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Electrochemical Properties of Substituted 2-Methyl-1-4-Naphthoquinones: Redox Behavior Predictions

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Abstract

© 2014 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim. In the context of the investigation of drug-induced oxidative stress in parasitic cells, electrochemical properties of a focused library of polysubstituted menadione derivatives were studied by cyclic voltammetry. These values were used, together with compatible measurements from literature (quinones and related compounds), to build and evaluate a predictive structure-redox potential model (quantitative structure-property relationship, QSPR). Able to provide an online evaluation (through Web interface) of the oxidant character of quinones, the model is aimed to help chemists targeting their synthetic efforts towards analogues of desired redox properties.

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Keywords

Cheminformatics, Cyclic voltammetry, Electrochemistry, Redox chemistry, Structure-property relationships