Abstract Submitted
for the OSS21 Meeting of
The American Physical Society

Stereochemical Analysis of Porphyrins and Chelators to Control Free Radicals JEEWON HAN, Cranbrook Kingswood Upper School — Photodynamic Therapy, or PDT, is a method of cancer treatment which uses a photosynthesizer, oxygen, and a light of a determined frequency. Normally, reactive oxygen species are damaging to normal cells around them and therefore should be eliminated, but their destructive properties also allow them to eliminate cells harmful to the body, such as cancer cells. In photodynamic therapy, the high reactive oxygen species interact with biomolecules and produce oxidative radicals, which is cytotoxic in action. The free radicals then destroy the tumor cell through inducing apoptosis or necrosis. In this study, various molecules that can help remove reactive oxygen species from normal cells and the different isomers of porphyrin and cyclodextrin, photosynthesizers, were analyzed and compared to reveal which compound would work best. Also, to eliminate the toxic levels of redox metals in nerve cells, especially copper and iron, through selective chelation, this research investigated various iron chelators (EDTA, DTPA among others) from multiple dimensions, including optimization energy, electrostatic potential map, and dipole moment.

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Date submitted: 28 Mar 2021 Electronic form version 1.4