

## Affinities to Oxaliplatin: Vitamins from B Group vs. Nucleobases

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### Streszczenie

Oxaliplatin, similar to Cisplatin, exhibits anticancer activity by interacting with DNA and inducing programmed cell death. It is biotransformed through a number of spontaneous and non-enzymatic processes. In this way, several transient reactive species are formed, including dichloro-, monochloro-, and diaqua-DACH platin, which can complex with DNA and other macromolecules. The molecular level suggests that such interactions can also take place with vitamins containing aromatic rings with lone pair orbitals. Theoretical and experimental studies were performed to investigate interactions of vitamins from the B group with Oxaliplatin, and the results were compared with values characterizing native purines. Quantum-chemical simulations were carried out at the B3LYP/6-31G(d,p) level, with the LANL2DZ basis set representing atomic orbitals of platinum atom, and at the MN15/def2-TZVP levels of theory with the use of Polarizable Continuum Model (IEF-PCM formulation) and water as a solvent. Additionally, time-dependent density functional theory (TD-DFT) was employed to study molecular properties in the electronic excited state. Interactions of vitamins and Oxaliplatin were investigated using UV-Vis spectroscopy. Values of the free energy ( $\Delta G_r$ ) indicate spontaneous reactions with monoqua  $[\text{PtH}_2\text{OCIDACH}]^+$  and diaqua  $[\text{Pt}(\text{H}_2\text{O})_2\text{DACH}]^{2+}$  derivatives of Oxaliplatin. However, diaqua derivatives were found to be preferable. The free energy ( $\Delta G_r$ ) values obtained for vitamins from the B group indicate lower affinity of Oxaliplatin compared with values characterizing complexes formed by guanine, adenine, and cytosine. The exception is the monoqua form of vitamin B1 (thiamine) at the MN15/def2-TZVP levels of calculations. An application of atoms in molecules (AIM) theory revealed non-covalent interactions present in the complexes studied. The comparison of computed and experimental spectroscopic properties showed a good agreement.

### Słowa kluczowe

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Oxaliplatin, platinum-based drugs, colorectal cancer, gastric cancer, esophageal cancer, cancer treatment, vitamins from B group, UV-Vis, DFT, TD-DFT, PCM

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