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Clinical Image

Title : 99Tc NMR as a Promising Technique for Structural Investigation of Biomolecules

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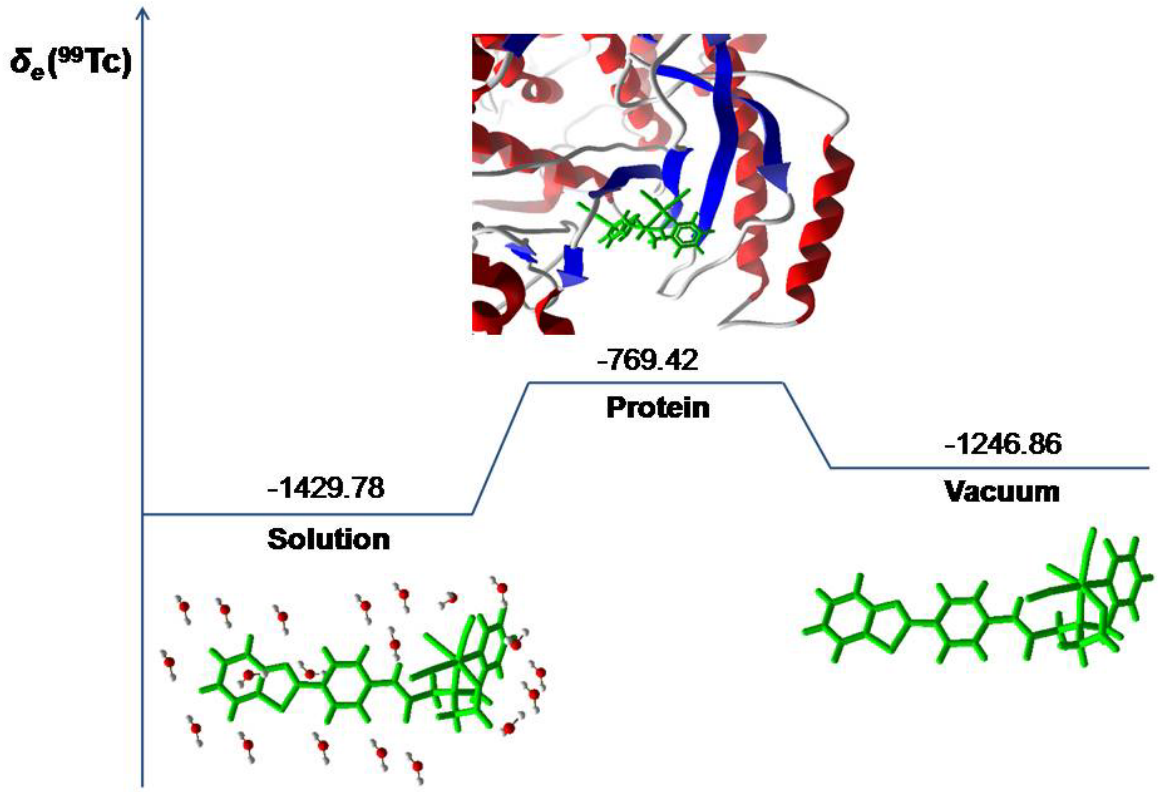

The breast cancer is one of the major health problems of the western world. Currently, drugs containing radionuclide, denominated radiopharmaceuticals, are used frequently in nuclear medicine for the diagnosis or therapy of cancer and various other diseases. In fact, a large number of different classes of radiopharmaceuticals can be employed. Among them, one of the most commonly used is based on Technetium (Tc) metallic complexes, highlighting the nuclides 99Tc and its metastable nuclear isomer 99mTc. Within this context, in 2006 Tzanopoulou et al. synthesized the (99mTc)(CO)3(NNO) complex conjugated to the antitumor agent 2-(4'-aminophenyl) benzothiazole (ABT). The phenyl benzothiazole (PBT) compounds show antitumor properties and are highly selective. The original lead compound in this series, ABT, exhibits nanomolar in vitro activity against certain human-breast cancer cell lines. Its chemical activity is connected to docking properties of this molecule to the protein Phosphoinositide 3-kinase (PI3K). We have calculated the 99Tc NMR chemical shifts of the complex in different environments vacuum, solution and protein, using the density functional theory, DFT- level BPW91/aug-cc-pVTZ for the Tc and BPW91/IGLO- II for the other atoms. The results highlight that the 99Tc NMR spectroscopy can be a promising technique for structural investigation of biomolecules, at the molecular level, in different environments.

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