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Commentary

A New Insight of Pharmacophore Modelling Hypothesis in Cancer Treatment

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ABOUT THE STUDY

Cancer is a major problem in the world it is a diverse group of diseases that can be identified by abnormal and uncontrolled growth of cells. It seriously threatens the healthy lives of people and is a major cause of human mortality and morbidity worldwide. Interestingly, GLOBOCAN estimates that approximately 19.3 million new cancer cases will lead to 10 million cancer deaths in 2020, with approximately 70% of cancer deaths occurring in low- and middle-income countries. In men, the most common cancers are lung cancer, colon cancer, prostate cancer, and gastric cancer, and in women, the most common cancers are breast cancer, lung cancer, cervical cancer, thyroid cancer, and colon cancer. Cancer treatment is a challenging task due to its diversity, diversity, and high drug resistance. Consistent efforts have been made over the last few decades to understand the biochemical processes involved in the survival of cancer cells to cure this disease. This is underpinned by advances in the development of effective anti-cancer molecules.

With the increasing number of cancer patients and the associated cancer resistance pathways, the demand for innovative new drug development is higher than ever. Coumarin (2H1benzopyran2one) is an effective antibiotic against various diseases. Breast and lung cancers were the focus of this study. To develop the pharmacophore hypothesis, biologically active coumarin derivatives were tested with IC50 values against the breast cancer cell line MCF7 and the lung cancer cell line A549. The AAARR-1 theory gave the highest score. Both types of cancer have been studied using the 3D QSAR model. A 3D QSAR model was generated using pIC50 of the compound of interest. The QSAR approach was used to develop 17 new drugs for breast cancer and 23 new drugs for lung cancer.

Pharmacophore features study of these compounds provided a 5-point AAARR_1 hypothesis. Using this hypothesis, we screened the coumarin library and obtained the top 20 ligands for both cancers. The 3DQSAR model was generated using the above dataset. The R2, Q2, and RMSE values were obtained for the training set (both breast and lung cancer). These statistical models have been used to design new molecules. A total of 17 structures have been developed for breast cancer and 22 structures for lung cancer. The compounds screened by the pharmaceutical company and the designed ligands were docked. Both the screened and designed ligands showed excellent activity of -9.7 and -0.3 kJ/mol for breast cancer VEGFR2 protein and -8.2 and -7/1 kJ/mol for breast cancer protein, respectively. Although known ligands show very high docking scores. The docking results were verified by MD simulation. The RMSD, Rg, SASA, and RMSF of both protein complex systems show good stability. The energy of interaction of both proteins with the corresponding ligand indicates lower energy. This designed ligand may be potentially more active.

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