

Poster Presentation

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Bioactive molecules modelised by numerical simulation: molecules against Escherichia Coli

R. Kakou Yao¹, J. Abodou Tenon¹, A. Abou¹

¹University FELIX houphouet BOIGNY, Department of Physics, Abidjan, Côte d'Ivoire

The work exposed in this paper joins in the research of medicine by means of the modelling by digital simulation (method in silico). This method allows to plan the biological activities of new molecules and to design others more active than existing molecules against a given infection. The generated and validated models are used here in the research for molecules potentially more active against Escherichia coli which causes diarrheic infections at the human beings. Here, we report works the synthesis of our works of structural determination, of forecast of biological activity and conception of molecules bioactive again Escherichia coli.

Keywords: bioactive molecules, modelisation