Spectroscopic studies of the interaction of 3-(2-thienyl)-[1,2,3]triazolo[1,5-a]pyridine with 2,6-dimethyl-beta-cyclodextrin and ctDNA

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Resumen

The inclusion complexation behavior of 3-(2-thienyl)-[1,2,3]triazolo[1,5-a]pyridine (TTP) with native beta-cyclodextrin and derivatized cyclodextrins was investigated. Stability constants for complexes with 1 : 1 molar ratios were calculated from phase solubility diagrams. The solubilizing efficiency of the TTP inclusion complex is enhanced in the order of DM beta CD > HP beta CD > beta CD. The TTP-DM beta CD inclusion complex was further characterized in solution by means of absorption, fluorescence, 2D NMR and molecular modeling methods. The thermodynamic studies indicate that the inclusion of TTP into the cyclodextrin cavity is mainly an enthalpy-driven process. The 2D NMR studies revealed that the thienyl moiety of TTP is inserted into the CD cavity while the triazolopyridine protrudes the primary rim of the DM beta CD, which are in good agreement with docking results. The fluorescence titration of TTP by ctDNA suggested that the quenching mechanism is a dynamic quenching procedure resulting from the temperature dependence of the TTP-ctDNA complex. Thermodynamics of the interaction revealed that the positive values of Delta H and Delta S announced that the binding process was primarily driven by hydrophobic forces indicating that TTP interacts with ctDNA by means of the minor groove. These results are in good agreement with docking experiments and iodide experiments which reinforce TTP's interactions in the minor groove.

Palabras clave

KeyWords Plus:DRUG-DNA INTERACTIONS; CYCLODEXTRINS; THERMODYNAMICS; BINDING; INTERCALATION; COMPLEXATION; REACTIVITY; SOLUBILITY; STABILITY; CHEMISTRY

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