**Keynote speaker at WASP Industry Days 2023**

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**Title of talk: Applying AI to drug design**

**Abstract**

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 talk 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. 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.

**Biography**

Professor Ola Engkvist is head of Molecular AI in Discovery Sciences, AstraZeneca R&D. He did his PhD in computational chemistry at Lund University followed by a postdoc at Cambridge University. After working for two biotech companies, he joined AstraZeneca in 2004. He currently leads the Molecular AI department, where the focus is to develop novel methods for ML/AI in drug design, productionalize the methods and apply the methods to AstraZeneca's small molecules drug discovery portfolio. His main research interests are deep learning based molecular de novo design, synthetic route prediction and large-scale

molecular property predictions. He has published over 140 peer-reviewed scientific publications. He is adjunct professor in machine learning and AI for drug design at Chalmers University of Technology and a trustee of Cambridge Crystallographic Data Center.