

**Correction to CSAR Benchmark Exercise of 2010: Selection of the Protein–Ligand Complexes** [*Journal of Chemical Information and Modeling* 2011, DOI: 10.1021/ci200082t]. James B. Dunbar, Jr.,\* Richard D. Smith, Chao-Yie Yang, Peter Man-Un Ung, Katrina W. Lexa, Nickolay A. Khazanov, Jeanne A. Stuckey, Shaomeng Wang, and Heather A. Carlson\*

This Erratum is to declare that the values reported for  $R^2$  in the paper are actually Pearson  $R$  values. The wrong column of data in a spreadsheet was used inadvertently. All correlation values in the paper are correct, just mislabeled with the squared superscript. One of the major conclusions noted in the abstract and discussed in the “Strengths and Weaknesses” Section should read:

“Inherent experimental error limits the possible correlation between scores and measured affinity; Pearson  $R$  is limited to  $\sim 0.91$  (Pearson  $R^2 \sim 0.83$ ) when fitting to the data set without over parameterizing. Pearson  $R$  is limited to  $\sim 0.83$  (Pearson  $R^2 \sim 0.70$ ) when scoring the data set with a method trained on outside data.”

For clarity, the Pearson  $R$  and  $R^2$  are given in Table 1 below for all the theoretical cases posed. It corrects the correlation coefficients in Figure 3 and in the discussion of signal over noise in the “Strengths and Weaknesses” section.

It should be noted that our use of  $R^2$  is based on squaring the Pearson value, not based on a calculation of the coefficient of determination (also called  $R^2$ ). The coefficient of determination measures the one-to-one correspondence between two values, requiring a slope of 1 and an intercept at 0 rather than least-squares-fit values.

**Table 1. Correlation Metrics when Random Error is Added to the 343 Affinity Data of the CSAR-NRC Data Set<sup>a</sup>**

	error with $\sigma = 0.5 \log K$	error with $\sigma = 1.0 \log K$	error with $\sigma = 2.0 \log K$	error with $\sigma = 3.0 \log K$
Random Error in One Coordinate (Ideal vs Lab Case)				
Pearson $R$	0.976	0.913	0.744	0.590
(Pearson $R$ ) <sup>2</sup>	0.952	0.834	0.554	0.348
Random Error in Both Coordinates (Lab vs Scoring Case)				
Pearson $R$	0.952	0.835	0.553	0.355
(Pearson $R$ ) <sup>2</sup>	0.907	0.696	0.305	0.130

<sup>a</sup> Values are the medians of 100 generations of random error.

## ACKNOWLEDGMENT

We thank Christian Kramer of Novartis Pharma AG for pointing out that the  $R^2$  values in the paper were likely  $R$  and for very stimulating discussions regarding Pearson  $R^2$  versus the coefficient of determination.

DOI: 10.1021/ci200363q

Special Issue: CSAR 2010 Scoring Exercise  
Published: August 19, 2011