THEORETICAL STUDIES OF THE MOLECULAR INTERACTIONS OF A PALLADACYCLE COMPOUND THAT PRESENT ANTITUMORAL ACTIVITY.

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In vitro, some N,N-dimethyl-1-phenethylamine enantiomers, derived from organometallic palladacycles compounds, showed an antitumoral activity by impeding in a significant way the formation of tumor. Experimental analysis of these molecules showed significant enantioselective related to antitumoral activity. The enantiomer S(-) presented an antitumoral activity, while the enantiomer R(+) showed inactive. To understand the difference of antitumoral activity of these two enantiomers, we studied possible routes of hydrolysis of enantiomers R(+) and S(-) through studies using quantum calculations and computational simulations. The study of the enantiomers, through quantum calculations, showed that antitumoral agent S(-) is more favorable energetically to hydrolysis than R(+). We also observed that the effect of the solvent in the hydrolysis process of the antitumoral agent R(+), which turns the process more endothermic. Computational simulations and the quantum calculations results showed that the hydrolysis of R(+) enantiomer enthalpy are 14.6 kcal/mol and 27.6 kcal/mol, respectively, for two different possible hydrolysis routes. For antitumoral S(-) was observed enthalpy of -6.1 kcal/mol, which suggest that its hydrolysis is more favorable than the other enantiomer. These results can be an important factor to explain the biological activity of the enantiomer S (-).