Calculating Solvation Energies of Fluoroquinolones.

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Abstract

The fluoroquinolones, examples of which include norfloxacin and ciprofloxacin, are important therapeutic antibiotics, especially useful in combating drug-resistant bacteria. Because the molecules of the class possess both a carboxylic acid group and a piperazinyl group, they can behave as acids, bases or zwitterions in solution. Their acid-base properties are important to their physiological activity, and it is desirable to be able to obtain accurate solvation energies when new members of the group are synthesized. We have optimized the structures of a number of fluoroquinolones in B3LYP/6-31+G* calculations, calculated solvation free energies by the self-consistent reaction field method, and compared these to known values of pK_a for the molecules to determine the accuracy of the solvation energies.