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DOCKING OF DITERPENE AS TOPOISOMERASE INHIBITOR

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Abstract: Introduction. In spite of the continued search for new anticancer drugs, cancer remains a leading cause of death. The chemotherapy most commonly used cytotoxic (tumor) chemotherapies are largely nonspecific, have narrow therapeutic indices, and undesirable side effects. DNA topoisomerases are nuclear enzymes that have important functions in DNA replication, and serve as a cancer chemotherapy target. **Methodology**. As we noted earlier, diterpenes isolated in our laboratory from Paraiban flora showed potential anticancer activity [1,2]. Here we evaluated the topoisomerase inhibition of three atisane and three trachylobane diterpenes extracted from the roots of *X. langsdorffiana*, [3-6]. The three-dimensional structures were drawn using HyperChem and the energy-minimized employing the MM+ and AM1 method. The ligands were submitted to docking with Topoisomerase I and II, using the Molegro Virtual Docker 6.0. program. **Discussion**. We note that the compound T1 do a hydrogen bond when submitted to docking with Topo I (with the ASP533 residue) and two with residues Top of II (THR213 and TYR188). The atisane diterpene form only steric interactions (between nonpolar atoms) with ARG364 Top of I and II Top of TYR188. **Conclusion.** We believe that the stability difference observed in the formation of the energy difference can be attributed to hydrogen interactions.

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