

Oncocalyxone A: Electrochemical, spectroscopic investigation and studies of its interaction with DNA, nucleobases and N-acetylcysteine

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The formation of paramagnetic species from oncocalyxone A in aprotic medium was confirmed by performing in situ electrochemical-electron spin resonance (E-ESR) experiments. The high delocalization of the radical generated at the first reduction potential is clearly evidenced by the hyperfine coupling of H-9 with the larger coupling constant, besides the couplings at the H-3 (close to quinone) and H-7 (far from the quinone nucleus) positions. In protic medium, together with pH dependence experiments, oncocalyxone A showed to be DNA-reactive through experiments with DNA sensors. Its reaction with N-acetylcysteine, with structural characterization of the addition products, proved its ability as Michael acceptor. Both aspects are important in terms of biological/pharmacological activities and indicate the present models as important tools in the screening of biologically active compounds. © 2012 Sociedade Brasileira de Química.