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Fusarium metabolites as electrolytes in Redox flow batteries.

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Fusarium species produces a plethora of secondary metabolites with a variety of functions, and many of these compounds contain quinone structures. Quinones are present in various other biological sources, and are found to act as natural electron transfer agents, e.g. as pigments in *Fusarium*, such as bikavarin and aurofusarin[3]–[5]. Here we present a screening of biological quinones and an investigation of redox potentials and solvation energies conducted using computational chemistry[6], [7].

Quinones have recently become of interest in the search of efficient organic electrolytes used in redox flow batteries. Nearly all published studies utilize synthetically produced quinones, which are often derived from waste products of the oil processing industry [8], [9]. To develop a sustainable technology that matches the green image of renewable energy production and the need of the storage to meet grid demands, we propose using natural quinones, extracted from Fusarium species, for this application.

The screening process was conducted using AntiBase, where 990 different quinones of various biological sources were identified; of these 73 quinones were found in Fusarium species. These compounds were compiled in a database, containing names, ID numbers from AntiBase, source of origin and molar mass. For the screening of the electrochemical potentials, Gaussian 09 was used.

A calibration curve containing 6 sets of experimental standard reduction potentials and calculated energies was obtained with a R^2=0.9827. The method was then used for estimating the reduction potentials in the screening process of the 990 biological quinones. The screening of the *Fusarium* compounds provided a distribution of reduction potentials of the biological quinones varying from -1.00V to 1.13V. This is useful for further development of an all quinone flow battery, as the overall cell potential may exceed 2V, if the extremes were used as anolytes and catholytes. In addition, the study revealed the theoretical solvation energy for each quinone, which indicates the solubility in aqueous solution. This was found by calculating the total energy for the oxidized form of the quinones both in gaseous phase (G_g^o) and solvated (G_s^o), using an implicit solvation model. The ΔG_{sol}^o was calculated by subtracting the two energies, $\Delta G_{sol}^o = G_s^o - G_g^o$. The screening showed distribution of solubilities that differentiated based on side groups and sizes of the molecules, both with molecules that show tendencies of good solubilities and molecules that do not.

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