Quantitative Structure-Activity Relationship of Morita-Baylis-Hillman Adducts with Leishmanicidal Activity

Rodrigo Octavio M. A. de Souza*, José C. Barros, Joaquim F. M. da Silva, and Octavio A. C. Antunes

Instituto de Química, Universidade Federal do Rio de Janeiro, Av. Athos da Silveira Ramos 146, 21944–910, Rio de Janeiro, Brazil. Fax: +55-21-2562-7556. E-mail: rodrigosouza@iq.ufrj.br

* Author for correspondence and reprint requests

Z. Naturforsch. **66 c**, 136–142 (2011); received June 18/November 23, 2010

Dedicated to the memory of Professor Octavio Antunes and his family

A quantitative structure-activity relationship model for Morita-Baylis-Hillman adducts with leishmanicidal activities was developed which correlates molecular orbital energy and dipole with percentage in the promastigote stage.

Key words: Leishmaniasis, Morita-Baylis-Hillman, QSAR