Finanziato dall'Unione europea NextGenerationUE
Ministero dell'Università e della Ricerca
Italiadomani PIANO NAZIONALE DI RIPRESA E RESILIENZA
VITALITY

Progetto VITALITY | Programma di Consulenza Specialistica | **Seminario**

In silico prediction of toxicity – from QSAR modelling to biological fingerprints

Abstract

The safety assessment of drugs is a critical factor of early development stages, necessitating rigorous testing to ensure efficacy and minimize harm to future patients. In recent years, new approach methods (NAMs) for animal free safety assessment have gained increasing importance, with in silico models becoming an integral part. However, due to the complexity of some endpoints such as hepatotoxicity, common molecular descriptors such as those used in conventional QSAR modeling are not sufficient to fully capture all processes involved. Thus, integrating mechanistic and structural insights by using fingerprints from various data domains such as compound-pathway interaction fingerprints should overcome this limitation and also aid to the explainability of the models.

martedì 1 aprile 2025 - Ore 10.30

Aula A

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Gerhard Ecker is Professor of Pharmacoinformatics and Head of the Pharmacoinformatics Research Group at the Department of Pharmaceutical Sciences, University of Vienna. Gerhard received his doctorate in natural sciences from the University of Vienna and performed his post-doctoral training at the group of J. Seydel in Borstel (Germany). His research focuses on computational drug design with special emphasis on drug-transporter interaction and in silico safety assessment. He participated in 5 EU-funded projects related to toxicity prediction and animal free safety assessment and coordinated the Open PHACTS project, which created an Open Pharmacological Space by semantic integration of public databases. Gerhard served 2009 – 2011 as President of the European Federation for Medicinal Chemistry, and from 2018 – 2022 as Dean at the Faculty of Life Sciences.