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Prediction of Biodegradation Rate Constants of Hydroxylated Polychlorinated Biphenyls by Fungal Laccases from *Trametes versicolor* and *Pleurotus ostreatus*

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Abstract Quantitative structure-activity relationship (QSAR) models for fungal laccase-catalyzed degradation of different hydroxylated polychlorinated biphenyls (OH-PCBs) were developed using some fundamental quantum chemical descriptors. The cross-validated $Q^2{}_{\mathrm{cum}}$ values for the two optimal QSAR models are as high as 0.958 and 0.961 for laccases from *Trametes versicolor* and *Pleurotus ostreatus*, respectively, indicating good predictive abilities for laccase-catalyzed degradation of OH-PCBs. Results from this study show that increasing heat of formation (ΔH_f) and frontier molecular orbital energy (i.e. $E_{\mathrm{LUMO}} + E_{\mathrm{HOMO}}$) values or decreasing frontier molecular orbital energy (i.e. $E_{\mathrm{HOMO-1}}$) and core-core repulsion energy (*CCR*) values leads to the increase of OH-PCB degradation rates by laccases.

Keywords Hydroxylated PCBs · QSARs · Laccases · Biodegradation

Hydroxylated polychlorinated biphenyls (OH-PCBs) are toxic metabolites of PCBs, which have been identified in human beings and the wildlife (Hovander et al. 2006). Due to their similarity in chemical structures to the natural estrogens and thyroid hormones, OH-PCBs have the potential to disrupt endocrine and metallothionein processes (Kitamura et al. 2005; Kimura-Kuroda et al. 2007). The wide occurrence of these toxic chemicals poses considerable threat to ecosystem and human health. Therefore, the development of methods for removing and transforming OH-PCBs has recently received increasing attention (Schultz et al. 2001; Keum and Li 2004). As effective detoxifying agents for organic pollutants, ozone and chloramine-T have been used to destroy toxic organic pollutants. For example, Cassidy et al. (2002) utilized ozone to oxidize PCBs and found that ozone sparging in the kaolinite slurries removed >90% of PCBs in 30 days. On the other hand, Laccases (benzenediol:oxygen oxidoreductases; E.C. 1.10.3.2) are widely distributed in higher plants and fungi. They are capable of removing a wide variety of organic pollutants due to their low specificity (Durán et al. 2002; Zille et al. 2005; Shumakovich et al. 2006). Consequently, laccase-catalyzed degradation of organic contaminants has received particular attention and been carried out by many researchers (Dodor et al. 2004; Pozdnyakova et al. 2006; Pedroza et al. 2007). Previous researches found that laccase-catalyzed oxidation appeared to be a feasible method to remove chlorinated phenols from the wastewater (Bollag et al. 1988, 2003). Dodor et al. (2004) utilized immobilized *Trametes versicolor* laccase to oxidize polycyclic aromatic hydrocarbons (PAHs) and found more than 80% of PAHs were oxidized after 24 h incubation. Pozdnyakova et al. (2006) found the laccase from white-rot fungus *Pleurotus ostreatus* D1 was an effective degrader for PAHs in the presence of 2,2′-azino-bis(3-ethylbenzothiazoline-6-sulfonic acid) (ABTS) or 1-hydroxybenzotriazole (HBT).

So far, limited research has been carried out on biodegradation of OH-PCBs (Schultz et al. 2001; Keum and Li

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2004). Keum and Li (2004) studied the degradation of OH-PCBs catalyzed by fungal laccases from *T. versicolor* and *P. ostreatus*. Their findings showed that the reactions followed pseudo-first order kinetics and lower chlorinated OH-PCBs could be rapidly decomposed. On the other hand, higher chlorinated OH-PCBs, such as tetra-, pentra- and hexa-chloro hydroxybiphenyls, could not be degraded by the two laccases. To some extent, sufficient data on the laccase-catalyzed degradation of OH-PCBs are necessary for choosing proper methods to remove their toxicity and getting insight into which aspect of the molecular structure influences the property (Niu et al. 2007). However, due to its costly and time-consuming characteristics of OH-PCBs bio-degradation process, along with the limitation in efficient detection method and lack of standard materials (Keum and Li 2004), most data on degradation rates of OH-PCBs by fungal laccases are unavailable in experimental conditions. Interestingly, quantitative structure-activity relationships (QSARs), which correlate and predict degradation rates of OH-PCBs from their molecular structural descriptors, may be able to give certain insight into the degradation mechanisms and degradation rates efficiently. Since quantum chemical descriptors can be easily obtained by computation and the defined molecular properties can be clearly described without restriction to related compounds, the development of QSAR models with quantum chemical descriptors are very useful and convenient. In the previous research, the QSAR models for the toxicity of OH-PCBs were developed (Niu et al. 2007). So far, little studies were reported about QSARs for prediction of the laccase-catalyzed degradation of OH-PCBs. Is it possible to develop QSAR models for fungal laccase-catalyzed degradation of different OH-PCBs by some fundamental quantum chemical descriptors? This current study is to answer this question. Moreover, reliable QSAR models may be used to investigate reaction mechanisms and generate predicted biodegradation rate constants efficiently. Partial least squares (PLS) algorithm, which can analyze data with strongly collinear, as well as noisy and numerous X variables (Wold et al. 2001) were used in this study.

