The underlying mechanism of how MALDI matrices work is poorly understood. Experimental literature suggests that the triplet excited state (T$_1$) of the matrix plays a significant role in its ability to transfer charge to the analyte effectively. The heavy atom substitution effect predicts that the addition of a heavy atom to an otherwise "dead" matrix, such as 2,4-dihydroxybenzoic acid, would increase the rate of Intersystem Crossing (ISC) to the T$_1$ state via spin-orbit coupling. This effect was observed experimentally as there was a visible decay in singlet lifetime and an increase in triplet lifetime, as well as a better matrix performance when compared to its original, unsubstituted partner. To provide insight into the photophysical properties of 2,4-dihydroxybenzoic acid and its halogenated isomers, calculations were performed using Gaussian09. Geometry optimizations, frequencies, and IR spectra of all isomers were calculated using Density Functional Theory (DFT) with B3LYP functional and the 6-31G+(d,p) basis set. UV-Vis and fluorescence spectra were generated using Time-Dependent DFT (TDDFT). The following values for the singlet ground state (S$_0$), triplet excited state (T$_1$), and singlet excited state (S$_1$) were tabulated and compared: optimization energies, HOMO-LUMO energies and orbital contours, and bond distances. In addition, the energy values for Proton Affinity (PA) and Gas Phase Acidity (GPA) were determined.