

Billev Pharma East



trust



commitment



expertise

The power of *in silico* methods in drug development and assessment

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QPPV
Billev Pharma East

In silico ... predicting versus testing



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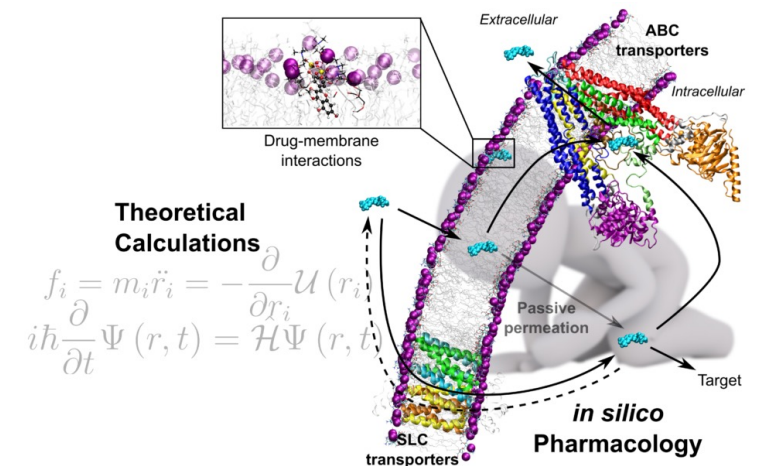
<https://brewminate.com/herbal-medicine-in-ancient-egypt/>



<https://kosheeka.com/how-do-primary-cells-differ-from-continuous-cell-lines/>

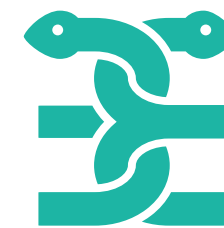


<https://www.healthline.com/health/bit-by-a-mouse>



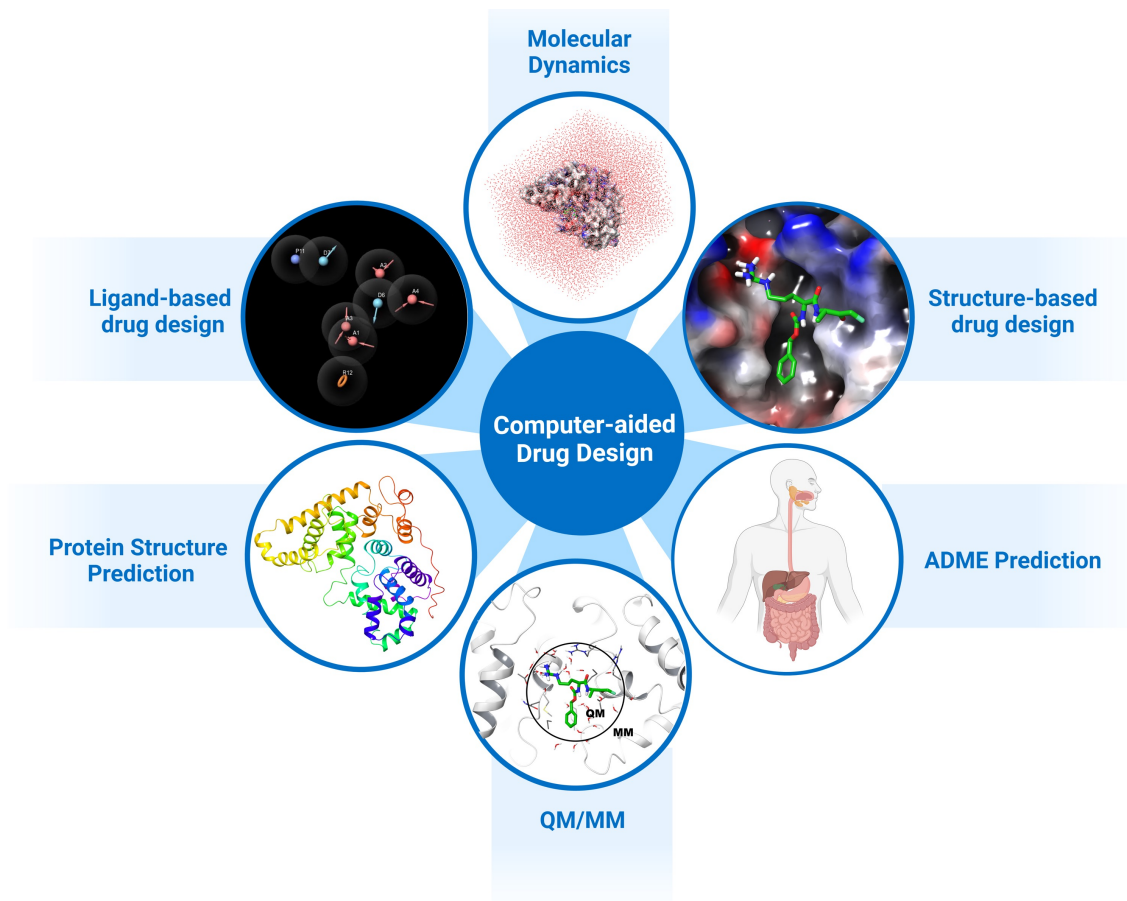
<https://www.unilim.fr/ippritt/wp-content/uploads/sites/56/2017/01/toc-1-1024x605.png>