Materials and Methods

Recently, biodegradation of OH-PCBs by laccases was investigated by Keum and Li (2004). The reaction rate constants catalyzed by fungal laccases (k_L, h^{-1}) from *T. versicolor* and *P. ostreatus* are expressed as $k_{L(T)}$ (h^{-1}) and $k_{L(P)}$ (h^{-1}), respectively. These data obtained from the literature (Keum and Li 2004) are reproduced in Table 1. The results show that almost an order of magnitude difference exists between the k_L values for 3-hydroxy-2′,5′-PCB ($k_{L(T)} = 0.053 \pm 0.002\ h^{-1}$ and $k_{L(P)} = 0.040 \pm 0.003\ h^{-1}$ for laccases from *P. ostreatus* and *T. versicolor*, respectively) and that for 4-hydroxybiphenyl ($k_{L(T)} = 0.401 \pm 0.032\ h^{-1}$ and $k_{L(P)} = 0.348 \pm 0.011\ h^{-1}$ for laccases from *P. ostreatus* and *T. versicolor*, respectively). In this study, these reaction rate constants were transformed in logarithm form and used as the training sets. Parameterized Model revision 3 (PM3) Hamiltonian method is the semi-empirical method based on the correct inclusion of one-center overlap. Results from our previous study indicated that the model using computed molecular descriptors by PM3 Hamiltonian method had a slightly better predictive capability than the models developed using AM1 or MNDO methods (Niu et al. 2007). Thus, in present study, PM3 Hamiltonian in MOPAC (2000) contained in the CS Chem3D Ultra was used to compute quantum chemical descriptors of OH-PCBs. The optimization of molecular structures was described in detail elsewhere (Chen et al. 2000).

A total of 18 MOPAC derived descriptors reflecting the overall character of the OH-PCB molecules were used in this study. The definitions of these molecular structure descriptors and the values of selected descriptors for OH-PCBs are listed in Tables 2 and 3, respectively. In addition, three combinations of frontier molecular orbital energies, e.g. $E_{LUMO} - E_{HOMO}$, $(E_{LUMO} - E_{HOMO})^2$ and $E_{LUMO} + E_{HOMO}$, were also selected as predictor variables. The $E_{LUMO} - E_{HOMO}$ and $E_{LUMO} + E_{HOMO}$ can be related to absolute hardness and electronegativity, respectively (Pearson 1986; Faucon et al. 1999). $E_{LUMO} - E_{HOMO}$, $E_{LUMO} + E_{HOMO}$ and $(E_{LUMO} - E_{HOMO})^2$ were proven to be significant in previous QSAR (Veith et al. 1995; Niu et al. 2007) and quantitative structure-property relationship (QSPR) studies (Chen et al. 2000).

QSAR models were developed using PLS regression, as implemented in the Simca (Simca-S Version 6.0, *Umetri AB and Erisoft AB*) software. The conditions for the computation were based on the default values of the software. The criterion used to determine the model dimensionality—the number of significant PLS components—is cross validation (CV). With CV, when the fraction of the total variation of the dependent variables that can be predicted by a component, Q^2, for the whole data set is larger than a significance limit, the tested PLS component is considered significant. Model adequacy was mainly characterized by the number of observations used for model building in the training set, the number of PLS principal components (A), Q^2_{cum}, the correlation coefficient between observed and fitted values (R), the general standard error (SE) and the significance level (p).

