

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

Iten Mamdouh Fawzy ,Sherif Ashraf Fahmy ,Fortuna Ponte,Emilia Sicilia ,Udo Bakowsky ,Hassan Mohamed El-Said Azzazy

## 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 para-sulfonatocalixarene (SC4) and a sixth-generation para-sulfonatocalixarene (SC6) with oxaliplatin were prepared and characterized by <sup>1</sup>H NMR, UV, Job's 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 × 10<sup>-5</sup> to 1.0 × 10<sup>-3</sup> mol/L. The stability constants for the complexes were 5.07 × 10<sup>4</sup> and 6.3 × 10<sup>4</sup> mol<sup>-1</sup> for SC4 and SC6, respectively. These correspond to complexation free energy of -6.39 and -6.52 kcal/mol for SC4 and SC6, respectively. Complexation of oxaliplatin with SC4 and 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.

*Molecules* 2020, December