Why *in silico*?

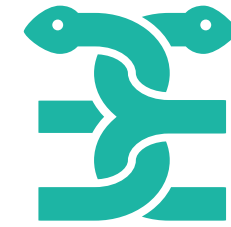


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Not only cost and time savings, but so much more!



Computational models are a basis for implementing 3R principles



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EUROPEAN MEDICINES AGENCY
SCIENCE MEDICINES HEALTH

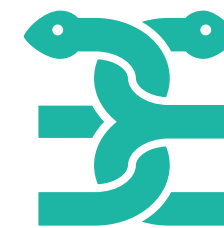
3Rs Working Party [← Share](#)

The 3Rs Working Party (3RsWP) is a joint working party of the Committee for Medicinal Products for Human Use (CHMP) and the Committee for Veterinary Medicinal Products (CVMP). It advises these committees on all matters concerning the use of animals in the regulatory testing of medicines, with particular focus on the application of the so-called 3Rs principles - replace, reduce and refine.

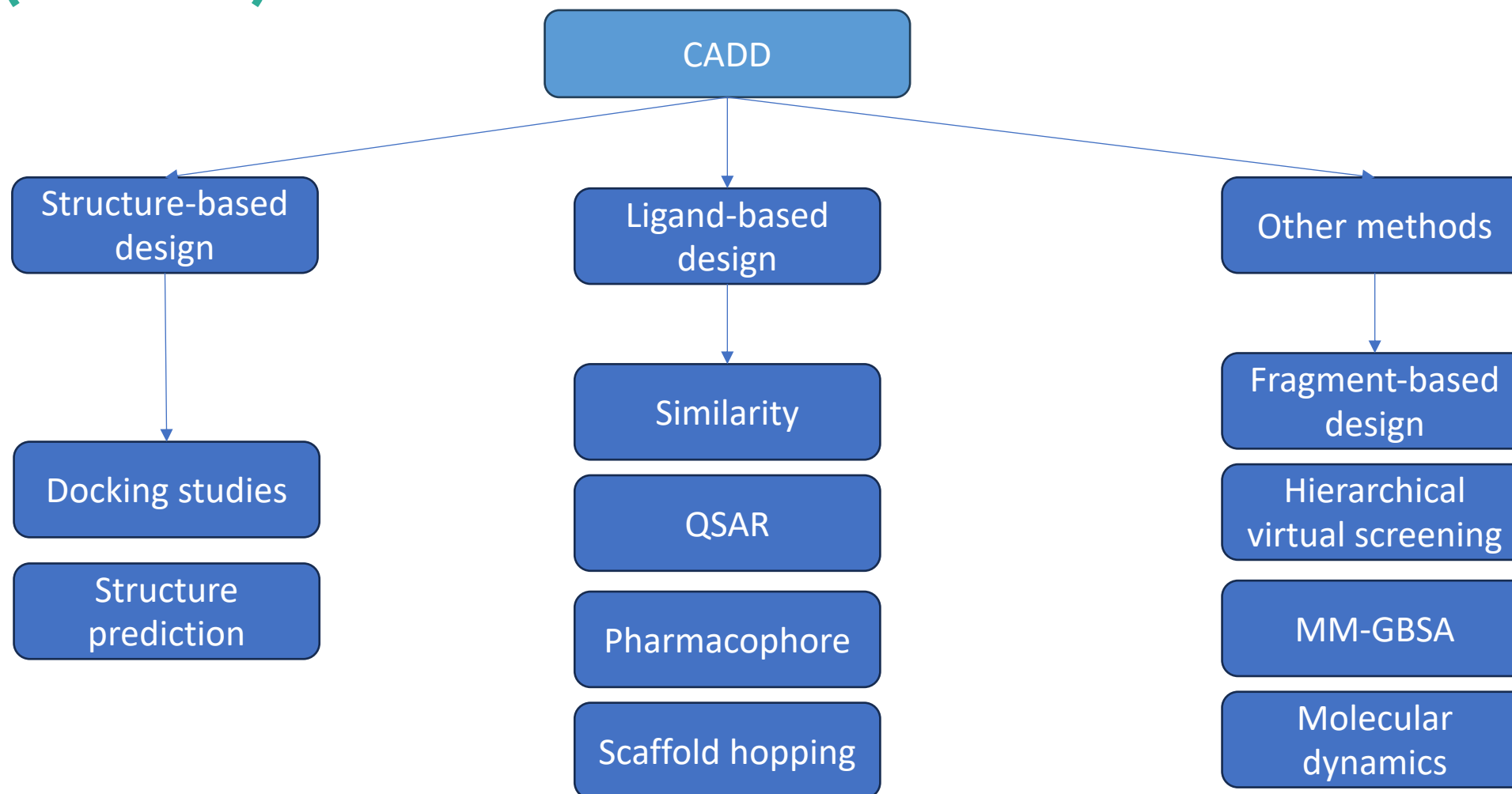
15 December 2016
EMA/CHMP/CVMP/JEG-3Rs/450091/2012
Committee for Medicinal Products for Human Use (CHMP)
Committee for Medicinal Products for Veterinary Use (CVMP)

Guideline on the principles of regulatory acceptance of 3Rs (replacement, reduction, refinement) testing approaches

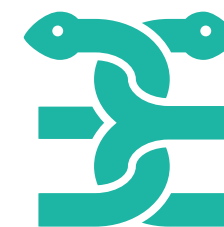
Computer-aided drug design (CADD)



