Computational Electrochemistry of Bio-Derived Quinone Derivatives for Organic Redox Flow Batteries

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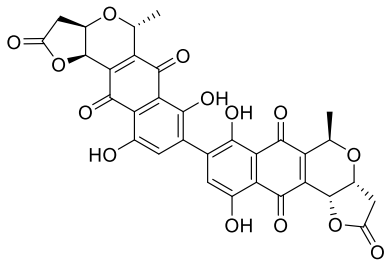
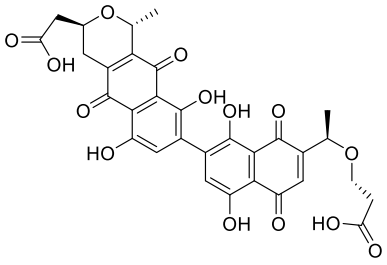
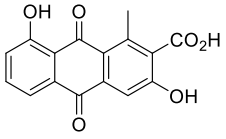
Large-scale, low-cost electrical energy storage is necessary for using intermittent renewable energy sources such as solar and wind. Redox flow batteries, particularly organic aqueous redox flow batteries, may be the solution to this problem. There are several factors to be accounted for when trying to decide which molecules to use for the redox flow batteries. The molecules need to have high solubility and extreme half-cell voltages. They also need to be synthesized in "green" and low cost ways. To overcome the problem of synthesizing molecules at low cost without too much environmental impact, we observed that *Streptomyces coelicolor* metabolites produce four quinone molecules (actinorhodin, gamma actinorhodin, DMAC, and aloe) in high yield. Using quantum chemistry calculations, we examined the capabilities of these molecules to serve as electroactive carriers in redox flow batteries. Several combinations of sulfonic acids and primary amines were added to these molecules to increase solubility. Of the 100 molecules tested with cheminformatics for high solubility, 74 molecules were determined to have a solubility of exceeding 1 M. Thermochemical calculations using the B3LYP/6-311+G (d, p) with the SMD solvation model were used to predict the voltages. So far, the lowest predicted voltage is 0.28 V and the highest predicted voltage is 1.04 V. This combination of high solubility, wide voltage range, and bio-based production offers a new strategy for high-performance redox flow battery materials.



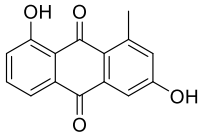
gamma actinorhodin
(major extracellylar product from S. coelicolor M510)



actinbrhodin
(major intracellular product from S. coelicolor M510)



DMAC
(one of two major products from SEK38)



Aloe
(one of two major products from SEK38)