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TOPIC SUMMARY

Smart Pharmacology: Exploring new frontiers with AI

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This is a brief summary of Symposium on **Smart Pharmacology: Exploring new frontiers with AI** developed on Dec 3th. 2025 at the Faculty of Pharmacy of the University of Barcelona, including experts on basic, clinical and social Pharmacology.

The symposium on **Artificial Intelligence (AI) and Drug Development** brought together leading scientists, innovators, and industry experts whose work is reshaping the landscape of biomedical research. The event highlighted how AI has evolved from a supportive computational tool to a **strategic driver of pharmaceutical innovation**, accelerating every stage of the drug discovery pipeline and opening new avenues for precision medicine.

Bridging expertise across academia, biotechnology start-ups, large pharmaceutical companies, and computational research centers, the symposium underscored the transformative power of AI to **shorten timelines, reduce costs, improve target selection, expand chemical and biological search spaces, and enhance patient impact worldwide**.

Across the talks, a consistent message emerged: AI now underpins critical decisions throughout the drug discovery continuum, including:

- **Target identification and validation**, integrating genomic, molecular, and systems-biology datasets.
- **Generative molecular design**, allowing the creation of novel chemical entities at unprecedented speed and scale.

- **Prediction of toxicity, off-target effects, and pharmacokinetic behavior**, reducing experimental burden and attrition rates.
- **Optimization of preclinical and clinical strategies**, supported by advanced simulations, digital twins, and virtual patients.

This paradigm shift reflects a move toward **data-driven, AI-enhanced, and patient-centered innovation**, positioning computational intelligence at the heart of tomorrow's therapeutics.

The Opening Vision: A Changing Landscape

The symposium opened with the reflections of **Andrés García Fernández**, whose career spans more than three decades of drug development. He did not speak as a futurist, but as someone who has lived through the historical cycles of pharmaceutical productivity—its rises, declines, and reinventions. Yet rather than a tale of decline, Andrés guided us through a narrative of renewal: the rise of biological therapeutics, the dismantling of old silos, the embrace of collaboration, and the emergence of new discovery platforms powered by computation and simulation. AI, he argued, is not simply accelerating processes; it is **rewiring the very logic of modern drug R&D**, enabling researchers to anticipate failures before they occur, to simulate biological complexity, and to design more safely and intelligently.

His perspective set the tone for the day: one of realism, but also of possibility.

From this broad strategic landscape, the symposium moved into the terrain of scientific creativity. **Patrick Aloy** took the stage with a story that felt almost futuristic—yet it is already reality in his laboratory.

He described a framework in which AI doesn't simply classify molecules or predict their properties, but **imagines new ones**. In pancreatic cancer models, his team screened thousands of compounds to understand how cells respond. These data then trained machine-learning models capable of distinguishing subtle differences between cell lines—differences often invisible to traditional approaches.

What followed sounded like science fiction: a generative model, guided by reinforcement learning, began producing virtual molecules tailored to kill cancer cells selectively. Many of these molecules bore little resemblance to those in the original screening set; they were novel designs. And when synthesized and tested, a surprising number worked as intended.

His story illustrated something profound: AI is not only helping us understand biology—it is beginning to **co-create therapeutics** with us.

Where Aloy explored chemical innovation, **David Torrents** delved into the genetic foundations of drug discovery. His narrative centered on a simple but powerful idea: our genomes contain the instructions not only for disease, but also for **how we will respond to therapy**.

He walked the audience through the ways genomic and functional-genetics data can guide every decision in drug development—from choosing the right targets, to identifying patients most likely to benefit, to foreseeing adverse effects long before a clinical trial begins. His team's work on detecting pleiotropic genetic effects—where one gene influences multiple traits—offers a way to anticipate safety liabilities before a single experiment is performed.

Running through the day's sessions was a thread that warranted a closer look: how to understand drug action at the systems level and design against resistance. This is where the contributions of Albert Antolín come into particularly sharp focus. His work treats polypharmacology—the fact that most drugs engage multiple targets—not as an inconvenience but as an opportunity for design. In recent group overviews and publications, this approach has been applied to understand drug metabolite biology and to unpack adverse-effect mechanisms reinforcing the idea that computational insight and wet-lab fidelity must move together if discovery is to keep pace with disease.

The conversation turned next to genomics, where David Torrents described the modern logic of target selection. In his telling, the genome is a map that not only points to the mechanisms that drive disease, but also forecasts how patients will respond to Torrents' story was a reminder that precision medicine is not built on algorithms alone; it is built on the vast and intricate language written in our DNA, which AI can now help decode at unprecedented scale.

The symposium then shifted focus toward a broader horizon—**global health**—through the work of the **Ersilia Open Source Initiative**.
When **Miquel Duran Frigola** spoke, the room was reminded that innovation is not only about cutting-edge science; it is also about equity.

They described laboratories in low-resource settings—places where diseases like malaria or tuberculosis remain urgent threats—yet where computational tools are scarce and data availability is limited. Ersilia's response has been to create an open-source hub

of AI/ML models for infectious diseases, specifically designed to work in *low-data environments*.

Their story was one of empowerment. With nothing more than a laptop and a stable internet connection, a scientist in Africa or Southeast Asia can now access models for drug design, predict activity of potential antibiotics, or analyze pharmacogenomic patterns relevant to their local populations.

It was a compelling reminder that AI can—and must—serve the world, not just the wealthiest health systems.

Nuria Campillo brought the narrative back to the central arc of the day: how AI accelerates the journey from a molecular idea to a therapeutic reality. She described a process that once took years—designing, filtering, and manually optimizing thousands of candidate molecules—and showed how AI now performs much of this work in silico. Models propose compounds, test them virtually for binding, predict toxicity, and refine designs, often within hours.Yet her message was not simply technical. It was about **redefining the scientist's role**: less manual screening, more strategic decision-making; fewer dead ends, more informed paths forward. Her story tied together many threads of the day: speed, intelligence, safety, and the growing interplay between chemical intuition and computational creativity.

This text has been grammatically refined using AI. The content remains original from the speakers and M.P.