

Predicting Degradation Half-life of Organophosphorus Pesticides in Soil Using Three-Dimensional Molecular Interaction Fields

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ABSTRACT

A simple and strong model, based on an alignment independent three-dimensional quantitative-structure activity relationships (3D-QSAR), is developed for prediction of degradation half-life (DT_{50}) of 47 organophosphorus pesticides in soil. Molecular descriptors derived from 3D molecular interaction fields (MIF) were calculated using the GRIND methodology. Fractional factorial design (FFD) applied to feature selection and modeling of the relationship between selected descriptors and DT_{50} data was achieved using partial least squares regression. Validation and reliability of the obtained model were checked by the prediction of external test set cross-validation and chance correlation. The value of the determination coefficient (R^2) was 0.817 for leave-one-out cross-validation procedure. The R^2 values for the training and test sets were 0.951 and 0.893 respectively. The obtained model confirmed that size and shape of the molecules as well as hydrophobic interactions are the main parameters influencing the degradation half-life of organophosphorus pesticides in soil.

KEYWORDS

3D-QSAR, Degradation Half-Life, Molecular Interaction Fields (MIF), Organophosphorus Pesticides

1. INTRODUCTION

Organophosphorus pesticides (OPPs) are among the most commonly employed pesticides worldwide because of their high activity, ease of use and rapid degradation under natural conditions (Zvinavashe et al., 2009). They have been widely applied as insecticides, herbicides, acaricides, fungicides, and plant growth regulators for controlling disease and growth (Cai, Liang, & Wen, 1995; Yan et al., 2008). Organophosphorus pesticides are generally degraded by the reactions including oxidation, reduction, hydrolysis, hydroxylation, dehydrochlorination, dealkylation, methylation, isomerization, and conjugate formation (Tomizawa, 1974). Their ability to degrade made them an attractive alternative to the persistent organochlorines pesticides, such as DDT, aldrin and dieldrin. Although the degradation process of pesticides in soils is complicated, the main factors may be soil constituents, soil microflora, and chemical structures of pesticides. Chemical structures are especially important for soil metabolism of organophosphorus pesticides, because the priority of the reactions mentioned above is decided by the structure (Tomizawa, 1974). The soil degradation half-life (DT_{50}) is a measure of the persistence of a pesticide in soil. Pesticides can be categorized on the basis of their half-life as non-persistent,

DOI: 10.4018/IJQSPR.2017070103

degrading to half the original concentration in less than 30 days; moderately persistent, degrading to half the original concentration in 30 to 100 days; or persistent, taking longer than 100 days to degrade to half the original concentration (Gavrilescu, 2005; Jenkins & Thomson, 1999).

The lack of experimental data for the majority of the organic compounds in commercial use has increased the importance of quantitative structure-activity relationships (QSAR) to evaluate and predict the activities of compounds not yet tested (Ghasemi & Zolfonoun, 2012; Livingstone, 2000). A QSAR model is a mathematical equation that correlates the physicochemical properties or biological activities of compounds under investigation to molecular structure represented by the chemical composition, connectivity of atoms, potential energy surface etc. (Chen, Li, Xie, Gao, & Zou, 2009; J. Ghasemi & Saaidpour, 2007). 3D-QSAR, which refers to use of force field calculations to compute spatial properties of three-dimensional structure (3D) of compounds, provides useful information of the forces and interactions between molecules (Langer & Bryant, 2008; Yuyin, Chunsheng, Hongyan, Zhongsheng, & Yang, 2008).

The GRid-INdependent Descriptors (GRIND) (Pastor, Cruciani, McLay, Pickett, & Clementi, 2000) derived from the 3D molecular interaction field (MIF) of a molecule are examples of 3D-based molecular descriptors. The principal advantage of these descriptors is that they do not require structural superimposition for a 3D-QSAR analysis, as is usually required when working with grid-field variables, and their numerical values are related to conformations submitted to computation (Ermondi & Caron, 2008). Recently, applications of 3D-QSAR models derived from GRIND descriptors in environmental science were reported (J. B. Ghasemi, Salahinejad, & Rofouei, 2011; J. B. Ghasemi, Salahinejad, Rofouei, & Mousazadeh, 2012; Rofouei, Salahinejad, & Ghasemi, 2014; Salahinejad & Ghasemi, 2014; Zhuang, Xiao, Li, Zhang, & Ruan, 2006).

In this work, a 3D-QSAR study is performed, to develop a model that relates the structures of 47 organophosphorus pesticides to their soil degradation half-life (DT₅₀) with the applicability of GRID independent descriptors.

2. MATERIAL AND METHOD

2.1. Dataset

The experimental values for the degradation half-life (DT₅₀) of 47 organophosphorus pesticides taken from the literature (Jenkins & Thomson, 1999) are presented in Table 1. The dataset was split into a training set (37 pesticides) and a test set (10 pesticides) by the Kennard-Stone algorithm (Daszykowski, Walczak, & Massart, 2002). The training set was used to adjust the parameters of the model, and the test set was used to evaluate their prediction ability.

2.2. Molecular Optimization and Descriptor Calculation

The structure of molecules was drawn in ChemDrawUltra version 11.01 (ChemOffice 2008, Cambridge Soft Corporation) software. The optimizations of molecular structures were done by the HyperChem version 8.05 using molecular mechanics and semi empirical AM1 tools with a convergence criterion of 0.01 kcal/molÅ. All calculations were run on a Dell Vostro 1310 Laptop computer with Intel (R) Core™ 2 Duo CPU with windows XP as operating system.

GRid-INdependent Descriptors (GRIND) was calculated automatically using the software Pentacle, version 1.05 (Molecular Discovery Ltd., Oxford, UK). The Pentacle software uses alignment independent descriptors derived from molecular interaction fields (MIF) (Pastor et al., 2000). In this study, DRY, N1 (amide), O (carbonyl) and TIP probes were used to generate MIFs which represent hydrophobic interactions, hydrogen bond donor, hydrogen bond acceptor, and shape-field respectively. All molecular interaction fields were computed with the grid resolution of 0.5 Å with the smoothing window 0.8 Å. ALMOND algorithm was used for the extraction of nodes from the obtained MIF, the distance and relative position of nodes were described by MACC2. After calculation of GRIND

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