- SUPPLEMENTARY MATERIAL -



Figure S1. ¹H-NMR spectrum of compound **1** (DMSO- d_6). A: full spectrum with detail of the aromatic region. B: aromatic region of the spectrum and signals of the molecule.



Figure S2. ¹³C-NMR spectrum of compound 1 (DMSO-d₆).



Figure S3. ESI-MS spectrum of compound 1 (positive ionization mode).



Figure S4. HPLC profile for compound 1 (254 nm, 96% area).



Figure S5. Docking of compound 1 (depicted in orange) to PDE5 (PDB ID: 2H42). View of the whole protein.



Figure S6. Compound **1** (depicted in orange) docked to PDE5 (PDB ID: 2H42): detailed view of the binding pocket.



Figure S7. Compound **1** (depicted in orange) docked to PDE5 (PDB ID: 2H42): detailed view of the binding pocket. In this figure, the residues present in the binding pocket have been highlighted.



Figure S8. Comparison between the docking poses of sildenafil (blue), quercetin (yellow) and compound **1** (orange). PDB ID: 2H42.



Figure S9. Comparison between the docking poses of sildenafil (blue), quercetin (yellow) and compound **1** (orange): detailed view. PDB ID: 2H42.



Figure S10. Comparison between the docking poses of sildenafil (blue), quercetin (yellow) and compound **1** (orange): detail of the binding pocket. PDB ID: 2H42.



Figure S11. Results of molecular dynamics simulation on the PDE5-compound 1 complex. A: protein root-mean-square deviation (RMSD) of atomic positions for alpha carbons (CA) and side chains. B: protein root mean square fluctuation (RMSF) of atomic positions for alpha carbons (CA) and side chains over simulation time.



Figure S12. Results of molecular dynamics simulation on the PDE5-compound 1 complex. A: ligand root-mean-square deviation (RMSD) of atomic positions. B: ligand root mean square fluctuation (RMSF) of atomic over simulation time.