

Outcome of the IHI JU Science and Innovation Panel on ideas submitted for potential IHI topics

Reference number of the idea: N° TI_001209

Harnessing data science and artificial intelligence to scale and democratize small molecule drug discovery

Overall opinion

The general aim of the idea is to increase the number of druggable proteins, lower the price for discovery of clinical candidates, and support a more open, robust, and equitable ecosystem for drug discovery. For this purpose, it is proposed to create an open public dataset of the interaction of billions of compounds with thousands of human proteins in a machine-learning readable format, and use this resource to train, benchmark, and test artificial intelligence (AI) models that can predict new protein/small molecule interactions.

Generally, the idea has a clear context, it addresses knowledge gaps and limitations of current approaches, it has a clear and relevant objective, promising impacts, and it perfectly fits the scope of IHI.

The SIP recommends supporting this idea in the following IHI calls.