BigChem

The Marie Skłodowska-Curie Actions in Horizon 2020 finance around 65,000 researchers between 2014 and 2020, including 25,000 doctoral candidates.

The 2016 Marie Skłodowska-Curie Actions are:
- Innovative Training Networks (ITN)
- Individual Fellowships (IF)
- Research and Innovation Staff Exchange (RISE)
- Co-funding of regional, national and international programmes (COFUND)

Visualization and data mining

ESR1: Machine learning methodologies for mining very large compound data sets

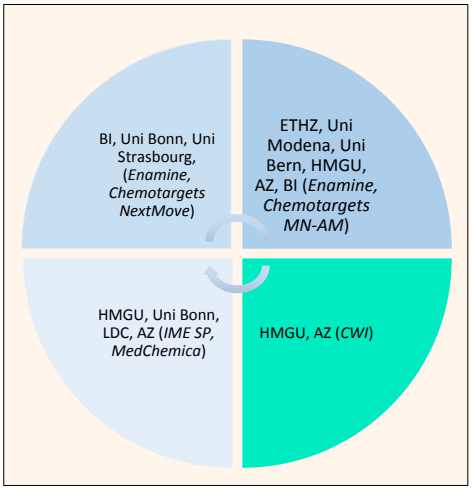
ESR2: Computational compound profiling by large-scale mining of pharmaceutical data

ESR3: Big data visualization and modeling using Generative Topographic Mapping (GTM)

Promiscuity analysis

ESR4: Development of frequent hitters filters for HTS screening

ESR5: Analysis of Compound Promiscuity Based on Bio-Assay Ontology



Accessing new chemical space

ESR6: Developing virtual screening methods to exploit large virtual chemical space

ESR7: Exploration of uncharted regions of the chemical space by reaction-driven de novo design

ESR8: Accessing new chemical space for lead optimization based on QSAR models

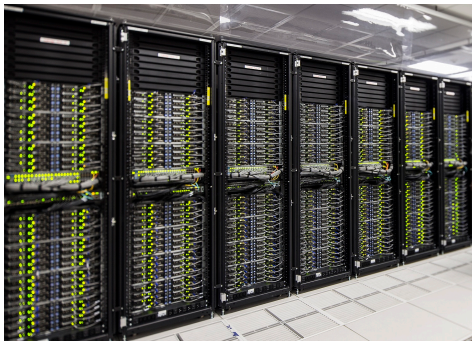
ESR9: Integrated ligand- and structure-based approaches for predicting compound polypharmacology based on big data

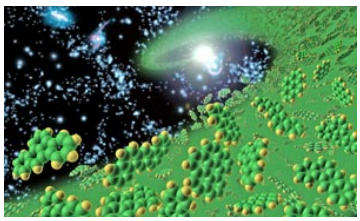
Secure sharing of data

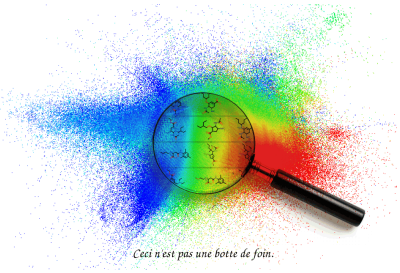
ESR10: Secure sharing of information using ensemble of machine learning methods and surrogate data

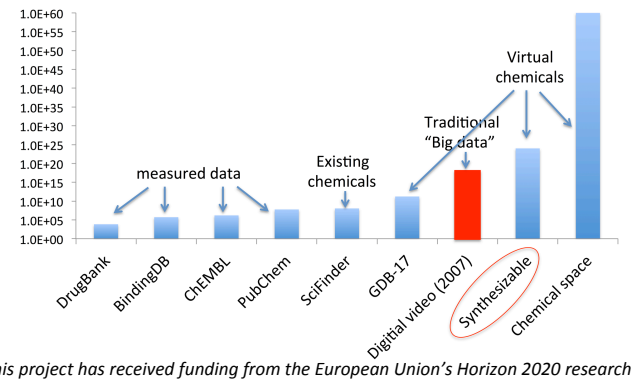
Beneficiaries:

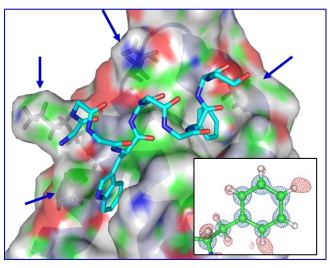
AstraZeneca, Boehringer Ingelheim, LDC, universitätbonn, Rheinische Friedrich-Wilhelms-Universität Bonn, Université de Strasbourg, Università degli Studi di Modena e Reggio Emilia, Universität Bern, HelmholtzZentrum münchen German Research Center for Environmental Health, ETH zürich





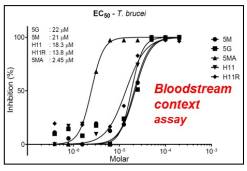




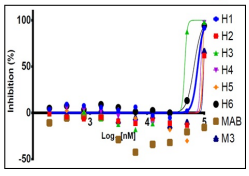


Sattler M. and Popowicz G., Biovaria 2017

Trypanocidal activity



Low mammalian cell toxicity



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