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Influence of the geometric isomers on the radical scavenging properties of 3,5-dica®eoylquinic acid: A DFT study in vacuo and in solution

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ABSTRACT:

3,5-Dica®eoylquinic acid (diCQA) is a part of the chlorogenic acid group of compounds, largely isolated from food sources and possessing potent antioxidant activity. Only the trans–trans isomer exists in nature, however, abiotic stresses, such as UV-radiation, give rise to cis isomers. There have been no reports on the antioxidant activity of the cis isomers. The current study, performed using the B3LYP/6-311þG(d,p) method, is aimed at investigating and comparing the antioxidant properties of the geometrical isomers of 3,5-diCQA. The study is conducted by checking the molecules' ability for two main radical scavenging mechanisms, hydrogen atom transfer (HAT) and electron transfer (ET). A separate DPPH assay experimental study performed in this study shows that all the geometrical isomers are potent radical scavengers. The lowest O_H bond dissociation enthalpy value (70.599 kcal/mol) corresponds to the trans–trans isomer and is comparable to that of gallic acid, a commercially available antioxidant. The lowest ionization potential value corresponds to the cis–cis isomer (149.54 kcal/mol), indicating that it is best antioxidant, in terms of ET mechanism.