-ERRATA

A Protein Folding Degree Measure and Its Dependence on Crystal Packing, Protein Size, Secondary Structure, and Domain Structural Class [J. Chem. Inf. Comput. Sci. 44, 1238–1250 (2004)] By E. Estrada. Molecular Informatics, X-ray Unit, RIAIDT, Edificio CACTUS, University of Santiago de Compostela, 15782 Santiago de Compostela, Spain

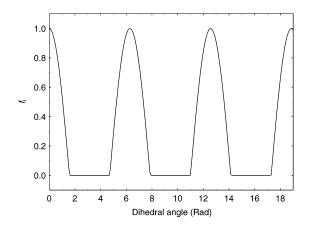
Pages 1242–1248. The function f_i used in the main diagonal of the matrices for the calculation of the I_3 index is not $f_i = \cos \theta_i$ as might be inferred from the text below eq 1 on page 1241. Instead we have used in all calculations the function

$$f_i = \frac{1}{2} [1 + \operatorname{sgn}(\cos \theta_i)] \cos \theta_i \tag{1}$$

where sgn(x) is the sign function defined as

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

The plot of this function is given below for illustration.



CI7001654

10.1021/ci7001654 Published on Web 06/01/2007