Computational Modeling of Lithium-specific Fluorescent Sensors to Better Treat Bipolar Disorder

Claridge, Sean, Dr Diane Nutbrown, Department of Physical Sciences, Emporia State University

Lithium carbonate has been prescribed as the gold-standard treatment for bipolar disorder for over fifty years, continuing to outperform newer, alternative mood stabilizers. Despite this, the pharmacological mode of action for lithium in treating bipolar disorder is still speculative. A lithium-specific fluorescent probe would aid researchers in fully understanding how lithium works, and help design more effective drugs for treatment. Calculations were performed using Gaussian as the computational engine and Density Functional Theory. These calculations were used to both identify potential probes and to complement experimental data with theoretical calculations. The ability of these proposed fluorescent sensors to selectively bind lithium was estimated by comparing absolute energies of the molecule with and without a metal ion present. Molecules that appeared to exclude competing ions (e.g. Mg^{2+}, Na^{+}, K^{+}) and yield reasonable complexes with Li^{+} will be targeted for synthesis in the lab. A small-molecule fluorescent sensor operates by exhibiting a change in absorbance and/or emission upon binding of a specific ion. This decrease in emission intensity (turn-off sensor), or a shift in the emission wavelength that changes the color of the light emitted, is preferred because the colors are directly related to gaps in molecular orbital energies. Calculated molecular orbitals predicted these potential emission changes.