

Chemistry - A European Journal 2015 vol.21 N8, pages 3415-3424

Electrochemical properties of substituted 2-methyl-1-4-naphthoquinones: Redox behavior predictions

Elhabiri M., Sidorov P., Cesar-Rodo E., Marcou G., Lanfranchi D., Davioud-Charvet E., Horvath D., Varnek A.

Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

© 2015 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

<http://dx.doi.org/10.1002/chem.201403703>

Keywords

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