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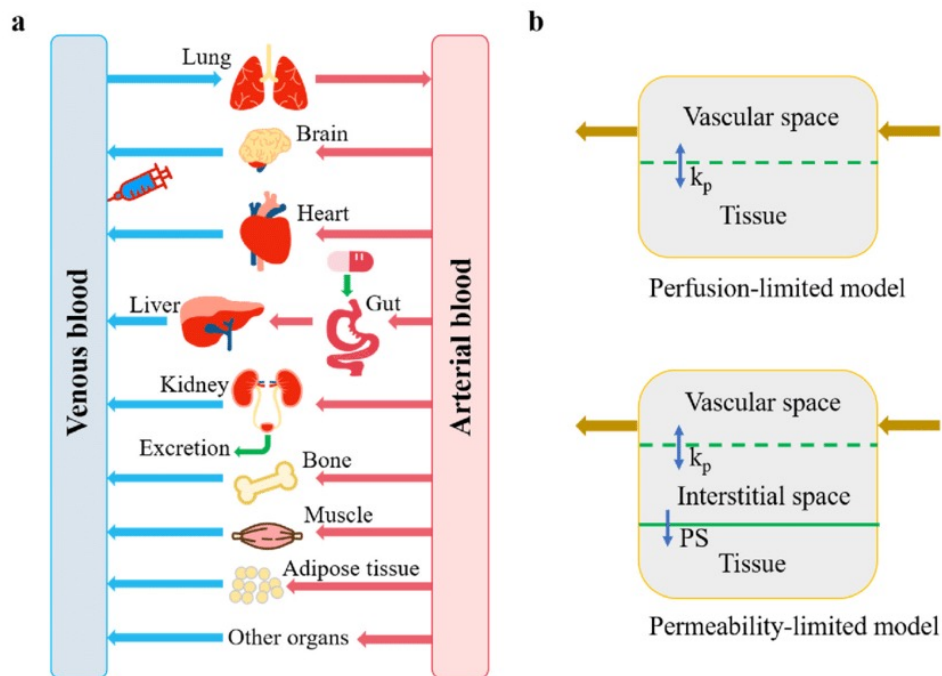


Evaluation of candidate molecules



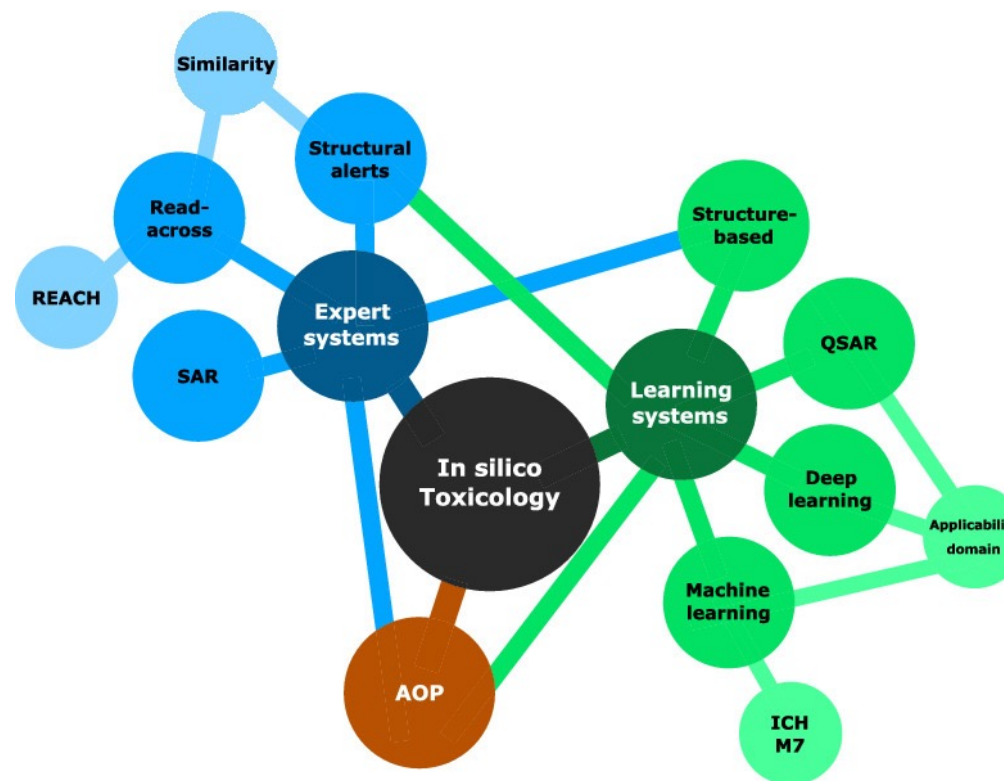
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PHARMACOLOGY PBPK modelling



