Host-Guest Complexation of Oxaliplatin and Para-Sulfonatocalix[n]Arenes for Potential Use in Cancer Therapy

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Abstract

P-sulfonatocalix[n]arenes have demonstrated a great potential for encapsulation of therapeutic drugs via host-guest complexation to improve solubility, stability, and bioavailability of encapsulated drugs. In this work, guest-host complexes of a third-generation anticancer drug (oxaliplatin) and p-4-sulfocalix[n]arenes (n = 4 and 6; p-SC4 and p-SC6, respectively) were prepared and investigated, using 1H NMR, UV, Jobôs plot analysis, and DFT calculations, for use as cancer therapeutics. The peak amplitude of the prepared host-guest complexes was linearly proportional to the concentration of oxaliplatin in the range of 1.0 Ĭ 10ī5 Mī1 to 2.1 Ĭ 10ī4 Mī1. The reaction stoichiometry between either p-SC4 or p-SC6 and oxaliplatin in the formed complexes was 1:1. The stability constants for the complexes were 5.07 Ĭ 104 Mī1 and 6.3 Ĭ 104 Mī1. These correspond to complexation free energy of ī6.39 and ī6.52 kcal/mol for p-SC4 and p-SC6, respectively. Complexation between oxaliplatin and p-SC4 or p-SC6 was found to involve hydrogen bonds. Both complexes exhibited enhanced biological and high cytotoxic activities against HT-29 colorectal cells and MCF-7 breast adenocarcinoma compared to free oxaliplatin, which warrants further investigation for cancer therapy.

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