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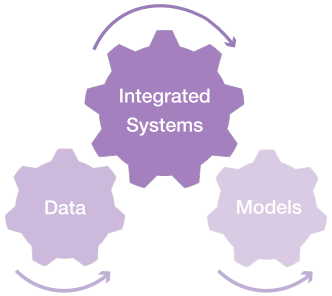
eTOX

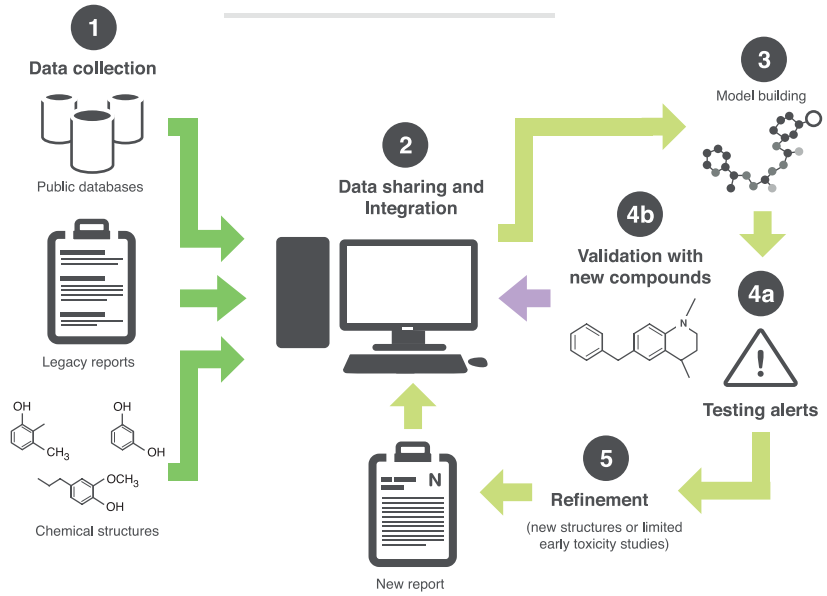
Integrating bioinformatics and chemoinformatics approaches
for the development of expert systems allowing the
***in silico* prediction of toxicities**

efpia · imi innovative medicines initiative

eTOX aims to develop innovative methodological strategies and novel software tools able to predict the in vivo toxicology of new molecular entities by ***sharing and exploiting legacy toxicological information stored in the archives of the participating pharma companies***



The **eTOX** project is carried out by a public-private partnering between 11 academic groups, 6 SMEs and 13 pharmaceutical companies, which works to set up an software platform (eTOXsys), which includes an integrative database and predictive models, in order to provide novel guidance in the design of new drug candidates on the basis of cumulative knowledge that is shared between pharma companies that participate in the project.



Achievements up to date

Creation of a database of toxicology-related data combining public data and legacy reports from participating pharmaceutical companies. **Over 7.000 study records available in the eTOX Database corresponding to 4.749 reports and 2.176 compounds.**

Development of a common ontology to allow mapping of the terms used across the different companies and also in public literature to a single preferred term essential for cross-study data analyses. **Ontology of over 10 million verbatim terms.**

At present eTOXsys includes **74 *in silico* models** for diverse endpoints: 28 on ADME, 5 on transporters, 2 on physicochemical properties, 2 on carcinogenicity, 2 on genotoxicity, 16 on organ toxicities, and 19 on safety pharmacology.

eTOXsys incorporates a powerful, flexible and user-friendly engine for interrogating the database on the basis of any of their chemical, biological or toxicological properties, or combinations of them. **Version 2.0 released in May 2014.**

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