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

\[
\begin{align*}
\left\{ 
\begin{array}{ll}
-1 & \quad r_{OH} < \sqrt{3}\sigma_{OH} \\
-\cos\left(\frac{\pi}{2}\frac{r^2 - 3\sigma^2}{\sigma^2}\right) \quad & \quad \sqrt{3}\sigma_{OH} \leq r_{OH} < 2\sigma_{OH} \\
0 & \quad r_{OH} \geq 2\sigma_{OH}
\end{array}
\right.
\end{align*}
\] (15)

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

\[
V_{\text{Hb, direct, 4body}} = -\epsilon_{\text{Hb}} \sum c_{\text{Hb, 4body,}ij,s.t.I,2,3;4,b(i,s.t.I,2,3;4,b)} u^{(\rho)}_{\text{Hb}}(r_{ij}) u^{(\rho)}_{\text{Hb}}(r_{kl}) .
\] (14)

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