Applying Artificial Intelligence in Drug Design

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Artificial intelligence is underway to transform the society through technologies like self-driving cars. Also, in drug discovery machine learning and artificial intelligence methods has received increased attention. [1] The increased attention is not only due to methodological progress in machine learning and artificial intelligence, but also progress in automation for screening, chemistry, imaging and -omics technologies, which have generated very large datasets suitable for machine learning.

While machine learning has been used for a long time in drug design, there has been two exiting developments during the last years. One is the progress in synthesis prediction, where deep learning together with fast search methods like Monte Carlo Tree Search has been shown to improve synthetic route prediction as exemplified by a recent Nature article. [2] In this talk I will focus on the second development, which is applying deep learning based methods for *de novo* molecular design. It has always been the dream of the medicinal and computational chemist to be able to search the whole chemical space of estimated 10^{60} molecules. This would be a step change compared to search enumerable chemical libraries of perhaps 10^{10} compounds. Methods to search the whole chemical space through generative deep learning architectures has been developed during the last 3-years. In the presentation there will be a focus de novo generation of molecules with the Recurrent Neural Network (RNN) architecture. The basis will be described and exemplified of how molecules are generated. After the concept has been introduced it will be described how the method is used within drug design projects at AstraZeneca. Current limitations will be discussed in conjunction with mitigation strategies to further enhance the potential of RNN based molecular de novo generation.

[1] The rise of deep learning in drug discovery, Hongming Chen, Ola Engkvist, Yinhai Wang, Marcus Olivecrona, Thomas Blaschke, Drug discovery today, 23, 6, 1241
[2] Planning chemical syntheses with deep neural networks and symbolic AI, Marwin HS Segler, Mike Preuss, Mark P Waller, Nature, 555, 7698, 604
[3] Molecular de-novo design through deep reinforcement learning, Marcus Olivecrona, Thomas Blaschke, Ola Engkvist, Hongming Chen, Journal of cheminformatics, 9, 1, 48