[L3] Cheminformatics in Drug Discovery, an Industrial Perspective

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Cheminformatics has established itself as a core discipline within large scale drug discovery operations. It would be impossible to handle the amount of data generated today in a small molecule drug discovery project without persons skilled in cheminformatics. In addition, due to increased emphasis on “Big Data”, machine learning and artificial intelligence, not only in the society in general, but also in drug discovery, it is expected that the cheminformatics field will be even more important in the future. Traditional areas like library design and high-throughput screening analysis are highlighted in this review. Applying machine learning in drug discovery is an area that has become very important. Applications of machine learning in early drug discovery has been extended from predicting ADME properties and target activity to tasks like de novo molecular design and prediction of chemical reactions.