## **Applying Density Functional Theory to Predict the Reduction Potential in the Indigo Dyeing Process**

Maha Abdelileh, Manel Ben Ticha, Nizar Meksi, Hatem Dhaouadi

The figures below illustrate the Mulliken atomic charge distribution of both monomers and [iron(II) salt-indigo] dimers

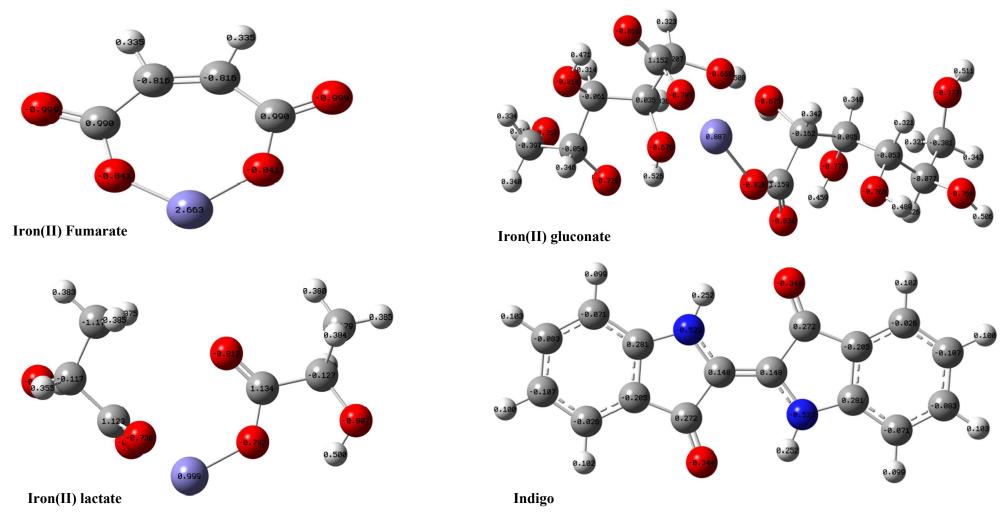
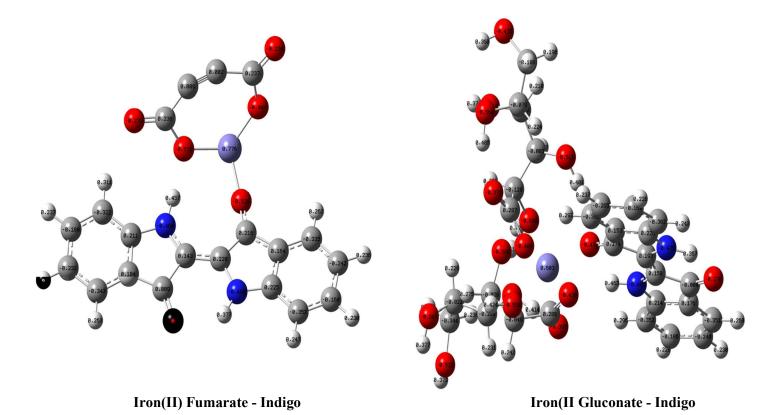


Figure S1. Mulliken atomic charge distribution of iron(II) salts and indigo.



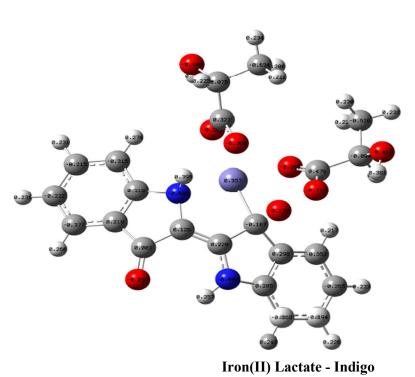


Figure S2. Mulliken atomic charge distribution of [iron(II) salt-indigo] dimers.