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Dynamics-based Computational Design of Anti-Cancer Drugs

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Condition: New. Publisher/Verlag: LAP Lambert Academic Publishing | An Emerging Approach to Drug Design | Computational drug design approach has a great potential in accelerating the drug discovery process. Structure-based drug design and ligand-based drug design are the two broad classes of computational drug design. Cancer is a class of highly complex diseases involving multiple genes and multiple cross-talks between signaling networks. Cancer cells may be developed from inherited defects or acquired damages of DNA. However, many cancers are resistant to treatment, and metastasis of cancers makes the disease even more intractable. Secondary malignancies are frequently observed after cancer chemotherapy. The call for more effective cancer therapy is obligatory. Using drug-cocktails that combine multiple anti-cancer agents working in different mechanisms has been a standard treatment of cancers to overcome the drug resistance problem. More recently, design of multiple ligands (may be more easily understood as "multiple target ligands"), i.e., single agents that target multiple biomolecules in a rational manner, receives increasing attention. Some recent methodological developments on computational drug design are reviewed, and a few recent drug design efforts in cancer is summarized. | Format: Paperback | Language/Sprache: english | 104 pp.



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