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SOLUBILITY OF BIPYRIMIDINE ELECTROLYTES FOR REDOX FLOW BATTERIES

Shelby Lynn Galinat (Matthew S. Sigman, Adam R. Pancoast)
Department of Chemistry

As the world seeks alternatives to traditional energy sources in the light of climate change and its damaging consequences, it is clear that improved energy storage systems for the grid are needed[1,2]. The intermittent supply of solar and wind energy requires large scale energy storage in order to provide consistent energy to meet grid demand. Redox flow batteries (RFBs) offer a potential solution to this energy storage problem. A main feature of RFBs is the decoupling of energy and power density, which satisfies the unique energy and power demands of different loads.

While the current state-of-the-art RFBs are run under aqueous conditions, their reliance on water as a solvent presents several notable limitations. The organic solvents and electrolytes employed by non-aqueous RFBs (NRFBs) expand temperature resilience, increase the potential window, and allow for the use of more sustainable and cheaper materials[3]. An important research area for NRFBs is developing highly soluble and stable electrolytes. In a study by Griffin *et al*, a highly stable o-trifluoromethyl phenyl bipyrimidine anolyte which undergoes two reductions in the solvent potential window of acetonitrile was reported (**Figure 1**).

Following the example of the previous bipyrimidine stability model and the solubility model developed by Robinson *et al.*, Adam Pancoast and I are continuing work on a project that aims to study solubility or stability trends in a library of bipyrimidine derivatives. Using laboratory solubility and cycling measurements, computationally derived molecular descriptors, and Multivariate Linear Regression for the 13 bipyrimidine derivatives shown in **Figure 2**, we hope to predict and test anolytes with improved battery performance in acetonitrile. If the experimental solubilities of the derivatives are

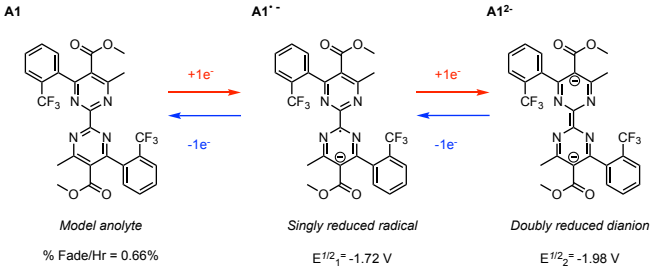

Figure 1. The o-trifluoromethyl phenyl bipyrimidine derivative **A1** was the highest energy density and lowest percent capacity fade anolyte from the recent study by Griffin et al.

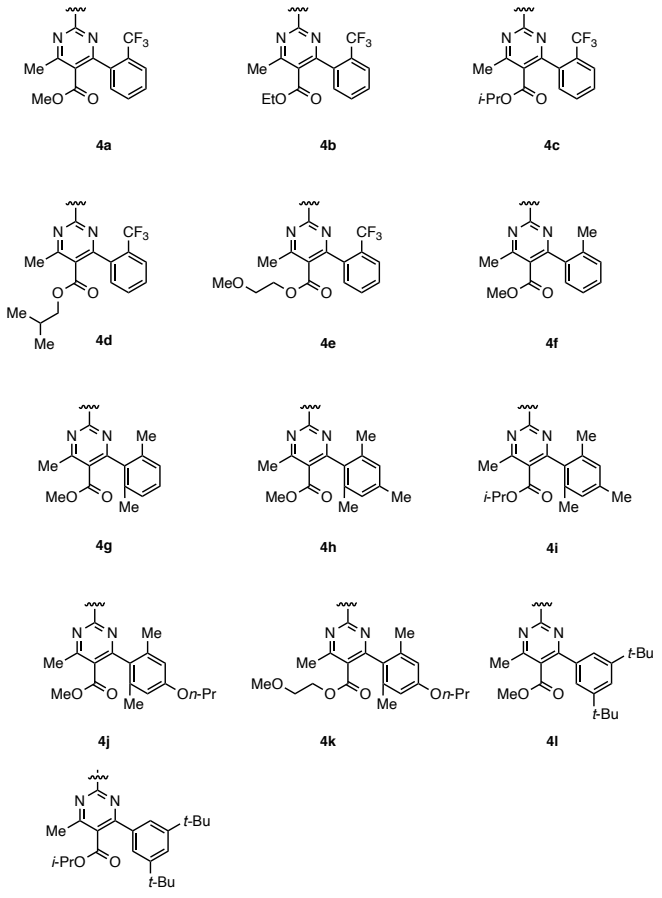

Figure 2. Novel additions to the original data set from the Griffin *et al*. paper.

sufficiently high for use in a battery with the bis(diisopropylamino)cyclopropenium-arene catholytes developed by Yan *et al*., we will incorporate the new derivatives in this training set to the stability model from the paper by Griffin *et al.*

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