PRESENTATION TITLE: *Machine Learning (ML) and Artificial Intelligence (AI) in the design of new drug lead compounds*

ABSTRACT: The hype surrounding the use of Machine Learning (ML) and Artificial Intelligence (AI) can be found in almost every field today. It is perhaps most prevalent in healthcare, and in drug discovery specifically. But in the rush to deploy AI for drug discovery, we should not overlook the obvious. Unlike text and image analysis, where data sets are abundant, the available data sets in chemistry tend to be sparse and small. In order to successfully use ML in Drug Design, one must choose the right dataset to begin with. An example of such set, that has been tested and deployed with multiple ML algorithms, is the EPO TOX21 set. However, such datasets are rare. We suggest here the use of Augmented Intelligence, the application of AI methods, such as big data and ML, to enhance computational chemistry and other non-AI algorithms and information. We will demonstrate the benefits of using Augmented Intelligence for drug design on several examples. One such example is the prediction of solvation energy of different conformers. Conformers are vectorized by Coulomb Matrix and applying Deep Tensor Neural Network algorithms, resulting in a reduction of the computational cost of deploying quantum chemistry to decide which conformers are relevant.