Results and Discussion

In a PLS model, variable importance in the projection (*VIP*) is a parameter that shows the importance of a variable in PLS analysis. Terms with a large value of *VIP* are the most relevant for explaining dependent variable. PLS

Table 1 The studied OH-PCBs and their biodegradation rate constants by laccases from *T. versicolor* ($k_{L(T)}$, h^{-1}) and *P. ostreatus* ($k_{L(P)}$, h^{-1})

No.	Compounds	*T. versicolor* model				
		Observed[a]		Predicted		Residues[b]
		$k_{L(T)}$	$\log k_{L(T)}$	$\log k_{L(T)}$	$k_{L(T)}$	
1	2-hydroxybiphenyl	0.386 ± 0.022	−0.413	−0.415	0.385	0.002
2	3-hydroxybiphenyl	0.228 ± 0.031	−0.642	−0.681	0.208	0.039
3	4-hydroxybiphenyl	0.401 ± 0.032	−0.397	−0.349	0.448	−0.048
4	4-hydroxy-3-PCB	0.202 ± 0.015	−0.695	−0.693	0.203	−0.002
5	2-hydroxy-2′,5′-PCB	0.092 ± 0.002	−1.036	−1.020	0.095	−0.016
6	3-hydroxy-2′,5′-PCB	0.053 ± 0.002	−1.276	−1.166	0.068	−0.109
7	4-hydroxy-2′,5′-PCB	0.115 ± 0.021	−0.939	−1.021	0.095	0.081
8	4-hydroxy-3,5-PCB	0.105 ± 0.032	−0.979	−1.052	0.089	0.073
9	4-hydroxy-2′,3,5′-PCB	0.052 ± 0.002	1.284	−1.264	0.054	−0.020
10	4′-hydroxy-2,3′,5,5′-PCB	n.d.[c]		−1.604	0.025	
11	4-hydroxy-2′,3,4′,5,6′-PCB	n.d.[c]		−1.774	0.017	
12	4-hydroxy-2′,3,3′,4′,5,5′-PCB	n.d.[c]		−2.103	0.008	

No.	Compounds	*P. ostreatus* model				
		Observed[a]		Predicted		Residues[b]
		$k_{L(P)}$	$\log k_{L(P)}$	$\log k_{L(P)}$	$k_{L(P)}$	
1	2-hydroxybiphenyl	0.248 ± 0.003	−0.606	−0.543	0.286	−0.063
2	3-hydroxybiphenyl	0.135 ± 0.022	−0.870	−0.931	0.117	0.061
3	4-hydroxybiphenyl	0.348 ± 0.011	−0.458	−0.455	0.351	−0.003
4	4-hydroxy-3-PCB	0.164 ± 0.022	−0.785	−0.796	0.160	0.010
5	2-hydroxy-2′,5′-PCB	0.081 ± 0.031	−1.092	−1.096	0.080	0.005
6	3-hydroxy-2′,5′-PCB	0.040 ± 0.003	−1.398	−1.317	0.048	−0.081
7	4-hydroxy-2′,5′-PCB	0.094 ± 0.011	−1.027	−1.128	0.074	0.101
8	4-hydroxy-3,5-PCB	0.072 ± 0.011	−1.143	−1.156	0.070	0.013
9	4-hydroxy-2′,3,5′-PCB	0.044 ± 0.003	−1.357	−1.312	0.049	−0.044
10	4′-hydroxy-2,3′,5,5′-PCB	n.d.[c]		−1.607	0.025	
11	4-hydroxy-2′,3,4′,5,6′-PCB	n.d.[c]		−1.630	0.023	
12	4-hydroxy-2′,3,3′,4′,5,5′-PCB	n.d.[c]		−1.961	0.011	

[a] Data from Keum and Li (2004)

[b] *Residues* = $\log k_L$(Observed) − $\log k_L$(Predicted)

[c] n.d.: Not detectable

analysis with the degradation rates ($\log k_L$) as dependent variable and the 18 quantum chemical descriptors as independent variables generated many results. Previous studies found that all the predictor's variables were not necessary for a PLS model (Niu et al. 2006). The optimal model, which has the largest Q^2_{cum}, was obtained through stepwise culling the model with the smallest *VIP* value out. Then the optimal PLS model was selected based on statistical values of Q^2_{cum}, *R*, and *p*.

