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PTML Model for Alignment-free Prediction of Protein Targets of Anti-Melanoma Drugs

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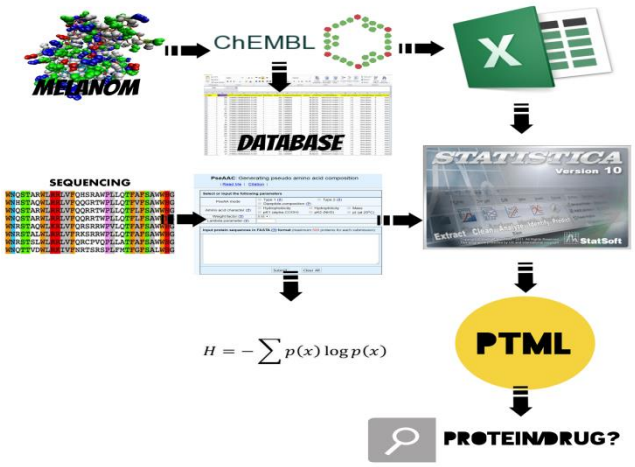
Graphical Abstract



Abstract.

Melanoma, the most serious type of skin cancer, develops in the cells (melanocytes) that produce melanin — the pigment that gives your skin its color. Worldwide Skin melanoma has an incidence of 1% in men and 0.9% in women in countries and of 0.7% in men and 0.6% in women in developing countries. In Mexico, skin melanoma has an incidence of 1.3% of all cancer patients. There is a little information about the target protein related to drug under test. There were 327480 preclinical test compounds and only 242 described the related protein. Knowing this fact could drastically changes the compound

Introduction

Melanoma is known as a malignant transformation of the melanocyte. Worldwide Skin melanoma has an incidence of 1% in men and 0.9% in women in countries and of 0.7% in men and 0.6% in women in developing countries. In Mexico, skin melanoma has an incidence of 1.3% of all cancer patients. Although there is a high number of antineoplastic drugs, the rate of mortality of this disease is highly. Collecting information in the database of CHEMBL we concluded the little information it has about the target protein related to drug under test. There were 327480 preclinical test compounds and only 242 described the related protein. Knowing this fact could drastically changes the compound.

Materials and Methods

The methodology used was basically a "statistical methodology", they were collected all melanoma-related compounds registered in CHEMBL, a manually curated chemical database of bioactive molecules with pharmaceutical-like properties. The number of test compounds found was 327480, of which a sample of

243 having the related target protein was taken. It was obtained Shannon entropy of each variable of the drug. In addition to calculating the entropy of the proteins with the FASTA format, PseAAC was used: Generating pseudo amino acid composition to obtain the lambda factor, which was also calculated entropy. The method used was the comparison of all the information on sequence, test conditions, entropies of the new drug with respect to the drug values of reference. The STATISTICA software was used to obtain the desired model.

Conclusions

From the present investigation it has been possible to obtain a predictive model that allows to recognize the biological activity of the new drug against the "j" conditions of a drug of reference in melanoma from a base of 243 proteins. Most of the drugs are unknown the related target protein, with this model we try to recognize the probability that one of the 243 base proteins is related to drugs that are unknown this variable.

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