

Abstract Submitted
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Assessment of the Biocompatibility of the Iron Oxide Nanoparticles Treating Cancer Disease Using Computational Simulation JOO HEE LEE, RICHARD KYUNG, Choice Research Group — Bio-metals such as copper, zinc, iron, and manganese have been widely used as prominent materials for medical applications including clinical treatment such as treating cancer disease. In the past, iodine and transitional metal oxides have been used in nanoparticles for cancer detection but some of them showed harmful effects to the body. In this research, the efficiencies of magnetic nanoparticles such as iron oxide compounds used the detection of the CTC (Circulating Tumor Cells) are modeled using computer software and explained through the compounds electron structure. Gamess is a program that allows performing such computations for a compound. It takes an input file of a defined format and converts it into an output describing the molecule and the reaction. Chemcraft and Avogadro are another programs that take the output from Gamess and expresses it as a model. These programs show the optimized geometry energy levels and they fully determines the theoretical values of the structures atomic properties. These computational programs were used to complement each other to produce a result that is useful to see the outcomes.

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