The above described PLS analysis procedure, for the nine OH-PCBs contained in the training set, led to QSPR *T. versicolor* Model for the degradation of OH-PCBs catalyzed by laccase from *T. versicolor*. Similarly, *P. ostreatus* Model was also developed for the degradation of OH-PCBs catalyzed by laccase from *P. ostreatus*. Based on the unscaled pseudo-regression coefficients of the independent variables and constants transformed from PLS results, analytical QSPR equations were obtained and expressed in Eqs. 1 and 2:

T. versicolor Model:

$$\begin{aligned}\log k_{L(T)} = {} & -5.767 \times 10^{-1} + 4.210 \times 10^{-3} \Delta H_f \\ & - 7.319 \times 10^{-5} CCR - 4.355 \times 10^{-1} E_{HOMO-1} \\ & + 3.864 \times 10^{-1} (E_{LUMO} + E_{HOMO})\end{aligned} \tag{1}$$

$A = 1$, $R^2_{X(adj.)(cum)} = 0.725$, $R^2_{Y(adj.)(cum)} = 0.968$, $Eig = 2.899$, $Q^2_{cum} = 0.958$, $R = 0.984$, $p = 1.713 \times 10^{-6}$, $SE = 0.064$

Table 2 List of molecular structural descriptors of OH-PCBs

Symbols	Description
*M*w	Molecular weight
ΔH_f (kCal)	Standard heat of formation
TE (eV)	Total energy
EE (eV)	Electronic energy
CCR (eV)	Core-core repulsion energy
E_{HOMO} (eV)	Energy of the highest occupied molecular orbital (Electronegativity)
$E_{\mathrm{HOMO\text{-}1}}$ (eV)	Energy of the second highest occupied molecular orbital
E_{LUMO} (eV)	Energy of the lowest unoccupied molecular orbital (Electronaffinity)
$E_{\mathrm{LUMO+1}}$ (eV)	Energy of the second lowest unoccupied molecular orbital
q_{H}^{+} (a.c.u)	The most positive net atomic charges on hydrogen atoms
M (Debye)	Total dipole moment
α (a.u)	Average molecular polarizability
n_{Cl}	The number of chlorine atoms
q_{C}^{-} (a.c.u)	The largest negative atomic charge on a carbon atom
q_{Cl}^{+}(a.c.u)	The largest positive atomic charge on a chlorine atom

Table 3 Selected quantum chemical descriptors used in this study

No.	Compounds	ΔH_f	CCR	$E_{\mathrm{HOMO\text{-}1}}$	$E_{\mathrm{LUMO}} + E_{\mathrm{HOMO}}$
1	2-hydroxybiphenyl	28.725	8577.351	−9.517	−8.998
2	3-hydroxybiphenyl	10.096	8383.796	−9.339	−9.319
3	4-hydroxybiphenyl	9.481	8336.814	−9.796	−8.977
4	2-hydroxy-4′-PCB	−0.302	9711.738	−9.540	−9.160
5	3-hydroxy-4′-PCB	−18.206	9499.206	−9.376	−9.476
6	4-hydroxy-3-PCB	−17.244	9605.506	−9.706	−9.235
7	4-hydroxy-4′-PCB	−18.967	9446.522	−9.848	−9.178
8	2-hydroxy-2′,5′-PCB	−27.221	11248.500	−9.265	−9.165
9	3-hydroxy-2′,5′-PCB	−34.998	11029.830	−9.288	−9.526
10	4-hydroxy-2′,5′-PCB	−10.419	10946.270	−9.462	−9.629
11	4-hydroxy-3,5-PCB	−38.218	10965.500	−9.484	−9.428
12	4-hydroxy-2′,3,3′-PCB	−53.961	12439.240	−9.333	−9.433

P. ostreatus Model:

$$\begin{aligned}\log k_{\mathrm{L(P)}} = {} & -2.014 + 5.396 \times 10^{-3} \Delta H_f \\ & - 6.456 \times 10^{-1} E_{\mathrm{HOMO-1}} \\ & + 5.365 \times 10^{-1} (E_{\mathrm{LUMO}} + E_{\mathrm{HOMO}})\end{aligned} \tag{2}$$

$A = 1$, $R^2_{\mathrm{X(adj.)\ (cum)}} = 0.687$, $R^2_{\mathrm{Y(adj.)(cum)}} = 0.968$, $Eig = 2.062$, $Q^2_{\mathrm{cum}} = 0.961$, $R = 0.984$, $p = 1.808 \times 10^{-6}$, $SE = 0.062$

where $R^2_{\mathrm{X(adj)(cum)}}$ and $R^2_{\mathrm{Y(adj)(cum)}}$ stand for cumulative variance of all the *X*'s and *Y*'s, respectively, explained by all extracted components. *Eig* stands for the eigenvalue which denotes the importance of the PLS principal components. One PLS principal component was selected in *T. versicolor* Model and *P. ostreatus* Model, respectively. For example, for *T. versicolor* Model, one PLS principal component explained 72.5% of the variance of the predictor variables, and 96.8% of the variance of the dependent variable.

