Ciprofloxacin (CPFX) is one of the most prominent members of the fluoroquinolone class of antibiotics and is used to treat a wide variety of bacterial infections. As with many drugs also the beneficial effects of fluoroquinolones are accompanied by undesirable side effects of which photosensitivity is characteristic to all members of this class of antibiotics. While the mechanism of the photosensitive reactions remains greatly unknown several photophysical and photochemical experimental studies exist on this subject. However, quite surprisingly this topic has received very little attention from the theoretical scientific world.[1,2]

Molecular dynamics (MD) simulations were performed to determine the solvation of the carboxylate neutral and zwitterionic forms of CPFX in water. A discrete-continuum solvation model comprising CPFX and up to ten explicit water molecules was employed in the subsequent density functional (DFT) and time dependent DFT (TD-DFT) calculations. The calculated absorption spectra of several protonated forms of CPFX are compared against experimental observations. This allows us to determine a correlation between the absorption peaks observed at different pH values and the originating protonated forms. Additionally, the analysis of the calculated absorption spectra in continuum and discrete-continuum with different number of explicit water molecules reveals that the calculated excitation wavelengths and oscillator strengths are greatly influenced by both the solvation model and the degree of solvation.

References