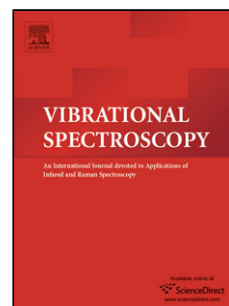


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A spectroscopic investigation into the binding of novel platinum(IV) and platinum(II) anticancer drugs with DNA

Rukshani Haputhanthi, Ruchika Ojha, Ekaterina I. Izgorodina, Si-Xuan Guo, Glen Deacon, Don McNaughton, Bayden R. Wood*

Centre for biospectroscopy and School of Chemistry, Monash University, Clayton, Victoria, 3800, Australia

*Corresponding Author: *Tel.*: +61 3 9905 5721; *fax*: +61 3 9905 4597.

E-mail address: Bayden.Wood@monash.edu (B.R. Wood).

Abstract

Platinum(II) complexes have had enormous success in cancer chemotherapy and novel Pt^{IV} complexes show potential for reduced toxic side effects and different mechanisms of action. While the action of Pt^{II} anticancer drugs with DNA has been well characterized with X-ray and many spectroscopic modalities, the mechanisms of binding Pt^{IV} complexes to DNA require further fundamental studies. In the present work using ATR-FTIR spectroscopy, we have extensively analyzed conformational changes in both single-stranded (ss) and double-stranded (ds) calf-thymus DNA, after binding to the Pt^{IV} anticancer complex, [Pt{((p-FC₆F₄)NCH₂)₂}(py)₂(OH)₂] (py = pyridine) (Pt103(OH)₂), and its Pt^{II} analogue, [Pt{((p-FC₆F₄)NCH₂)₂}(py)₂] (Pt103) in buffered aqueous acetone (55% water), under which conditions no hydrolysis of drugs occurs. To aid in band assignments of the Pt derivatives, DFT calculations using the M062X/cc-pVDZ level of theory were performed. The ssDNA is distorted and its conformation changes more towards the A-like DNA of dsDNA upon binding to both Pt103 and Pt103(OH)₂. This conclusion is derived from the changes in the PO₂⁻ symmetric stretching vibrations (1086 to 1093 cm⁻¹) and C-O (1055 to 1062 cm⁻¹) and C-C

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