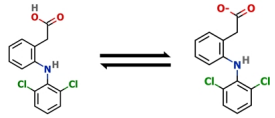
Layla Hosseini-Gerami[1,2], Rasmus Leth[1], Peter Hunt[1], Matthew Segall[1].

1 Optibrium Limited, Cambridge, UK
2 University of Leeds, Leeds, UK

This presentation was given at the ACS Spring 2017 National Meeting & Exposition held in San Diego, USA.

Abstract

The equilibrium between charged and neutral species has an important impact on a wide variety of properties relevant to pharmaceutical and agrochemical compound design and development. The accurate prediction of the pKa of any centre in a molecule would be of value in all stages of research from synthetic planning to biological activity and on to formulation and delivery. We will present our efforts to model the pKa of any hydrogen in a compound, based on ab initio density functional theory, semi empirical Hamiltonians and empirical quantitative structure activity relationships. We will compare these approaches and illustrate how they can be combined to balance speed, accuracy and transferability.



You can download this presentation as a PDF .