

2002, Volume 45

Nathalie Marchand-Geneste, Kimberly A. Watson, Bjørn K Alsberg, and Ross D. King: New Approach to Pharmacophore Mapping and QSAR Analysis Using Inductive Logic Programming. Application to Thermolysin Inhibitors and Glycogen Phosphorylase *b* Inhibitors

Page 402. In line 26, second column, “For model A, ILP indicator variables led to a cross-validated coefficient $r^2_{cv} = 0.82 \dots$ ” should be “For model A, ILP indicator variables led to a cross-validated coefficient $r^2_{cv} = 0.74 \dots$ ”.

Page 404. In Table 4, the cross-validated squared correlation coefficients r^2_{cv} using only ILP attributes for the three lowest conformations of thermolysin inhibitors were reported incorrectly. For model A, the corrected cross-validated squared correlation coefficient is $r^2_{cv} = 0.74$, and for model B, the corrected r^2_{cv} is $r^2_{cv,ILP} = 0.67$. In line 10, first column, “Model B yielded a cross-validated coefficient $r^2_{cv} = 0.80$ using only ILP attributes ...” should be “Model B yielded a cross-validated coefficient $r^2_{cv,ILP} = 0.67$ using only ILP attributes ...”. In line 27, second column, “... to correlations having cross-validated coefficient $r^2_{cv} = 0.85$ (model A) and $r^2_{cv} = 0.79$ (model B).” should be “to correlations having cross-validated coefficient $r^2_{cv} = 0.75$ (model A) and $r^2_{cv} = 0.76$ (model B).”

Page 405. In Table 5, the cross-validated squared correlation coefficient r^2_{cv} , using only ILP attributes for GP inhibitors, should be $r^2_{cv,ILP} = 0.55$ instead of $r^2_{cv,ILP} = 0.72$. In line 2 below Table 5, second column, “ILP indicator variables yield a cross-validated coefficient $r^2_{cv} = 0.72 \dots$ ” should be “ILP indicator variables yield a cross-validated coefficient $r^2_{cv} = 0.55 \dots$ ”.

Page 406. In Table 6, the r^2_{cv} using only ILP attributes for the 10 lowest conformations of thermolysin inhibitors were reported incorrectly. For model A, the corrected cross-validated squared correlation coefficient is $r^2_{cv,ILP} = 0.69$, and for model B, the corrected $r^2_{cv,ILP}$ is 0.74. In line 18 below Table 6, column 1, “... AM1 Monte Carlo search, produced a correlation having a cross-validated $r^2_{cv} = 0.80$.” should be “... AM1 Monte Carlo search, produced a correlation having a cross-validated $r^2_{cv} = 0.69$.” In line 18, second column “Model B yields a cross-validated coefficient $r^2_{cv} = 0.84 \dots$ ” should be “Model B yields a cross-validated coefficient $r^2_{cv} = 0.74 \dots$ ”. In line 37, second column, “Importantly, using the CoMFA and ILP descriptors led to lower cross-validated $r^2_{cv} = 0.79$ and $r^2_{cv} = 0.81 \dots$ ” should be “Importantly, using the CoMFA and ILP descriptors led to lower cross-validated $r^2_{cv} = 0.71$ and $r^2_{cv} = 0.78 \dots$ ”.

JM020948Z

10.1021/jm020948z

Published on Web 01/15/2003