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SimFold Energy Function for De Novo Protein Structure Prediction: Consensus with Rosetta

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In the paper, we found a crucial typo in eq.(15), which should be read as

$$u_{HB}^{(\beta)} = \begin{cases} -1 & r_{OH} < \sqrt{3}\sigma_{OH} \\ -\cos\left(\frac{\pi}{2}\frac{r^2 - 3\sigma^2}{\sigma^2}\right) & \sqrt{3}\sigma_{OH} \le r_{OH} < 2\sigma_{OH} \\ 0 & r_{OH} \ge 2\sigma_{OH} \end{cases} \quad (15)$$

Moreover, eq. (14), although not wrong, was somewhat misleading: Since eq. (15) is always non-positive, eq. (14) can be simplified as

$$V_{\mathrm{HB,direct,4body}} = -\varepsilon_{\mathrm{HB}} \sum_{ij(\mathrm{s.t.}I \ge J+3),kl(\mathrm{s.t.}I \ge J+3),x} c_{\mathrm{HB,4body},x} u_{\mathrm{HB}}^{(\beta)}(r_{ij}) u_{\mathrm{HB}}^{(\beta)}(r_{kl}) . \quad (14)$$

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