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Prediction of Activity for Antimalarial Nanoparticle Delivery Systems

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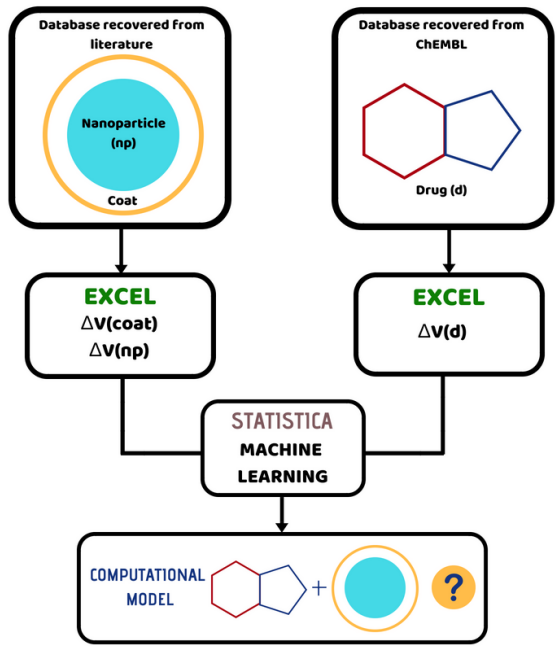
Graphical Abstract



Abstract.

For the development of the project different activities were carried out, starting with the analysis of databases downloaded from ChEMBL. These databases collect information on thousands of drugs that are used to treat several diseases. In this case, we used bases related to Plasmodium which causes malaria in humans. Additionally, a compilation of information on multiple nanoparticles was analyzed. Finally, with help of Excel application and a statistical package named STATISTICA, we found a computational model that can help us to select more effective drug-nanoparticles pairs instead of wasting resources and time creating many samples.

Introduction

Today we can see how nanotechnology has become increasingly integrated into our daily lives, that is why in the field of medicine it could not be lacking. For one example, an important application is the use of nanoparticles in drug delivery systems, since using this method a controlled and efficient release can be achieved.

However, it is also true that it presents some drawbacks because the synthesis of nanoparticles can be expensive and also involves a lot of time, even more if different samples have to be prepared.

Therefore, in this work a mathematical model was developed that allows the prediction of the antimalarial activity of the drugs bound to nanoparticles, in this way, in the laboratory, only the

experiments that comply with a good percentage of effectiveness in the model, reducing the waiting time and the resources necessary to carry out the synthesis.

Materials and Methods

For the development of the project different activities were carried out, starting with the analysis of databases downloaded from ChEMBL. These databases collect information on thousands of drugs that are used to treat several diseases. In this case, we used bases related to Plasmodium which causes malaria in humans. Additionally, a compilation of information on multiple nanoparticles was analyzed. Finally, with help of Excel application and a statistical package named STATISTICA, we found a computational model that can help us to select more effective drug-nanoparticles pairs instead of wasting resources and time creating many samples.

Conclusions.

From the present work we managed to create a mathematical model that serves as a prognostic predictor for the synthesis of nanoparticles, that together with a drug improve the effectiveness of treatments to fight malaria. In addition, the use of computational technology is highlighted to benefit the processes that are carried out in a laboratory.

References

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