

AI for drug design an industrial perspective

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Artificial Intelligence has become impactful during the last few years in chemistry and the life sciences, pushing the scientific boundaries forward as exemplified by the recent success of AlphaFold2. In this lecture I will provide an overview of how AI have impacted drug design in the last few years, where we are now and what progress we can reasonably expect in the coming years. There will be an emphasis on how AI for drug design is applied in the industry. The presentation will have a focus on deep learning based molecular de novo design, however, also aspects of synthesis prediction, molecular property predictions and chemistry automation will be covered.