

The hybrid models, containing hydrolytic and electron-driven processes, in theoretical study of oxaliplatin biotransformation.

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Streszczenie

The results of theoretical simulations of reaction paths for oxaliplatin from pro-drug into its active form responsible for cytostatic effect are presented. The studies based on the quantum-chemical density functional theory approach were performed considering environmental influence resulting from the aquation or electron donation. The hybrid mechanisms: hydrolytic mixed with electron driven were found to be the energetically favourable.

Słowa kluczowe

Oxaliplatin transformation, Electron-driven reactions, DFT calculations, Hybrid mechanism, Nonclassical Pt-water interactions

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