phases of 2,9-dichloro- and 4,11-difluoro-quinacridone solved from powder patterns with 14-20 peaks only.

References:

[1] Habermehl, S. et al. (2014). Acta Cryst. B70, 347-359.
[2] de Gelder, R. et al. (2001). J. Comput. Chem. 22, 273-289.
[3] Coelho, A. A. (2007). TOPAS-Academic 4.1. Coelho Software, Brisbane, Australia.

Keywords: structure determination from powder data, global optimization, cross-correlation functions

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Associating X-ray structure and antioxidant activity through UV-vis spectroscopy, cyclic voltammetry and DFT methods in Emodin

Miriam Rossi[1], Stuart Belli[1], Kelly Wen[1], Francesco Caruso [1]

1. Department of Chemistry, Vassar College, Poughkeepsie, NY, United States of America

email: rossi@vassar.edu

Regulation of reactive oxygen species such as the superoxide ion is an important chemical process. Emodin (1,3,8-trihydroxy-6-methyl anthraquinone) is present in the root and rhizome of *Rheum palmatum*, and the goji berry (*Lycium barbarum* and *Lycium chinense*). Elucidating the manner in which emodin carries this out may provide insight into the chemical properties described in the literature.

The scavenging of the superoxide radical in this study was analyzed using a combination of several methods. We quantify the ability of emodin in scavenging the superoxide ion $O_2^{\bullet -}$ in an aprotic solvent, dimethyl sulfoxide (DMSO); since water interferes with superoxide, highly dehydrated DMSO was used. We describe the results of our antioxidant assay using the electrochemical method of cyclic voltammetry with a novel rotating ring disk electrode (RRDE) method. This powerful technique provides a quantitative measurement of a redox reaction and allows us to detect products, side-products or even short-lived intermediates of electrode reactions. Since this process was accompanied by a variation of color, the time evolution of this antioxidant process was followed using *in situ UV-Vis* spectroelectrochemistry. At the molecular level, the reactivity of this process was followed using DFT methods which could be applied after determination of the crystal structure using single crystal X-ray diffraction. The combination of these different methods allowed us to demonstrate the unusual manner in which emodin behaves when scavenging superoxide radical. Our results point to the importance of the electron transfer in this scavenging mechanism.

Keywords: antioxidant activity, cyclic voltammetry, emodin