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Showcasing research from the group of Prof. Gabriel de Souza at Federal University of São Carlos - Lagoa do Sino, Buri-SP, Brazil

A density functional theory benchmark on antioxidant-related properties of polyphenols

This work presents general guidance for researchers working with DFT for investigating antioxidant activity mechanisms of polyphenols. Descriptors of a series of compounds were computed using twenty-three exchange-correlation functionals and four basis sets in the gas-phase, water, and methanol. The final verdict was achieved from calibration against the Domain-based Local Pair Natural Orbital CCSD(T) and statistical analysis. M05-2X, M06-2X, LC-PBE, and LC-ωPBE were declared the most suitable!

The authors acknowledge Tempo 3D Studio for creation of the image.

As featured in:

See Gabriel L. C. de Souza *et al.*, *Phys. Chem. Chem. Phys.*, 2024, **26**, 8616.

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