

Correction

## Roy *et al.* On Two Novel Parameters for Validation of Predictive QSAR Models. *Molecules*, 2009, 14, 1660-1701

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Received: 25 January 2010 / Published: 26 January 2010

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The authors wish to make the following corrections to this paper [1]:

**Abstract:** The sentence “The parameter  $r_{m^2(\text{overall})}$  penalizes a model for large differences between observed and predicted values of the compounds of the whole set (considering both training and test sets) while the parameter  $R_p^2$  penalizes model  $R^2$  for large differences between determination coefficient of nonrandom model and square of mean correlation coefficient of random models in case of a randomization test.” should read as: The parameter  $r_{m^2(\text{overall})}$  penalizes a model for large differences between observed and predicted values of the compounds of the whole set (considering both training and test sets) while the parameter  $R_p^2$  penalizes model  $R^2$  for a small difference between determination coefficient of nonrandom model and square of mean correlation coefficient of random models in case of a randomization test.

**Section 2.3.2.4:** The sentence “We have used a parameter  $R_p^2$  [32] in the present paper, which penalizes the model  $R^2$  for the difference between squared mean correlation coefficient ( $R_r^2$ ) of randomized models and squared correlation coefficient ( $R^2$ ) of the non-randomized model.” should read as: We have used a parameter  $R_p^2$  [32] in the present paper, which penalizes the model  $R^2$  for a small difference between squared mean correlation coefficient ( $R_r^2$ ) of randomized models and squared correlation coefficient ( $R^2$ ) of the non-randomized model.

**Conclusions:** The sentence “The parameter  $R_p^2$  penalizes model  $R^2$  for large differences between determination coefficient of nonrandom model and square of mean correlation coefficient of random models in case of a randomization test and thus confirms whether a model has been obtained by chance or not.” should read as: The parameter  $R_p^2$  penalizes model  $R^2$  for a small difference between determination coefficient of nonrandom model and square of mean correlation coefficient of random models in case of a randomization test and thus confirms whether a model has been obtained by chance or not.

## Reference

1. Roy, P.P.; Paul, S.; Mitra, I.; Roy, K. On Two Novel Parameters for Validation of Predictive QSAR Models. *Molecules* **2009**, *14*, 1660–1701.

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