

Electrochemical, ESR and theoretical insights into the free radical generation by 1,1'-hydrocarbylenebisindazoles and its evaluation as potential bio-active compounds

Aguilera-Venegas, Benjamín

Olea-Azar, Claudio

Arán, Vicente J.

Maya, Juan Diego

Kemmerling, Ulrike

Speisky, Hernán

Mendizábal, Fernando

A comprehensive multidisciplinary study is conducted here in order to assess the electrochemical behavior of a series of 1,1'-hydrocarbylenebisindazoles derivatives and its potential use as anti-T.cruzi drugs. At first, we have determined the electrochemical reduction mechanisms of this family by cyclic voltammetry (CV) studies, from which three kind of reduction mechanisms -depending on the substituent at positions 3 and 3'- were established, but sharing a first common step corresponding to the generation of a nitro anion radical, which was corroborated by ESR spectroscopy, showing a comparable hyperfine splitting pattern and a strong influence on the ESR spectral linewidths due to the radical-solvent interactions. Furthermore, in order to give a rational description about the electrochemical and ESR results, open- and closed-shell structures of bisindazoles were subjected to theoretical estimations at different levels of theory. For open-shell structures, the hyperfine splitting patt