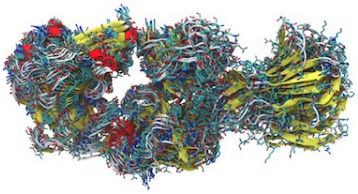

IV ASBioSim – Advanced School on Biomolecular Simulation: Protein Engineering with Rosetta, from fundamental principles to tutorials
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In silico study of the interaction between the Purine Nucleoside Phosphorylase of *Plasmodium falciparum* with Beta-Caryophylene

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Abstract: Every year millions of people die around the world due to viral, bacterial and parasitic infections. Malaria is the fifth leading cause of death for infectious diseases in the world, after respiratory infections, HIV / AIDS, diarrheal diseases and tuberculosis, with the number of victims 3 times higher than the number of victims of current armed conflicts. Malaria is caused by parasites of the genus *Plasmodium*, family Plasmodidae, filo Apicomplexa, with about 156 species that infect several vertebrates, and five of them can infect humans: P. falcipa- rum, P. malarie, P. Vivax, P. Knowlesi and P. Ovale, and malaria caused by P. falciparum is the most severe form of the disease.The increasing resistance of the parasite to antimalarial chemotherapy has worried the medical community and intensified the search for new antimalarial drugs.The purine nucleoside phosphorylase enzyme (PfPNP) catalyzes the formation of hypoxanthine, essential for the purine salvage pathway. Beta Cariophilene is a sesquiterpene found in various plants such as cinnamon (Cinnamomum spp.), Black pepper (Piper nigrum L.), clove (Syzygium aromaticum), cannabis (Cannabis sativa L.) lavender (Lavandula angustifolia), oregano (Origanum vulgare L.), rosemary (Rosmarinus officinalis) Copaíba (copaífera reticulata), and exhibit anti-inflammatory, anticarcinogenic, antimicrobial, antioxidative and analgesic therapeutic properties. In this work, three-dimensional models for the enzymes were constructed from structures obtained in the Protein Data Bank database using Modeller 9.19 software and Verify3D, MolProbity and ModFold validation techniques were used to determine the stereochemical quality of the models. The Molecular Dynamics (DM) of the enzyme and the topology of the ligand were performed using the GROMACS 5.1.4 software package, with the Gromos 96.1 force field (53A6) under NTP. Calculations of Root Mean Square Deviation (RMSD), and radius of rotation (Rr) were used for comparison and analysis of the systems with binders in relation to the free form. The binding sites of the enzymes with the ligands were obtained with Autodock Vina 1.1.2 and Autodock Tools 1.5.6 molecular docking software.