QSTR analysis and combining DFT of the toxicity of heterogeneous phenols

A. Ousaa[1*], B. Elidrissi[1], M. Ghamali[1], S. Chtita[1], A. Aouidate, M. Bouachrine[2], T. Lakhlifi[1]

[1]*Molecular Chemistry and Natural Substances Laboratory, Faculty of Science, University Moulay Ismail, Meknes, Morocco*
[2]*MEM, ESTM, University Moulay Ismail, Meknes, Morocco*
*Corresponding Author: E-mail: *abdellahousaa@gmail.com* ; Tel. +21271310939

Abstract

Quantitative structure–toxicity relationship (QSTR) models are useful to understand how chemical structure relates to the toxicity of natural and synthetic chemicals. The chemical structures of 70 heterogeneous phenols have been characterized by electronic and physic-chemical descriptors. Density functional theory (DFT) with Beck's three parameter hybrid functional using the LYP correlation functional (B3LYP/6-31G(d)) calculations have been carried out in order to get insights into the structure chemical and property information for the study compounds. The present study was performed using principal component analysis (PCA) method, multiple linear regression method (MLR), multiple non-linear regression (MNLR) and artificial neural network (ANN). The quantitative model of the toxicity of these compounds was accordingly proposed and interpreted based on the multivariate statistical analysis.

The statistical quality of the MLR and MNLR models was found to be efficient for the predicting of the toxicity, but when compared to the obtained results by ANN model, we realized that the predictions achieved by this latter one were more effective. This model provided statistically significant results and showed good internal stability and powerful predictability. The squared correlation coefficients were 0.801, 0.802 and 0.824 for MLR, MNLR and ANN models respectively. The obtained results suggested that the proposed descriptors could be useful to predict the toxicity of heterogeneous phenols to *Tetrahymena pyriformis.*

Keywords: QSTR model, DFT study, heterogeneous phenols, *Tetrahymena pyriformis.*

Informations	
Nom :	Ousaa
Prénom :	Abdellah
Fonction :	Doctorant
Université / Entreprise :	FS-Meknes
Laboratoire / Département :	MCNS Laboratory, Faculty of Science, University Moulay Ismail, Meknes, Morocco
Adresse postale :	Ait aissa taghzout tinghir
Ville :	Meknes
Pays **:**	Maroc
Téléphone :	0671310939
Fax :	
E-mail :	Abdellahousaa@gmail.com

Participation

- ■ Présentation de communication orale
- ■ Présentation de communication par affiche