

Corrigendum

Small-molecule inhibitor starting points learned from protein–protein interaction inhibitor structure

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Bioinformatics (2011) 28(6), 784–791

The authors regret that the equation for information gain was typeset incorrectly. The correct equation that was used to compute all reported results is:

$$\begin{aligned} IG = & \frac{1}{N+P} \left(-P \log_2 \left(\frac{P}{N+P} \right) - N \log_2 \left(\frac{N}{N+P} \right) \right. \\ & + TP \log_2 \left(\frac{TP}{TP+FP} \right) + FP \log_2 \left(\frac{FP}{TP+FP} \right) \\ & \left. + TN \log_2 \left(\frac{TN}{TN+FN} \right) + FN \log_2 \left(\frac{FN}{TN+FN} \right) \right) \end{aligned}$$