InSilicoTrials

InSilicoDISCOVERY

Early screening mutagenicity risk

Mutagenicity testing is a standard step in determining the genotoxic potential of chemicals as part of the genetic toxicology battery.

The ICH M7 guideline provides a practical framework for the assessment of mutagenic impurities to limit potential genotoxic risk. It states that a computational toxicology assessment can be performed in lieu of in vitro testing using two complementary (quantitative) structure-activity relationship (Q)SAR prediction methodologies [1].

In fact, the combined use of the two approaches increases the sensitivity and accuracy of predictions and is required by the authorities.

What is early screening mutagenicity risk

The early screening mutagenicity risk tools assess the mutagenic potential of a compound and are generally based on two approaches:

- Expert rule-based (Q)SAR
- Statistical-based (Q)SAR

The results of both approaches can be submitted to regulators, reducing the need for time consuming and expensive in vitro tests.

Advantages

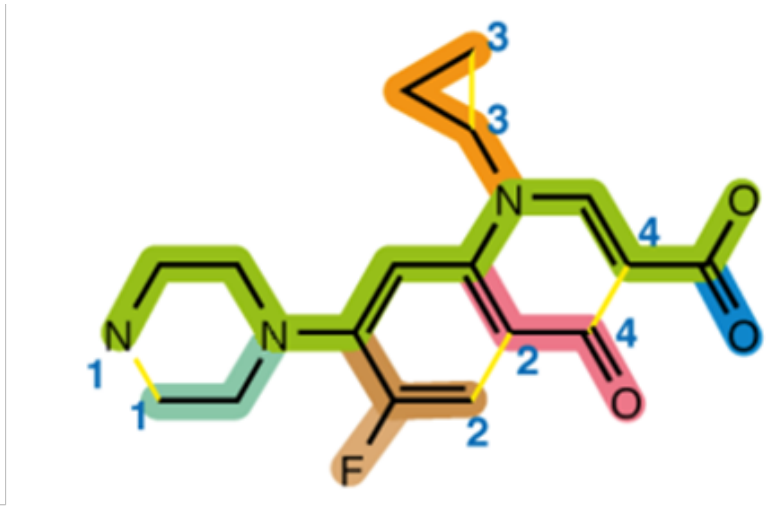
- Quick and easy assessment of a compound mutagenic potential
- Reduce need for time consuming and expensive experiments
- Support the design of non-mutagenic compounds
- Enables early screening toxicological assessments on large compound libraries

How it works?

Early screening mutagenicity risk requires the structure of the molecule in SMILE format or any other chemical structure file format.

The tools predict the mutagenicity either of the compound or of the compounds' library of interest.

Example of SMILE format



The results are provided in a pdf report following the ICH M7 guidelines.

Why working with InSilicoTrials

TECHNOLOGY-ENABLED SERVICES

Ask us for support on technology integration, in silico trials planning, execution and reporting, in line with regulatory requirements

VIRTUAL PATIENTS

Design and accelerate your clinical trials with the virtual patient populations you need

ON DEMAND & CUSTOM

Ask us for the models and simulations you need, or ask us to evaluate where modeling and simulation can support you

SaaS

Buy tokens and use the online products of your choice among those available on the platform

In silico methods can innovate drug research and development

Today, the very long and expensive development and the complex registration processes for new drugs are becoming financially unsustainable.

Regulatory agencies have been encouraging the use of in silico methods in drug research and development for years [2] because the use of these methods can significantly reduce costs and greatly accelerate the go-to-market of new medicines, allowing companies to exploit patents for a longer period. Solvers, IT infrastructure and computational specialists require a continuous investment from companies.

To help solve these challenges, InSilicoTrials Technologies has developed a game-changing-solution. Our experts:

- Select computational models from excellence research centers around the world
- Integrate them in our cloud-based platform
- Make them available through user-friendly online products

This solution enables companies to leverage cutting-edge in silico methods at low costs without specific computational expertise, IT infrastructure and solvers investments requirements. On our cloud-based platform, users can select the online computational product of their choice in pay-per-use or ask us to build the digital product they need.

References:

[1] Romualdo Benigni, Arianna Bassan & Manuela Pavan (2020) In silico models for genotoxicity and drug regulation, Expert Opinion on Drug Metabolism & Toxicology, 16:8, 651-662, 2020. DOI: 10.1080/17425255.2020.1785428

[2] U.S. Department of Health and Human Services and Food and Drug Administration, "Innovation or stagnation? Challenge and Opportunity on the Critical Path to New Medical Technologies," 2004.