

Abstract Submitted
for the TSP21 Meeting of
The American Physical Society

Study on the DNA-photocleavage Ability of Metalloporphyrins

RICHARD KYUNG, CRG-NJ, SEOYEON CHOI, CRG-NJ(KMLA) — Alzheimers Disease (AD) is one of the most common neurodegenerative diseases and Familial AD(fAD), an inherited form of Alzheimer's disease caused by gene mutations. Through efficient cleavage and elimination, porphyrin-DNA complexes can help repair mutations at specific locations in the human genome in order to cure hereditary causes of AD. During a photocatalytic reaction, a light of a specific wavelength activates the photosynthesizer to produce highly reactive oxygen species that interact with molecules and produce oxidative radicals. This paper focuses on the stability and activity of various porphyrins and porphyrin-DNA complexes for their DNA-photocleavage ability by measuring their thermodynamic characteristics using a molecular editing program. Optimized energy, dipole moment, and electrostatic potential maps were used as the main criteria for analysis. These factors were investigated when the porphyrins attach to DNA when they were attached to the nucleobase, phosphate group, or to the ribose moiety.

Richard Kyung
CRG-NJ

Date submitted: 26 Sep 2021

Electronic form version 1.4