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ORIGINAL ARTICLE

# QSAR study of the toxicity of nitrobenzenes to *Tetrahymena pyriformis* using quantum chemical descriptors

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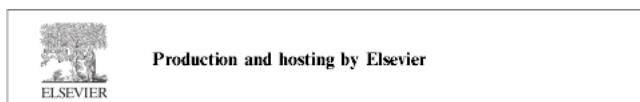
**Abstract** Quantitative Structure–Activity Relationship (QSAR) models are useful in understanding how chemical structure relates to the biological activity and the toxicity of natural and synthetic chemicals. The present study shows that Parr’s electrophilicity index  $\omega$  in combination of two other descriptors, namely, the LUMO energy and the hydrophobicity index  $\log P$ , prove their utility for the prediction of the toxicity of a series constituted by 50 nitrobenzene derivatives. The QSAR models are developed using the Multiple Linear Regression (MLR) method. It turns out that the best model, which its stability is confirmed using the leave-1/3-of-set-out validation, is able to describe about 87% of the variance of the experimental toxicity. The satisfactory obtained results show that Parr’s electrophilicity index is a useful quantum chemical descriptor for the toxicity modeling of nitrobenzene derivatives. Finally, the elaborated model shows that the most toxic nitrobenzenes are characterized by large hydrophobicities and high electrophilicity powers and could be efficiently applied for the estimation of the toxicity of nitrobenzenes for which the experimental measures are unavailable.

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## 1. Introduction

The rapid development of new compounds by the chemical industry in general and in particular by the agrochemical, petrochemical and pharmaceutical industries is accompanied by an increasing toxic burden in the environment. Because of this, the development of tools able to assess hazardous effects on living species should receive high attention (Smiesko and Benfenati, 2004).

Quantitative Structure–Property/Activity Relationship (QSPR/QSAR) methods are among the most practical tools in computational physical chemistry. These methods are based on the axiom that the variance in the physicochemical