Computational Molecular Design in Pharmaceutical Drug Discovery

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The incorporation of computational approaches into the early drug design process is a relatively young discipline compared to the long-standing history of drug discovery research. Considerable advances in hardware architecture, speed, accuracy and usability of computational algorithms have paved the way towards a quickly developing branch of research within the pharmaceutical industry. This talk will provide a general overview of computational molecular design in a pharmaceutical industry setting, highlight recent methodological advances and discuss their impact on real-world drug discovery projects.