

Effect of Protein Folding on the Stability of Protein–Ligand Complexes *J. Proteome Res.* **2006**, **5**, 105–111. Ernesto Estrada,* Eugenio Uriarte, and Santiago Vilar

Page 106. The diagonal entries of the matrix **T** used for the calculation of the I_3 index are not $T_{ii} = \cos\theta_i$, where θ_i are the dihedral angles of the protein backbone as indicated on this page. Instead we have used in all calculations the function

$$T_{ii} = \frac{1}{2} [1 + \operatorname{sgn}(\cos \theta_i)] \cos \theta_i \quad (1)$$

where $\operatorname{sgn}(x)$ is the sign function defined as

$$\operatorname{sgn}(x) = \begin{cases} -1 & x < 0 \\ 0, & x = 0 \\ 1, & x > 0 \end{cases} \quad (2)$$

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