*p*K$_a$s in Dicarboxylic Acids by Constant-*p*H Molecular Dynamics Simulations

M. Długosz and J. M. Antosiewicz

Department of Biophysics, Warsaw University,
Warsaw 02-089, Poland

Reprint requests to Dr. J. M. A.;
e-mail: jantosi@biogeo.uw.edu.pl

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A method for performing constant-*p*H molecular dynamics, where *p*H is one of the external parameters of the solution, is applied for computation of protonation equilibria in a series of small dicarboxylic acids. Proton dissociation constants for succinic, glutaric, adipic and cork acids were determined. Very good agreement with experimental measurements is achieved.

Key words: *p*K$_a$; Constant-*p*H Molecular Dynamics; Dicarboxylic Acid.