



Review

Anticancer Drug Discovery Based on Natural Products: From Computational Approaches to Clinical Studies

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Abstract: Globally, malignancies cause one out of six mortalities, which is a serious health problem. Cancer therapy has always been challenging, apart from major advances in immunotherapies, stem cell transplantation, targeted therapies, hormonal therapies, precision medicine, and palliative care, and traditional therapies such as surgery, radiation therapy, and chemotherapy. Natural products are integral to the development of innovative anticancer drugs in cancer research, offering the scientific community the possibility of exploring novel natural compounds against cancers. The role of natural products like Vincristine and Vinblastine has been thoroughly implicated in the management of leukemia and Hodgkin's disease. The computational method is the initial key approach in drug discovery, among various approaches. This review investigates the synergy between natural products and computational techniques, and highlights their significance in the drug discovery process. The transition from computational to experimental validation has been highlighted through in vitro and in vivo studies, with examples such as betulinic acid and withaferin A. The path toward therapeutic applications have been demonstrated through clinical studies of compounds such as silvestrol and artemisinin, from preclinical investigations to clinical trials. This article also addresses the challenges and limitations in the development of natural products as potential anti-cancer drugs. Moreover, the integration of deep learning and artificial intelligence with traditional computational drug discovery methods may be useful for enhancing the anticancer potential of natural products.

Keywords: natural product; anticancer drug discovery; computational drug design; clinical trials; molecular dynamics; drug design