

Calculations of Dissociation Constants of Carboxylic Acids by Empirical and Quantum-Chemical DFT Methods

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Abstract—Dissociation constants of 15 carboxylic acids in water, methanol, and DMSO were calculated by empirical and quantum-chemical DFT methods. The maximal error of the empirical calculation was 1.4%. A comparative analysis of the results obtained was carried out.

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