Lestón, Jose Manuel Santamaría and Marta Solla (*USC*).

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### Workshop Welcome and Introduction

09:00-09:30

Chair: Mabel Loza-Innopharma coordinator (*USC*).

Facilitators:

- Kiera McNeice- *eScience Support Specialist in the Strategic Innovation Group at RSC.*
  - Begoña Roibás-*Business Developer Manager at Innopharma (USC).*
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09:30-11:30

### Contributors' presentations (listed in alphabetical order)

- Ola Engkvist-*Team Leader, Computational Chemistry, Chemistry Innovation Centre, Discovery Sciences, AstraZeneca R&D.*
- Edgar Jacoby- *Senior Principal Scientist Molecular Informatics at J&J.*
- Marta Piñeiro- *Director, Open Innovation Drug Discovery, at Eli Lilly and Company.*
- María Jesús Blanco- *Director, Discovery Chemistry Research & Technologies Eli-Lilly and Company.*
- Ceara Rea- *Investigator within the Computational Chemistry dept.at GSK.*
- Jose Miguel Vela- *Director of Drug Discovery & Preclinical Development at ESTEVE.*
- Javier Burgueño- *Director of Screening In Vitro and Assay Development at ESTEVE.*
- Bryn Williams-Jones (OPF)- *CEO of the Open PHACTS Foundation.*

Chair: Derek Marren-*Director IT–Research Biology systems at Lilly & Erl Wood Research site director.*

Facilitator: Kiera McNeice- *eScience Support Specialist in the Strategic Innovation Group at RSC.*

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11:30-12:00

Coffee Break

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## Roundtable discussion among Contributors, Challengers and Attendants

### Challengers (listed in alphabetical order)

- Petr Bartunek- *Group leader at the Institute of Molecular Genetics and Director of CZ-OPENSSCREEN: National Infrastructure for Chemical Biology.*
- Iván Cornella- *Sr. Principal Scientist-Chemistry Capabilities Enhancement – Chemical Biology Lead at Merck Research Laboratories.*
- Willem Van Hoorn (pending)- *Head of Chemoinformatics at ex scientia Ltd.*
- David Wild (Indiana University)- *Chief Executive Officer at Data2Discovery Inc.*

12:00-13:00

Chair: Edgar Jacoby- *Senior Principal Scientist Molecular Informatics at J&J.*

Facilitator: Begoña Roibás-*Business Developer Manager at Innopharma (USC).*

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13:15-14:15

Lunch

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### Breakout sessions

Chairs:

- Pepo Brea-*Senior Scientist at Innopharma (USC).*
- Christine Chichester- *Open PHACTS, Chief Information Officer. Senior Researcher at CALIPHO group SIB-Swiss Institute of Bioinformatics*
- Ola Engkvist- *Team Leader, Computational Chemistry, Chemistry Innovation Centre, Discovery Sciences at AstraZeneca R&D.*
- Bryn Williams-Jones (OPF)- *CEO of the Open PHACTS Foundation.*

14:15-15:45

Facilitator: Kiera McNeice- *eScience Support Specialist (RSC).*

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15:45-16:15

Coffee Break

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### Conclusions and Wrap-up

16:15-17:15

Chair: Stefan Senger- *EFPIA coordinator of the IMI Open PHACTS Project.*

Facilitator: Begoña Roibás-*Business Developer Manager at (USC).*

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### Session Closure

Chairs:

- Edgar Jacoby-*Senior Principal Scientist Molecular Informatics at J&J.*
  - Mabel Loza-*Innopharma coordinator at (USC).*
  - Stefan Senger *EFPIA coordinator of the IMI Open PHACTS Project.*
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17:15-17:30

20:00-22:00

**Dinner hosted by USC Team**

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**February 17th, Tuesday. Venue: CiMUS Research Center (Av/ de Barcelona s/n)**

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|-------------|-----------------------|
| 08:30-09:00 | <b>Welcome Coffee</b> |
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| 09:00-12:00 | <b>Researchathon</b> |
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|-------------|---|
|             | <b>Prioritise use cases</b>   |
| 09:00-10:00 | Chair: Stefan Senger- <i>EFPIA coordinator of the IMI Open PHACTS Project.</i><br>Facilitator: Begoña Roibás- <i>Business Developer Manager at USC.</i> |

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|             | <b>Develop strategy, set up working groups</b>   |
| 10:00-11:00 | Breakout discussion groups to brainstorm strategies to address key use cas   |
| 11:00-12:30 | Group discussion of strategy, set up working groups  |
|             | Chair: Edgar Jacoby- <i>Senior Principal Scientist Molecular Informatics at J&amp;J.</i><br>Facilitator: Kiera McNeice- <i>eScience Support Specialist in the Strategic Innovation Group at RSC.</i> |

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| 12:30-13:30 | Lunch |
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|             | <b>Wrap-up Discussion and Conclusions</b>   |
|             | Chairs:   |
| 13:30-14:00 | <ul style="list-style-type: none"><li>• Edgar Jacoby-<i>Senior Principal Scientist Molecular Informatics at J&amp;J.</i></li><li>• Mabel Loza- <i>Innopharma coordinator at USC.</i></li><li>• Stefan Senger-<i>EFPIA coordinator of the IMI Open PHACTS Project.</i></li></ul> |

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