Editorial

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Cheminformatics and System Chemistry of Cisplatin, Carboplatin, Nedaplatin, Oxaliplatin, Heptaplatin and Lobaplatin as Anti-Cancer Nano Drugs: A Combined Computational and Experimental Study

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Editorial

The anti-cancer Nano drugs Cisplatin, Carboplatin, Nedaplatin, Oxaliplatin, Heptaplatin and Lobaplatin were characterized by ^{1}HNMR, ^{13}CNMR, ^{31}PNMR, Attenuated Total Reflectance Fourier Transform Infrared (ATR-FTIR), FT-Raman, HR Mass and UV-Vis spectroscopies and also by Scanning Electron Microscope (SEM), Transmission Electron Microscope (TEM), Differential Thermal Analysis-Thermal Gravim Analysis (DTA-TGA), Energy-Dispersive X-Ray Spectroscopy (EDX) and X-Ray Diffraction (XRD) analysis and crystallography. *Ab initio* and Density Functional Theory (DFT) calculations have been carried out for the title anti-cancer Nano drugs by performing HF, PM3, MM2, MM3, AM1, MP2, MP3, MP4, CCSD, CCSD(T), LDA, BVWN, BLYP and B3LYP levels of theory using the standard 31G, 6-31G*, 6-31+G*, 6-31G(3df, 3pd), 6-311G, 6-311G* and 6-311+G* basis sets of the Gaussian 09. The computational results show that the predicted geometries can well reproduce the structural, thermodynamic and spectroscopic parameters. Predicted vibrational frequencies have been assigned and compared with experimental ^{1}HNMR, ^{13}CNMR, ^{31}PNMR, Attenuated Total Reflectance Fourier Transform Infrared (ATR-FTIR), FT-Raman, HR Mass and UV-Vis spectra and they are supported each other comparison between the experimental and the computational results indicates that *ab initio* and Density Functional Theory (DFT) HF, PM3, MM2, MM3, AM1, MP2, MP3, MP4, CCSD, CCSD(T), LDA, BVWN, BLYP and B3LYP levels of theory using the standard 31G, 6-31G*, 6-31+G*, 6-31G(3df, 3pd), 6-311G, 6-311G* and 6-311+G* basis sets of the Gaussian 09 are able to provide satisfactory results for predicting dynamic NMR shielding tensors and vibrational frequencies properties. On the basis of vibrational analyses, the structural, thermodynamic and spectroscopic properties of the title anti-cancer Nano drugs at different temperatures have been calculated.

Anti-cancer Nano drugs Cisplatin, Carboplatin, Nedaplatin, Oxaliplatin, Heptaplatin and Lobaplatin are widely used mild analgesic drugs that cause liver necrosis in human and also experimental animals when high doses are ingested or administered [1-13]. Studies on the metabolism of anti-cancer Nano drugs Cisplatin, Carboplatin, Nedaplatin, Oxaliplatin, Heptaplatin and Lobaplatin **(Figure 1)** [13-23] have shown that major routes of elimination involve Sulfation or Sulfurylation and Glucuronidation, while a minor route involves oxidation and subsequent conjugation of the oxidation product with the sulfhydryl-containing tripeptide and Glutathione (GSH). Evidence strongly implicates a role for this minor oxidation product in the hepatotoxic reaction caused by anti-cancer Nano drugs Cisplatin, Carboplatin, Nedaplatin, Oxaliplatin, Heptaplatin and Lobaplatin, although the exact chemical nature of these anti-cancer Nano drugs and the mechanism (s) by which it leads to human cancer cells death are unknown [24-44].

