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TD-DFT and UV-visible spectroscopic investigation of the solute-solvent interactions of efavirenz

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Efavirenz (EFV) commercially known as Sustiva® or Stocrin® is a first-line antiretroviral treatment for HIV/AIDS. It is categorized as class 2 on the biopharmaceutical classification system (BCS) and therefore has a low aqueous solubility but high lipophility and permeability. The low water solubility reduces oral bioavailability which subsequently leads to decreased efficacy. The objective of this study was to use UV-visible spectrophotometry and time-dependent density functional theory (TD-DFT) calculations to investigate the solute-solvent interactions of efavirenzin different solvents ranging from polar protic to non-polar solvents. The theoretical and experimental results are in agreement and an overview of the dispersion interactions is given for each solvent. The theoretical free energy of solvation has also been predicted to find the most suitable solvent with the best dispersion results as the biodistribution is dependent on the solubility of EFV in the blood. The results from this study will contribute to the formulation of EFV nanosuspensions for use in nanotechnology-based drug delivery system to increase bioavailability.

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