Electrochemical and spectroscopic investigation of bioactive naphthoquinones

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The present work aims to investigate the electrochemical behavior of nine naphthoquinones, in aprotic and protic media. The reduction mechanism of the quinones in aprotic medium was proposed, with involvement of anion radical species, confirmed by performing in-situ Electrochemical-Electron Spin Resonance (E-ESR) experiments. Theoretical calculations using DFT method (U)B3LYP/6-31 were developed in order to rationalize the experimental hyperfine coupling constants. The results were in good agreement with the experimental data when solvent effects were included in the DFT models.