INTEGRATED *IN-SILICO* APPROACH TO DRUG DISCOVERY AND SAFETY EVALUATION

Seminari Tecnològic
Facultat de Farmàcia
Universitat de Barcelona

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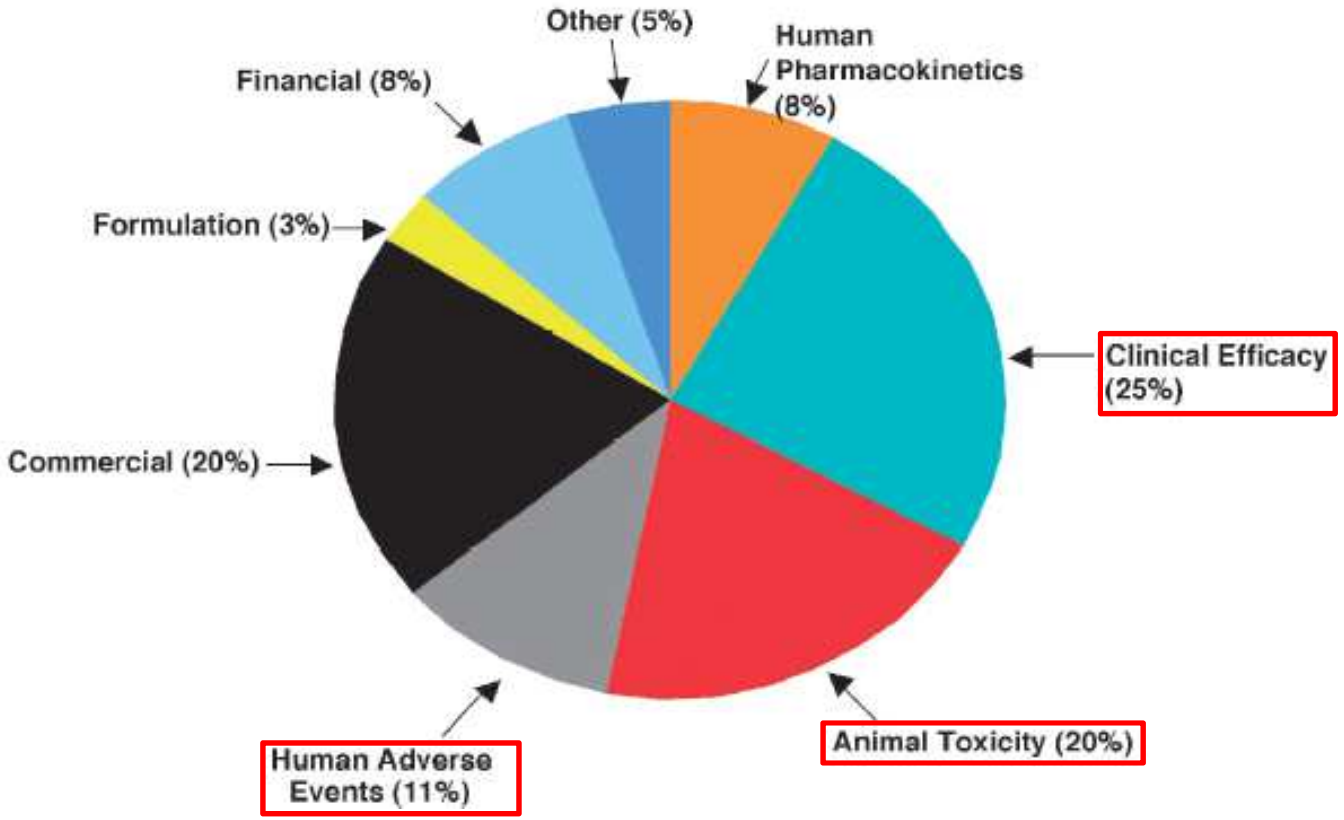
PROUS INSTITUTE
for Biomedical Research

Josep Prous, Jr., Ph.D., MBA
Vice President R&D

MAJOR ATTRITION REASONS OF DRUG CANDIDATES IN PRECLINICAL AND CLINICAL DEVELOPMENT



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F. Peter Guengerich, Drug Metab Pharmacokinet 26(1):3-14 (2011)

DEFINITION

- In-silico pharmacology and toxicology consist of the study of bioactive compounds by computational means

- This definition includes developing models and performing simulations to acquire knowledge on the mode of action of molecules and their associated toxicity, side effects and pharmacokinetics profile

APPLICATIONS

Predictive pharmacology and toxicology tools can help the biomedical community in the discovery and development of newer and safer drugs

The **predictive pharmacology** component assists in:

- Discriminating between active and inactive compounds for specific pharmacological activities
- The discovery of unknown mechanisms of action for compounds with a demonstrated therapeutic effect
- Determining areas in which recently patented or established compounds can be repurposed

