AI4SAFEMED

Artificial Intelligence for Safe Medicines

Timeline | 10/2022 to 4/2024

Budget | 100.000€

ICIQ People | Feliu Maseras Research Group

Call | Ajuts d'Indústria del Coneixement - Producte 2021

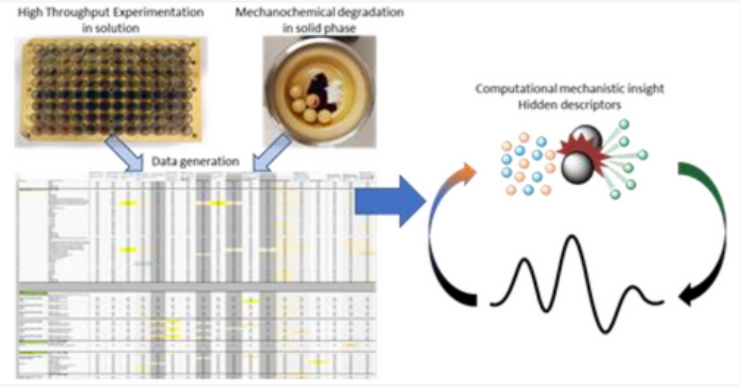
SUMMARY

AI4SAFEMED will develop a computational toolset (degradation prediction software + degradation product database (DB)) from TRL 3 to 6 to support mandatory forced degradation testing of active pharmaceutical ingredients (APIs) and formulated drug product, as well as support formulation activities to improve stability. The computational toolset will be licensed to pharmaceutical industry, CROs, CMOs and analytical companies to be deployed in a "software as a service" model.

Drugs in solid dosage form account for >80% of marketed drugs. Due to the lack of specific testing methods for solid formulations, most mandatory forced degradation testing is performed in solution. ICIQ's computational toolset will support both current commercial testing (solution) and upcoming mechanochemical approaches (solid phase) which more closely mimic real-life degradation of drugs during storage. The predictive software and DB will build on pre-existing results using the following strengths:

- Computational expertise: Prof. Maseras leadership in molecular modelling of mechanochemical reactions (few groups worldwide).
- Accelerated data generation for DB expansion: ICIQ's high-throughput experimental platform (HTE) which generates large datasets with minimized effort (solution experiments), combined with mechanochemical experiments.
- Highly sensitive analytics for nitrosamine detection following EMA and FDA-recognized methods.
- IoChem-BD for data handling and protection as industrial secret: this ICIQ-developed chemical data repository is used in several industrial projects, and is currently commercialized in Japan through company Itochu.
- RD&C (industrial mentor) as regulatory and pharmaceutical development experts (including leading experts in mechanochemical testing of drugs) and key allies in the commercialization strategy.

The project will place a strong focus on the prediction of (carcinogenic) nitrosamine degradation products. There is a tremendous need and pain point for pharma customers starting mid-2018 resulting in several product recalls (including in 2022 by Pfizer and Novartis) and ensuing drug shortages of highly needed medicines (blood pressure, heart disease, diabestes, oesophagal reflux disease and many more). Currently, a proper nitrosamine risk assessment is mandatory for all marketed and new medicines. Available testing and software options are often failing to predict and find the root cause of nitrosamine formation.



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Reference: 2021 PROD 00042