

Title: Novel Computational Methods for Cancer Drug Design

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Abstract: Cancer is a complex and debilitating disease that is one of the leading causes of death in the modern world. Computational methods have contributed to the successful design and development of several drugs. The recent advances in computational methodology, coupled with the avalanche of data being acquired through high throughput genomics, proteomics, and metabolomics, are likely to increase the contribution of computational methods toward the development of more effective treatments for cancer. Recent advances in the application of neural networks for the prediction of the native conformation of proteins have provided structural information regarding the complete human proteome. In addition, advances in machine learning and network pharmacology have provided novel methods for target identification and for the utilization of biological, pharmacological, and clinical databases for the design and development of drugs. This is a review of the key advances in computational methods that have the potential for application in the design and development of drugs for cancer.

Keywords: Anti-cancer drug design; Computational drug design; Convolutional neural networks; Generative adversarial networks; Graph neural networks; Reinforcement learning variational autoencoders.

DOI: <https://doi.org/10.2174/0929867330666230403100008>

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