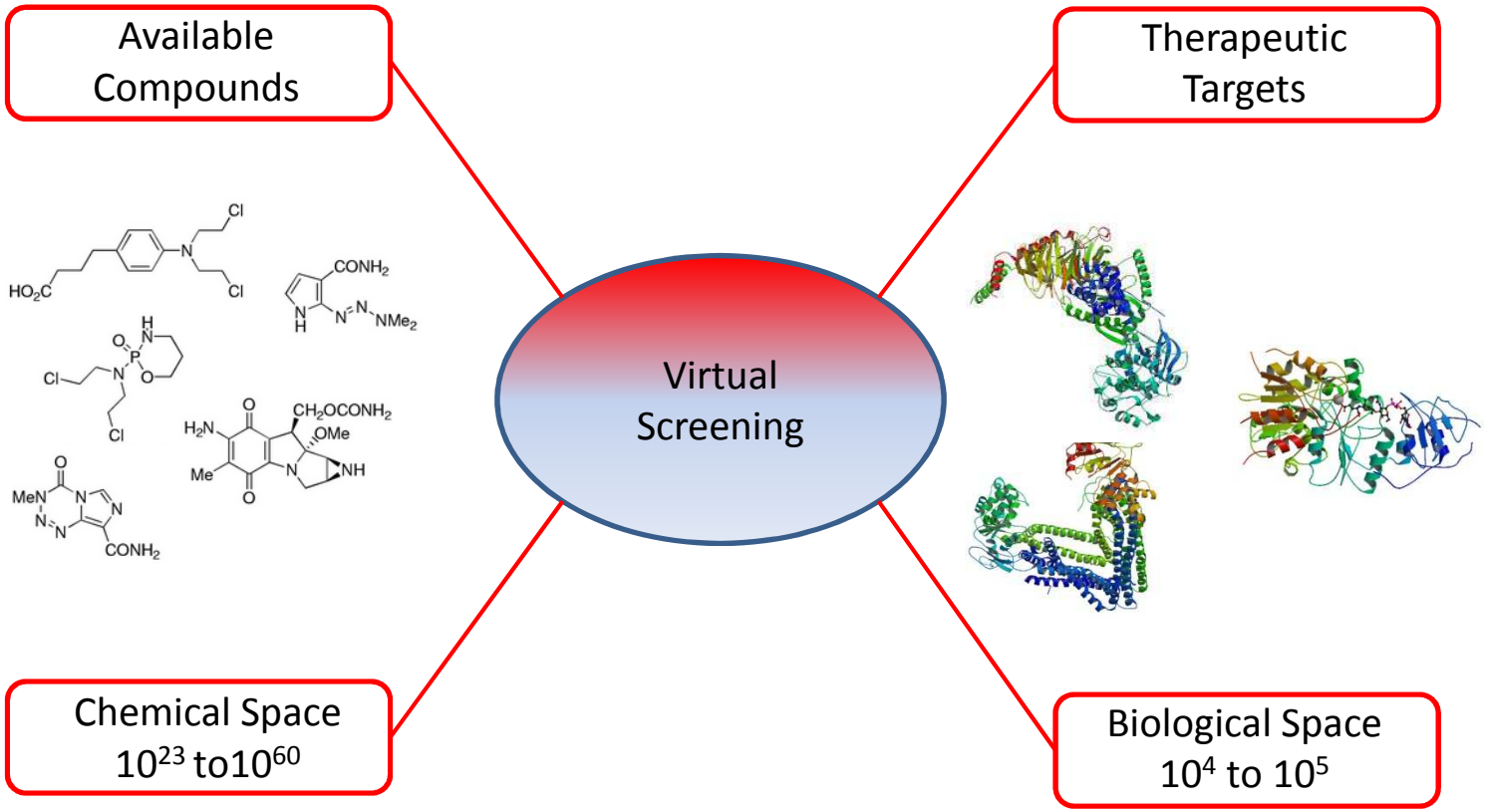
Predictive toxicology technologies can be applied in:

- Identifying early off-target activities, prior to the synthesis of the compounds
- Raising red flags for potential human safety events which may be encountered during clinical development

TYPES ON IN SILICO TOOLS

- Databases (provide comprehensive information on bioactive molecules and their corresponding targets)
- Virtual screening (evaluates the binding of a chemical to a biological target)
- Predictive modeling (delineates the pharmacological and toxicological effects of chemicals on human health)

The basic goal of virtual screening is the comprehensive reduction of the enormous virtual chemical space to a manageable number of compounds that could inhibit a target protein responsible for disease



PROUS INSTITUTE SYMMETRY

- Prous Institute Symmetry® integrates computational tools and methods aiming to replicate all the processes through which new drugs are discovered, developed and approved
- It enables the generation of new research hypotheses and predicts with accuracy the pharmacological and toxicological profile of a molecule
- Aims to “de-risk” and prioritize projects and speed up drug discovery and development, reducing time, costs and attrition rates

Experimental validation

In silico research

<= Higher Quality Lead Candidates

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