The optimized structural, thermodynamic and spectroscopic parameters of the anti-cancer Nano drugs Cisplatin, Carboplatin, Nedaplatin, Oxaliplatin, Heptaplatin and Lobaplatin by *ab initio* and Density Functional Theory (DFT) HF, PM3, MM2, MM3, AM1, MP2, MP3, MP4, CCSD, CCSD(T), LDA, BVWN, BLYP and B3LYP levels of theory using the standard 31G, 6-31G*, 6-31+G*, 6-31G (3df, 3pd), 6-311G, 6-311G* and 6-311+G* basis sets of the Gaussian 09 were calculated. The aim of this editorial is to give optimal molecular geometries and vibrational modes of these anti-cancer Nano drugs. Furthermore, in this editorial, vibrational frequencies were calculated at HF, PM3, MM2, MM3, AM1, MP2, MP3, MP4, CCSD, CCSD(T), LDA, BVWN, BLYP and B3LYP levels of theory using the standard 31G, 6-31G*, 6-31+G*, 6-31G (3df, 3pd), 6-311G, 6-311G* and 6-311+G* basis sets of the Gaussian 09. Gauss View 5 program was used to assign the computational harmonic frequencies. On the basis of the comparison between computational and experimental results, assignments of fundamental modes were examined. The assignment of the experimental frequencies are based on the observed band frequencies in the ^{1}HNMR, ^{13}CNMR, ^{31}PNMR, Attenuated Total Reflectance Fourier Transform Infrared (ATR-FTIR), FT-Raman, HR Mass and UV-Vis spectra of this species were confirmed by establishing one to one correlation between experimental and computational frequencies. The *ab initio* and Density Functional Theory (DFT) HF, PM3, MM2, MM3, AM1, MP2, MP3, MP4, CCSD, CCSD(T), LDA, BVWN, BLYP and B3LYP levels of theory using the standard 31G, 6-31G*, 6-31+G*, 6-31G (3df, 3pd), 6-311G, 6-311G* and 6-311+G* basis sets of the Gaussian 09 calculations were performed for anti-cancer Nano drugs

Cisplatin, Carboplatin, Nedaplatin, Oxaliplatin, Heptaplatin and Lobaplatin.

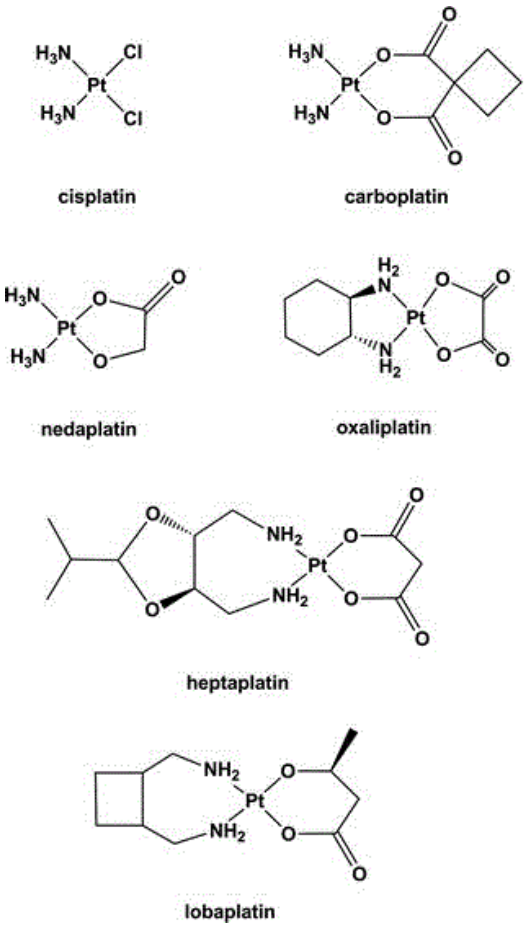

Figure 1: Molecular structure of anti-cancer Nano drugs Cisplatin, Carboplatin, Nedaplatin, Oxaliplatin, Heptaplatin and Lobaplatin.

The computational results show that the predicted geometries can well reproduce the structural, thermodynamic and spectroscopic parameters. Predicted vibrational frequencies have been assigned and compared with experimental ^{1}HNMR, ^{13}CNMR, ^{31}PNMR, Attenuated Total Reflectance Fourier Transform Infrared (ATR-FTIR), FT-Raman, HR Mass and UV-Vis spectra and they are supported each other. On the basis of vibrational analyses, the structural, thermodynamic and spectroscopic properties of the anti-cancer Nano drugs Cisplatin, Carboplatin, Nedaplatin, Oxaliplatin, Heptaplatin and Lobaplatin at different temperatures have been calculated, revealing the correlations among the structural, thermodynamic, spectroscopic parameters and temperatures.

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