

## عنوان مقاله:

Organometallic Pd (II) complexes of stabilized phosphorus ylide with  $\alpha$ -amino acids: Synthesis, structure, DNA/BSA binding, in vitro cytotoxicity and molecular dynamic simulation studies

## محل انتشار:

پانزدهمین همایش بیوشیمی فیزیک ایران (سال: 1397)

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## خلاصه مقاله:

A new series of biological active cyclometallated Pd (II) complexes bearing  $\alpha$ -amino acids have been synthesized and fully characterized by  $^1\text{H}$ ,  $^{13}\text{C}$ - $\{^1\text{H}\}$ ,  $^{31}\text{P}$ - $\{^1\text{H}\}$  NMR spectroscopy, FT-IR technique and CHN test. Single crystal X-ray crystallography showed the presence of Pd (II) atom in a slightly distorted square-planar environment surrounded by orthometallated phosphorus ylide as well as NO-chelated amino acid. Treatment of new synthesized orthopalladated complexes against a series of human cancer cell lines, demonstrated considerable cytotoxic activities in comparison with standard cisplatin. Binding interaction ability of the most bio-efficient complex with calf-thymus deoxyribonucleic acid (CT-DNA) and bovine serum albumin (BSA) has been investigated. UV-Vis spectroscopy, competitive emission titration and circular dichroism (CD) methods have demonstrated the intercalative binding of Pd (II) complex to DNA. The BSA interactions of complex using fluorescence quenching and synchronous fluorescence spectra suggested a static quenching procedure for the fluorescence quenching of BSA by complex. Evaluating site marker displacement experiments, the Sudlow's site I in the subdomain IIA was suggested to be the location of the complex binding to BSA. Furthermore, molecular docking method was applied to predict the binding modes of interactions that effectively confirmed the spectral data. These results can help on drug designing of new metal-based antitumor agents in near future.

## کلمات کلیدی:

Organopalladium complex, Amino acid, DNA/BSA, Antitumor, DFT

## لینک ثابت مقاله در پایگاه سیویلیکا:

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