Abstract Submitted
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Thermodynamic Analysis of Nanoparticles for the Treatment of Neurodegenerative Disease SEOYEON CHOI, RICHARD KYUNG, CRG-NJ — Photodynamic therapy(PDT) is one of the most common treatments for AD. It utilizes photoirradiation to activate photosensitizers, which produce ROS to kill tumor cells. Moreover, as metal ion imbalance is found to be associated with Alzheimers Disease(AD), chelation therapy has been proposed. It makes use of chelators to capture and remove metal ions. This paper is focused on using the computer software Avogadro to find the stability and activity of nanoparticles used for PDT and chelation therapy through assessing their thermodynamic characteristics. As for chelators, metal-EDTA compounds and metal-DTPA compounds were compared. As for photosensitizers, porphyrins, chlorins, and phthalocyanines were analyzed. Optimized energy, dipole moment, and electrostatic potential map were used as the main criterion for analyzing thermodynamic characteristics. As a result, EDTA was found to have higher stability than DTPA. Cu-EDTA and Mg-EDTA were the most stabilized EDTA compounds, whereas Cu-DTPA was the most stabilized DTPA compound. Out of the porphyrin isomers, N-confused porphyrin and doubly N-confused porphyrin were found to be the most stable and reactive molecules. Also, chlorin and isobacteriochlorin were found to have better thermodynamic characteristics than bacteriochlorin.

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