عنوان مقاله:

Molecular Structure Determination and Stability Parameters Study of 99mTc-MDP (Technetium 99m Methylene Diphosphonate) Cold Kit and Analysis of Its Binding to Osteocalcin Receptor as a Bone Scan Agent

محل انتشار:

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خلاصه مقاله:

This work evaluates the stability of tecnethium-99m methylene diphosphonate (99mTc-MDP) radiopharmaceutical and identifying its precise molecular structures and analyzing their binding to osteocalcin receptor. At first, different formulations of 99mTc-MDP cold kit were made in various conditions. Then, various molecular structures were evaluated and optimized using B3LYP/Lanl2DZ level of theory by Gaussian software at room temperature. The stability and reactivity properties of the optimized molecular structures were calculated using Frontier molecular orbitals (FMOs) theory. The binding of the molecular structures with the said receptor was analyzed using the molecular docking study. The investigation results indicated that the interactions between the molecular structures and osteocalcon receptor were related to the residues Leu 25, Asn 26, Asp 30, Cys 29, Tyr 42, Tyr 46 and Phe 38

کلمات کلیدی:

Medronate, methylene diphosphonate, Molecular docking, Molecular Simulation, Nuclear medicine, Osteocalcin receptor