DFT CALCULATIONS ON NMR CHEMICAL SHIFTS FOR PLATINUM BASED METALODRUGS

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Platinum-based drugs remain significant components in treatment of cancer. Recently however, there has been a surge of activity aimed at developing non-classical platinum complexes that operate a different mechanism from those of approved drugs that tantamount to a better delivery [1]. In this study, we demonstrate a protocol that is used to calculate NMR chemical complexation shifts for a series of Pt (IV) complexes derived from oxaliplatin.

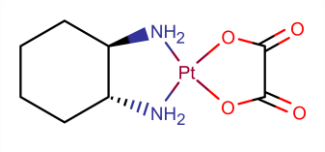

Fig. 1: Oxaliplatin

The standard PBE functional was used for optimizations and PBE0 functional was used for chemical-shift calculations using zeroth-order regular approximation (ZORA) for treatment of relativistic effects and solvation models to mimic the solvent environment [2]. We use experimental results as a benchmark for the calculated numbers. NMR shifts for Platinum and Hydrogens were evaluated.

[1] Johnstone T.C.; Suntharalingam K.; Lippard S.J. *Chem. Rev.*, 116. (2016) 3436-3486.
[2] Vicha J.; Patzchke M.; Marek R. *Phys. Chem. Chem. Phys*., 15 (2013) 7740-7754.