Artificial Intelligence (AI) is now being applied everywhere at least according to the news. Needless to say that also includes drug discovery. In this session we would like to give the audience a sense of what is going on in applying AI and machine learning (ML) in drug discovery by covering several important aspects.

The background and historical development of ML and AI in drug discovery will be presented. We will also take a look at the most important ingredient to successfully apply ML and AI in drug discovery project, namely the data and how it can be integrated. Applying ML to large datasets is an important topic that pushes the current machine learning algorithms to the limit. Another important topic to be covered is the integration of ML/AI with automation and the sizeable synergy effects when combining them.

Finally, application of deep learning in drug design has now become common, so it is time to hear from a medicinal chemist expert if there has been any real impact on the drug design process or if it just has been another hype.