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Insilco studies in breast cancer drug design

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Everyone agrees that finding new drugs is a hard, expensive, time-consuming and complicated task. On average, the traditional drug development pipeline takes about 12 years and costs about $2.7 billion to bring a new drug to market. How to lower the cost of research and speed up the process of developing new drugs has become a difficult and important question for the pharmaceutical industry. Computer-aided drug discovery (CADD) has become a powerful and promising way to design drugs that are cheaper, work better and can be made faster. In recent years, the rapid growth of computational tools for drug discovery, such as anticancer therapies, has had a big and positive effect on the design of anticancer drugs and given us new insights into cancer therapy. G protein-coupled receptor 116 (GPR116), which is an orphan adhesion receptor, plays a key role in how eukaryotic cells stick together and move. Since abnormal GPCR expression has been found in many cancers, it can be a matter of interest to find a drug that targets GPCR. Even though the role of GPR116 in the spread of metastasis in triple-negative breast cancer (TNBC) has been studied, no drugs that target GPR116 have yet been found. TNBC is an aggressive type of breast cancer that is not caused by hormones and can happen to young women. Since there is no therapy target receptor for TNBC, GPR116 would be a good choice. Chemotherapy is the only treatment that shows promise for TNBC right now, but these drugs cause chemoresistance. Therefore, newer drug molecules can be identified using CADD approach to overcome this problem.

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