SPANISH DRUG DISCOVERY NETWORK MEETING

BARCELONA, 20 – 21 NOVEMBER 2023

DAY 1 - MONDAY NOVEMBER 20, 2023

09:00 – 09:30 **General Assembly – SDDN Association**

09:30 – 10:00 **Welcome and Presentation of the XV SDDN Meeting**

10:00 - 10:30 **Coffee Break**

10:30 – 12:30 **Session 1:** The impact of AI-based tools and data science in Drug Discovery.
Chair: Xavier Barril (Universidad de Barcelona).

12:30 – 13:00 **Presentations SDDN Partners and Event Sponsors I**

13:15 – 14:15 **Lunch**

14:30 – 16:30 **Session 2:** Drug Discovery projects in public - private collaborations.
Chair: Anabel Sanz (CRG).

16:30 – 17:00 **Presentations SDDN Partners and Event Sponsors II**

17:00 – 19:30 **Poster & networking session at exhibitors hall**
(Coffee and refreshments)

20:30 **Conference Dinner**

DAY 2 - TUESDAY NOVEMBER 21st, 2023

09:00 – 11:00 **Session 3.** Using patient omics for the discovery of personalized medicines.
Chair: Francesc Fernández (Almirall)

11:00 – 11:30 **Presentations SDDN Partners and Event Sponsors III**

11:30 - 12:15 **Poster & networking session at exhibitors hall**
(Coffee and refreshments)

12:15 - 12:30 **Poster presentations and poster prizes ceremony**

12:30 – 14:30 **Session 4.** Advanced Cell and Gene Therapies.
Chair: Marjorie Pion (Health Research Institute Gregorio Marañón)

14:30 – 15:00 **Concluding remarks & announcement of SDDN 2024 meeting**

15:00 – 16:00 **Lunch**

16:00-18:00 **Additional networking**

SPANISH Drug Discovery Network

CRG Centre for Genomic Regulation

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Session 1: The impact of AI-based tools and data science in Drug Discovery.

Chair: Xavier Barril (Universidad de Barcelona).

Machine Learning (ML) is a rapidly evolving technology that has penetrated our daily lives and all scientific disciplines. In the drug discovery arena, ML applications can be found at all stages of the process, from target identification to clinical trials, and has had (or will have) a disruptive effect on the daily operations of all scientists involved, starting with computational chemistry and structural biology, but rapidly moving to medicinal chemistry, biology and pharmacology. ML not only enables more efficient processes, but also affects how we generate usable and systematic data to feed those algorithms. In this session we aim to provide an overview of achievements, current directions, challenges and next frontiers in the field of ML applied to drug discovery. In particular, we aim to highlight three distinct areas of application:

- Classic quantitative structure-activity relationships (QSAR) was a natural entry point for ML in drug discovery. ML algorithms appear to be superior and gain ground over traditional regressiion models. But they have not diminished the need for clean datasets and for careful consideration of the scope of the models and proper validation with external datasets.
- ML methods are a great complement to high-throughput and information rich biological assays, such as high-contents analysis or omics data. Internal data can, potentially, be complemented with large publically available datasets. The speakers will discuss what kind of breakthroughs can be expected in this area.
- The combination of physics-based computational methods with ML is a promissing strategy to obtain the best of both worlds: the accuracy and general applicability of computation based on first-principles with the speed of ML. This is also uniquely suited to integrate data generation with model training and validation.

Session 2: Drug Discovery projects in public - private collaborations.

Chair: Anabel Sanz (CRG).

Drug discovery can be performed by both private and public entities, and both have their own advantages and disadvantages. Their priorities and incentives are also different. In general, companies are better equipped and have better access to specialized resources, expertise, and funding. Companies focus is on moving promising drug candidates through the regulatory approval process and bring them to market, while public entities may be more interested in advancing basic research and understanding disease mechanisms, rather than in commercial purpose.

That being said, nowadays pharmaceutical have adopted new paradigms in the process of drug discovery thereby opening to collaborate with academic institutions, spin off and biotech companies with the aim to accelerate the drug development process, reduce costs, and increase the likelihood of success.

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In turn, academic institutions and governmental agencies and charities are making significant efforts to build capacities, technology platforms, and to fund early drug discovery projects that can efficiently transform innovative biomedical research into drugs to be further developed by the pharmaceutical industry.

The objective of this session is to present examples and capacities that hold the potential to foster public-private collaboration to advance Drug Discovery.

Session 3. Using patient omics for the discovery of personalized medicines.

Chair: Francesc Fernández (Almirall)

There have been many important advancements in omics data generation technologies in recent years. These developments have led to the generation of large amounts of data that enables an unprecedent level of molecular characterisation of biological mechanisms. In this context, the integration of different types of patient-derived omics data provides insights into better understanding disease mechanisms, potentially identifying new drug targets and finally enabling the development of new personalized medicines. In this conference track, we will explore recent progress in using and integrating different flavours of patient-derived omics data for personalized medicine, with special focus on the challenges and opportunities associated with this rapidly evolving field.

Session 4. Advanced Cell and Gene Therapies.

Chair: Marjorie Pion (Health Research Institute Gregorio Marañón)

Advanced cell and gene therapies (ACGTs) are medicinal products intended for human use that rely on genes, tissues, or cells. They provide revolutionary new opportunities for the treatment of diseases and injuries. ACGTs can be classified into three main types:

Gene therapy medicines designed to introduce recombinant genes into the body to achieve therapeutic, prophylactic, or diagnostic effects. In the field of genetic modifications, a broad range of techniques exists that may or may not directly modify the DNA, including but not limited to CRISPR/Cas9, ZF, AAV, and mRNA.

Somatic-cell therapy medicines contained cells or tissues that have been manipulated to alter their biological characteristics. They can be used to cure, diagnose, or prevent diseases.

Tissue-engineered medicines are composed of cells or tissues that have been modified to enable their use in the repair, regeneration, or replacement of human tissue.

In some cases, these therapies may include medical devices as an integral part of the medicine, which are referred to as combined ACGTs. For instance, cells embedded in a biodegradable matrix or extracellular vesicles.

Currently, the level of knowledge and technical advancement achieved make advanced therapies ideal for treating rare diseases or unmet medical needs. In this session we would like to introduce some recent advances in this field.