T. versicolor Model and *P. ostreatus* Model include four and three predictor variables, respectively. As shown in Table 1, the predicated $\log k_{\mathrm{L(T)}}$ and $\log k_{\mathrm{L(P)}}$ values for the degradation of OH-PCBs are close to their corresponding experimental values. All the correlations between experimentally observed and model predicted values are statistically significant. The cross-validated Q^2_{cum} values of the two models are higher 0.95, suggesting that the two models are stable and having good predictive abilities.

For the nine OH-PCBs involved in the training set, the correlations between observed and predicted $\log k_{\mathrm{L(T)}}$ values of both *T. versicolor* Model ($R = 0.984$, $p < 0.0001$) and Model ($R = 0.984$, $p < 0.0001$) are statistically significant. Based on *T. versicolor* Model and *P. ostreatus* Model, $\log k_{\mathrm{L(T)}}$ and $\log k_{\mathrm{L(P)}}$ for the other OH-PCBs were predicted, respectively (see Table 1). It can be seen from Table 1 that the predicted biodegradation rate constants for 4′-hydroxy-2,3′,5,5′-PCB, 4-hydroxy-2′,3,4′,5,6′-PCB and 4-hydroxy-2′,3,3′,4′,5,5′-PCB are very low and lower than all the OH-PCBs in the training set, which is in agreement with the conclusions from Keum and Li (2004), who found that the reaction rate constants of the three OH-PCBs are not detectable. Thus, the predictions in this study may give an initial estimation of biodegradation of OH-PCBs by laccases from *T. versicolor* and *P. ostreatus*.

As shown by Eqs. 1 and 2, the same quantum chemical descriptors, i.e. ΔH_f, E_{HOMO-1} and $(E_{LUMO} + E_{HOMO})$, were selected in both *T. versicolor* Model and *P. ostreatus* Model. Additionally, the descriptor *CCR* in *T. versicolor* Model was also found to be one main factor affecting the degradation rates by laccase from *T. versicolo*. For *T. versicolor* Model, The *VIP* values of *CCR* and ΔH_f are higher than 1.0, which shows a relative importance compared to other two descriptors, i.e. E_{HOMO-1} and $(E_{LUMO} + E_{HOMO})$. While for *P. ostreatus* Model, the *VIP* values of ΔH_f and $(E_{LUMO} + E_{HOMO})$ are higher than 1.0, which shows a relative importance compared to the descriptor E_{HOMO-1}. The effects of each independent variable on the $\log k_L$ values of OH-PCBs can be evaluated from the positive and negative symbols of the coefficients of the independent variables. As indicated by the Eq. 1, increasing ΔH_f and $E_{LUMO} + E_{HOMO}$ values of OH-PCBs could lead to the increase of $\log k_{L(T)}$ values. Contrarily, increasing CCR and $E_{HOMO\text{-}1}$ could lead to the decrease of $\log k_{L(T)}$ values.

The results obtained from the two models show that, under the same reaction condition, molecular structural characteristics of OH-PCBs did affect on laccase-catalyzed degradation of these molecules significantly. Among the descriptors selected in *T. versicolor* Model and *P. ostreatus* Model, the descriptor $E_{HOMO\text{-}1}$ correlates significantly with E_{HOMO} negatively ($R = 0.848$, $p < 0.01$). The descriptor E_{HOMO} accounts for the electron donor ability of the OH-PCBs in the process of degradation. The result of this study demonstrates that the higher E_{HOMO} values will lead to higher reaction rate constants of OH-PCBs, which agrees with several previous studies showing that increasing E_{HOMO} values results in higher reactivity (Soffers et al. 2001). Statistically significant positive correlation is found between *CCR* and *M*w ($R = 0.997$, $p < 0.01$). Thus, this indicates that increasing M_w values can lead to the decrease of the $\log k_L$ values of OH-PCBs. The conclusion was consistent with the findings from Keum and Li (2004) who found that higher chlorinated hydroxy PCBs were more resistant to laccase degradation than lower chlorinated analogues because high chlorinated OH-PCBs have high hydrophobicity and ionization potentials. Absolute electronegativity can be defined as $-(E_{LUMO} + E_{HOMO})/2$ (Pearson 1986). The result from *P. ostreatus* Model shows that PCB derivatives with higher absolute electronegativity values tend to have lower $\log k_L$ values, i.e. the reaction rate constants of such PCB derivatives are lower.

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