

In silico approach to cisplatin toxicity. Quantum chemical studies on platinum(II)-cysteine systems.

Autorzy

Henryk Chojnacki

Janina Kuduk-Jaworska

Iwona Jaroszewicz

Jerzy Jański

Rok wydania

2009

Czasopismo

Journal of Molecular
Modeling

Numer woluminu

15

Strony

659-664

DOI

10.1007/s00894-009-0469-2

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The behaviour of cisplatin in serum, and the drastic differences between the properties of this drug and its trans-isomer were the main motivations for this work. In a search for model "thiol-platin(II)" interactions, the first steps of the following reaction systems were evaluated: (1) cisplatin-thiomethanol; (2) transplatin-thiomethanol; (3) cisplatin-cysteine; and (4) transplatin-cysteine. In each case, calculations for the associative mode of reactions were performed. The electronic structure of these molecular systems was studied at the non-empirical all-electron level using density functional theory (DFT) within the Huzinaga and WTBS basis sets including polarisation Gaussian functions and full geometry optimisation. B3LYP or EPBO density functionals were applied throughout. The calculated molecular electrostatic potentials are presented graphically. Assuming that electrostatic effects are dominant, cisplatin should interact more strongly with the sulfur atom of CH₃S- and deprotonated CYS-S- than transplatin. This fact has been documented in the supermolecule model of the relevant interaction energies in both gas phase as well as within the solvent polarisable continuum model. The opposite relationship was observed when we compared values of energy differences between products and substrates for both isomers. The data obtained here could be applied to search for correlation between the biological activity of platinum complexes and their properties as estimated by various physico-chemical and in silico methodologies.

Słowa kluczowe

cisplatin, transplatin, interactions with deprotonated thiomethanol and cysteine

Adres publiczny

<http://doi.org/10.1007/s00894-009-0469-2>

<http://link.springer.com>

Plik został wygenerowany dnia 2026-10-06 20:34:30

Adres w repozytorium <https://old.chem.uni.wroc.pl/pl/repozytorium/iLDun80>.