Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supplementary material

The study of Mg(II) and Ca(II) ions influence on caffeic acid autoxidation in weakly alkaline aqueous solution using MCR-ALS analysis of spectrophotometric data

Slavoljub C. Živanović [1], Aleksandar M. Veselinović [2*], Žarko J. Mitić [2], Goran M. Nikolić [2]

[1] Research Center for Biomedicine, Faculty of Medicine, University of Niš, Bulevar dr Zorana Đinđića 81, 18000 Niš, Serbia

[2] Department of Chemistry, Faculty of Medicine, University of Niš, Bulevar dr Zorana Đinđića 81, 18000 Niš, Serbia

Table of contents

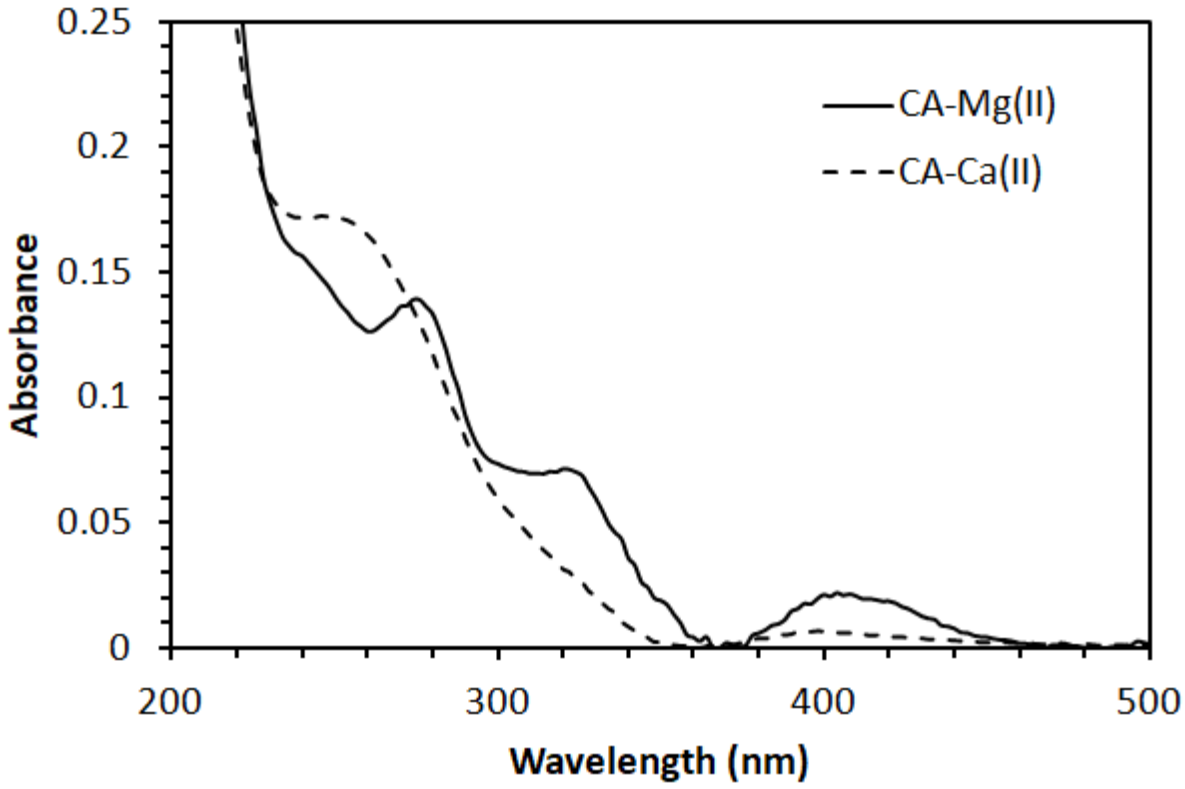

Fig. S1 MCR-ALS resolved UV-Vis spectra of the second component (C2) for the spectrophotometric data obtained during the caffeic acid autoxidation in weakly alkaline aqueous solution in the presence of Mg(II) and Ca(II) ions

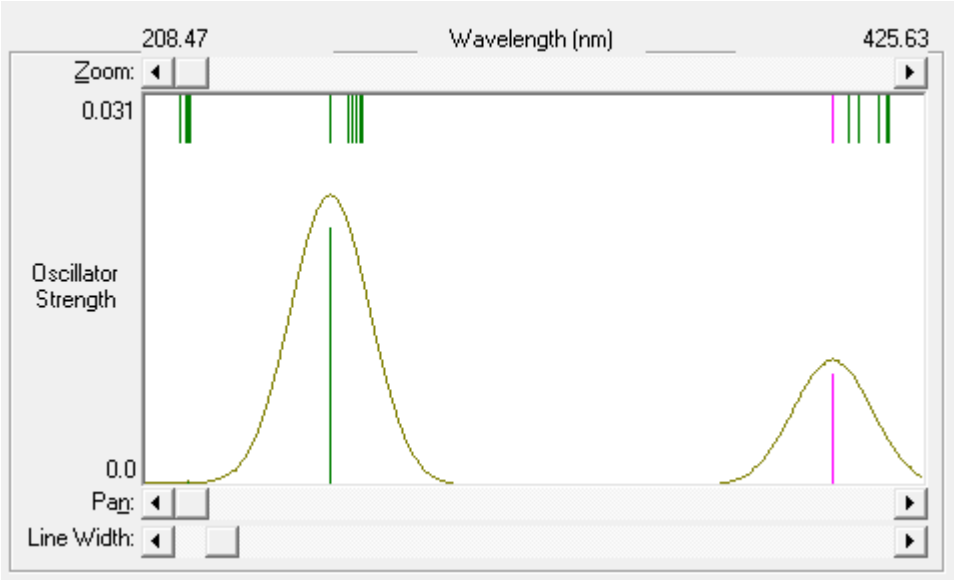

Fig. S2 Electronic absorption spectrum of caffeic acid quinone anion obtained by the semiempirical quantum chemical calculation using HyperChem software (release 8.0; Hypercube Inc., USA) by applying ZINDO/S method with PM3 geometry optimization