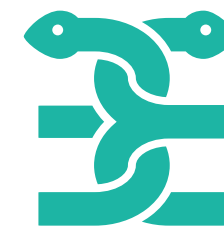
https://www.researchgate.net/figure/A-generic-physiologically-based-pharmacokinetic-PBPK-model-a-adapted-from-Shin-HK_fig2_348829940

TOXICOLOGY



<https://wires.onlinelibrary.wiley.com/doi/full/10.1002/wcms.1475>

In silico models are based on AOPs and enhanced by AI

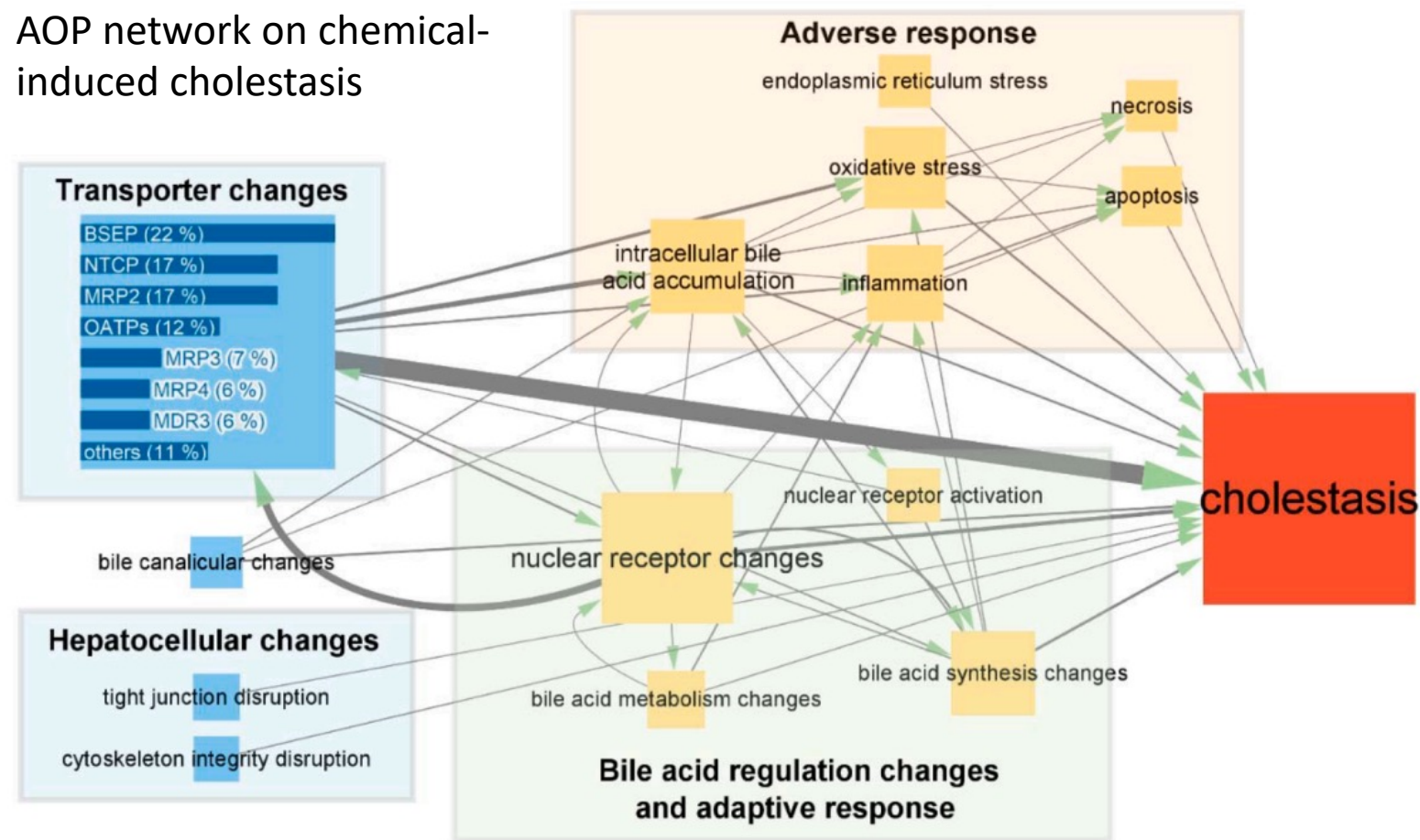


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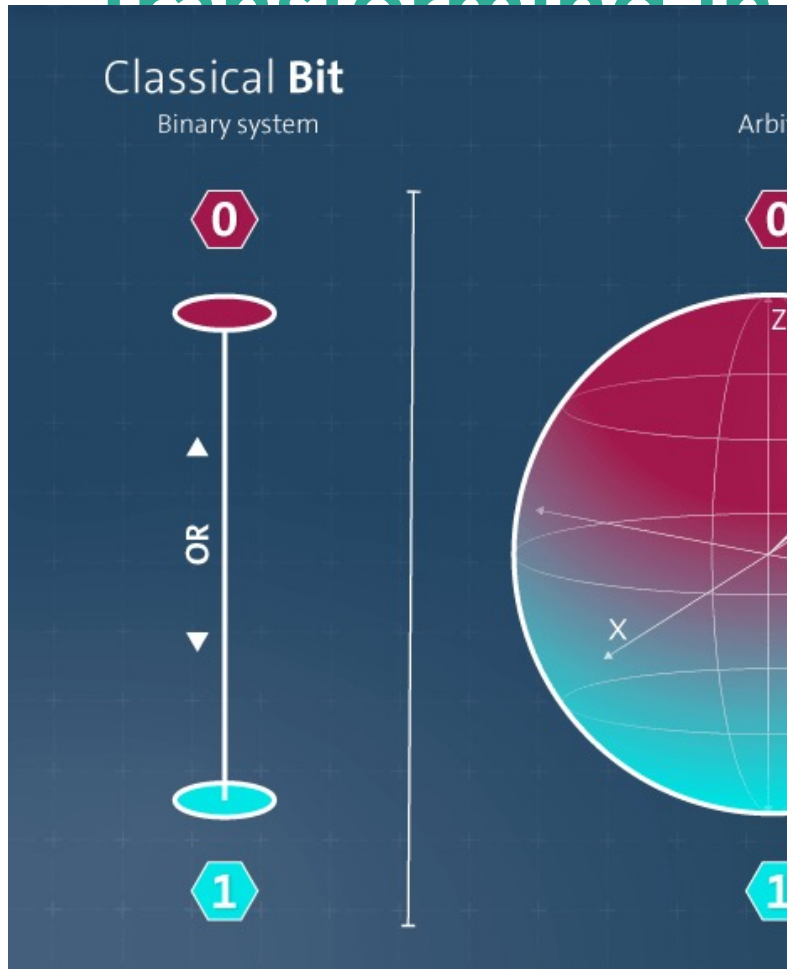
Ever growing database of interconnected pathways

AI assists in data collection and WoE calculations.

