**RESPONSE TO REVIEWERS**

**QSAR Study of octanol/water partition coefficient of organophosphorous compounds: Hybrid (GA/ MLR) Approach and Hybrid (GA/ ANN) Approach.**

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**1-Supplement table should be relocated to main text.**ok

**2-Introduction is missing review on QSAR used for Kow prediction. This is needed in order to evaluate the novelty of current paper.**

We are highly appreciating this comment, which give us the chance to improve the quality of the manuscript. we have cited in introduction (page3)

**3-Line 89: ..."PM3 method using14**

14 is reference, we are complete the phrase in the main text

**4-Line 123: Can be confusing, since it is unclear is it 5^19 or 19 is reference. Please rephase.**19 is reference

**5-Table I is unclear. Pred. stands for? R&D**Std.Err.Pred: standardized error prediction

Err.Pred: error prediction

**6-Line 203: Descriptors must be described after Eq is presented.**

In Eq. (6), four different kinds of molecular descriptors appear describe in the following table:

|  |  |  |
| --- | --- | --- |
| Descriptors | Class | Meaning |
| Polarizability | Hyperchem descriptor | polarizability defined as the dipole moment of a molecule induced by an electric field of unit intensity |
| O-058 | Atom-centred fragments | Defined hydrophobicity |
| nHAcc | Functional group counts | Total number of Ns, Os and Fs in the molecule, excluding N with a formal positive charge, higher oxidation states and pyrrolyl form of N |
| E1u | WHIM descriptors | 1st component accessibility directional WHIM index / unweighted |

**7-Table II should be transposed. Table II describes training or test results?  
These should be separately presented anyway.**

The table describes the statistical parameters of training and test results and we have separated them in the following table:

|  |  |  |
| --- | --- | --- |
| statistical parameters | Training set= 28 | Test set= 15 |
| Q2ext |  | 92.43% |
| SDEP ext |  | 0.533 |
| R2 | 94.09% |  |
| Q2 | 91.39% |  |
| Q2boot | 89.36% |  |
| Q2adj | 93.06% |  |
| SDEP | 0.569 |  |
| SDEC | 0.471 |  |
| S | 0.520 |  |
| F | 91.53 |  |
| Kxx | 30.91 |  |
| Kxy | 46.59 |  |

**8-Table IV is not needed, and it does not sufficient to support conclusion that this is "optimal regression equation "**

Table V shows a hight correlation between Polarizability and Kow. The correlation between the 3 descriptors (O-058, nHAcc, E1u) and the kow is less than 0.5, but their presence in the model improves the good results. The elimination of this descriptors reduce the quality of the model. (R2=47%, Q2= 42%, Q2ext= 12%).

**9-ANN model is poorly described. What were the inputs? Why the number hidden  
of neurons is fixed to only 2? Validation methods used for MLR are not  
reported for ANN, etc.**

The purpose of this work is to compare the results of linear and nonlinear quantitative structure property relationships of kow of organophosphorous compounds and we chose ANN because the last one has become an important and widely used nonlinear modeling.

Thus, in order to compare the predictive ability of the MLR model with an ANN model, the dataset was modeled by ANN using the descriptors selected by the MLR model. After optimization of the model several times. The number of neurons in the hidden layers was 2 and the number of iterations was 50.

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