Abstract Submitted
for the NEF19 Meeting of
The American Physical Society

Study on the Chelators Used in Treatment for Neurodegenerative Disease Using Bio-chemical and Computational Analysis MIA MOON, Bergen County Academies, AMANDA KYUNG, NVRHS at Demarest — Iron homeostasis is currently emerging as a key factor in maintaining brain health and preventing disease. In several neurodegenerative diseases such as Alzheimers disease, Parkinsons disease, or macular degeneration, iron homeostasis has been disrupted and elevated levels of redox active metals were detected in the brain. In this research, computational methods employing quantum chemistry were used to model various chelator candidates for iron and other metal ion chelation therapy in the brain. The molecules were assessed for thermodynamic stability, reactivity, and polarization. For certain hydroxyquinoline chelates, moderate molecules and EDTA series were tested for their thermodynamic stabilities, which were measured through the optimized energies. The reactivity and conductivity were also measured through the dipole moments to calculate the activity level the molecule could have with other nearby molecules. Lastly, electrostatic potential maps were utilized to visualize the polarization and assess the reactivity level of each molecule. As antioxidants, hydroxyquinoline chelates showed good activity and stability. However, as multimodal agents, EDTA analogues showed less activity compared to the hydroxyquinoline chelates due to their geometrical aspects.

Richard Kyung
CRG-NJ

Date submitted: 27 Sep 2019 Electronic form version 1.4