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Chemoinformatics in drug development

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It would be unimaginable to prosecute a drug discovery program without applying appropriate chemoinformatics analyses. In recent years a focus on target affinity and activity has been complemented by techniques to address physico-chemical properties such as lipophilicity and solubility, biological properties such as absorption, distribution, metabolism, elimination and toxicity. As such, a rounded package of studies can be performed to help in the generation and selection of molecules as clinical development candidates. Medicinal chemists are often well-served by their computational chemistry colleagues. Not so the development chemist.

Having successfully produced a clinical candidate the attention of chemoinformaticians in the pharmaceutical industry usually turns to the next molecule and scant regard is given to the contributions that can be made as a candidate molecule progresses towards becoming part of a drug substance.

This presentation will highlight the opportunities for the application of chemoinformatics techniques to the area of pharmaceutical materials science, a critical and complex phase in the creation of a drug.

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