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Erratum

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Correction to On the Applicability of Elastic Network Normal Modes in Small-Molecule Docking

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We present the following corrections to the paper "On the Applicability of Elastic Network Normal Modes in Small-Molecule Docking". The corrections remove errors that do not change or invalidate the results of the original paper.

- Page 845. Equation 1 should read as follows:

$$V(\mathbf{R}) = \frac{1}{2}\sum_{i=1}^{N}\sum_{j=i+1}^{N} k(|\mathbf{R}_i^0 - \mathbf{R}_j^0|) \\ (|\mathbf{R}_i - \mathbf{R}_j| - |\mathbf{R}_i^0 - \mathbf{R}_j^0|)^2 \quad (1)$$

- Page 845. Equation 2 and the preceding sentence "Taylor Expansion of $V(\mathbf{R})$ around the minimum $\mathbf{R}^0$ up to second order yields" should more precisely read as follows: To apply NMA to an ENM, one assumes that $V(\mathbf{R})$ can be approximated by quadratic Taylor Expansion around $\mathbf{R}^0$:

$$V(\mathbf{R}) \approx \frac{1}{2}(\mathbf{R} - \mathbf{R}^0)^{\mathrm{T}}\mathbf{H}(\mathbf{R} - \mathbf{R}^0) \quad (2)$$

- Page 845. Equation 3 should read as follows:

$$\mathbf{H} = \mathbf{U}\Lambda\mathbf{U}^{\mathrm{T}} \quad (3)$$

- Page 847. Equation 7 and the preceding sentence "Given the space $\mathbf{S}$ spanned by such a subset," should read as follows: Let $\mathbf{S}$ be the matrix containing the first m modes,

$$\mathbf{S} = [\mathbf{U}_1\, \mathbf{U}_2\, \ldots\, \mathbf{U}_m] \quad (7)$$

- Page 847. Equation 8 should read as follows:

$$\mathbf{P} = \mathbf{S}^{\mathrm{T}}(\mathbf{R}_{\mathrm{H}} - \mathbf{R}_{\mathrm{A}}) \quad (8)$$

- Page 847. Equation 10 should read as follows:

$$\mathbf{R}_{\mathrm{H}}^{*} = \mathbf{R}_{\mathrm{A}} + \mathbf{SA} \quad (10)$$

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