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Abstract

Steroids Conjugated to Carbon Nanoforms as Potential Inhibitors of Viral Proteases, Synthesis, DFT Calculations, and Molecular Docking †

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Abstract: Steroid [60]fullerene hybrids have been synthesized by the Bingel−Hirsch reaction as a contribution to the chemistry of carbon nanoforms. The hybrids were characterized by different spectroscopic experiments and analytical techniques. Theoretical calculations using the Density functional theory and the PBE functional were performed to predict the most stable conformations for the synthesized compounds and the frontier molecular orbitals energy. Some properties, such as polarizability, dipole moment, lipophilicity, solvent-accessible surface area, and topological polar surface area, were calculated. Fullerenes and their derivatives have potential antiviral activity due to their specific binding interactions with biological molecules. The ability of fullerene derivatives to interact with the active site of HIV and SARS-Cov-2 proteases was studied by the Autodock Vina program. The C_{60} cage exhibited an interaction with the phenyl group of phenylalanine residues through π–π and T-shape interactions. Furthermore, it was observed that the steroid moieties formed H-bonds with the amino acid residues in the active sites of proteins. In addition, van der Waals contacts with the nonpolar protease surface, thereby improving the binding relative to the tested compound. Protein-ligand docking revealed several important molecular fragments that are responsible for the interaction, thus paving the way to study the possible application of these hybrids in medicinal chemistry.

Keywords: steroid hybrids; antivirals; theoretical calculations; fullerenes

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