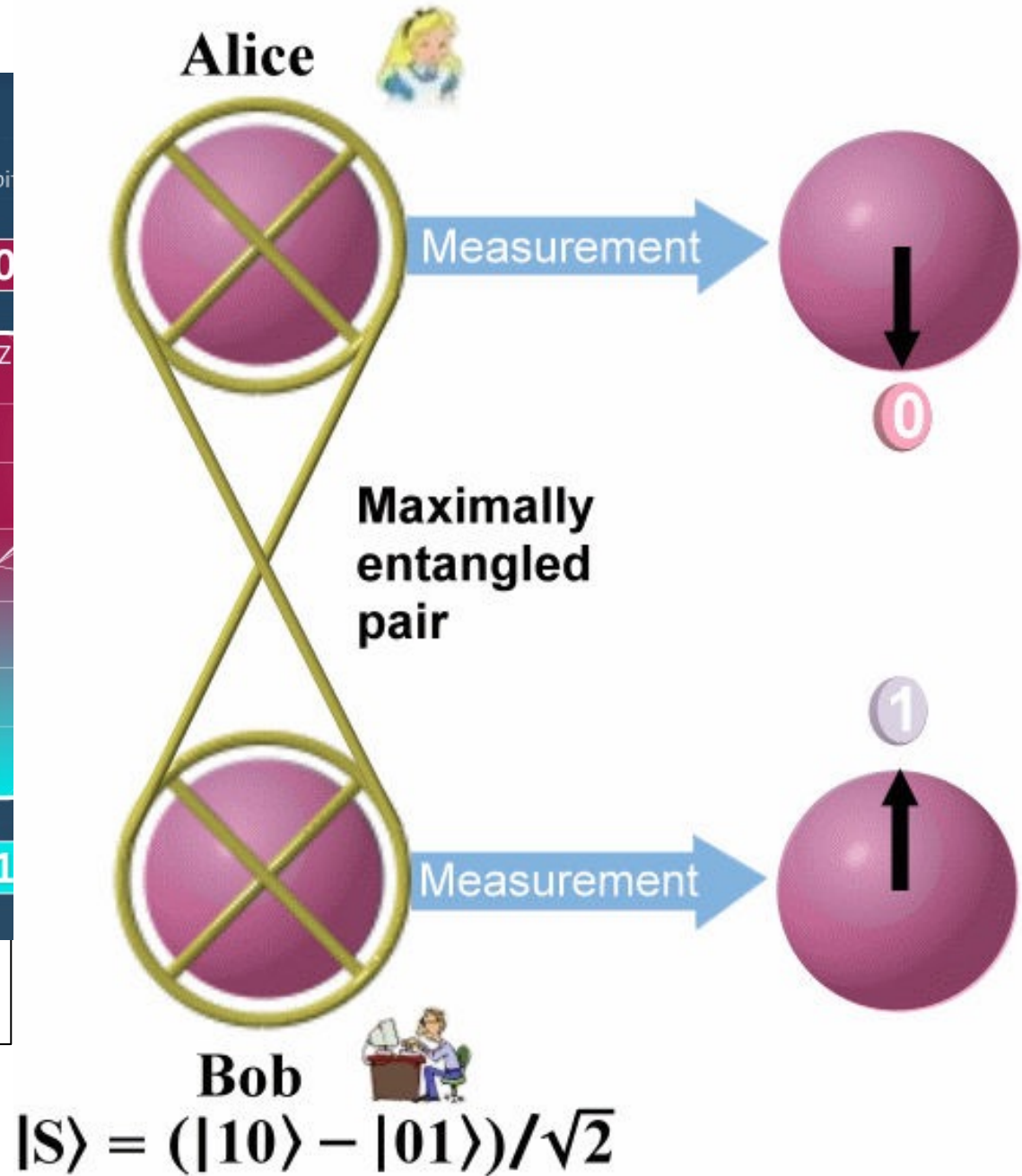
AOP network on chemical-induced cholestasis



Transforming in



- Future: quantum computing



$$|S\rangle = (|10\rangle - |01\rangle)/\sqrt{2}$$

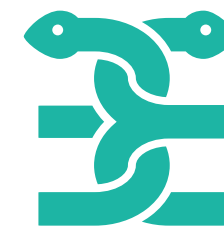
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ynamics

s at the atomic levels
al role in molecular

es (accuracy time)

Added value & future of CADD



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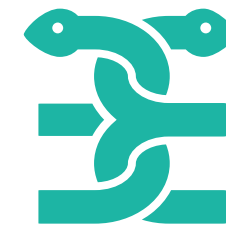
Fast, cost-effective generation of new candidate molecules



Auto-generation and evaluation



DL/ML in early-stage drug development could result in an additional 50 novel therapies over a period of 10 years, a 50-billion-dollar market



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Thank You.