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Series approximation of protein structure and constructing conformation space☆

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Abstract

Series approximations of the three-dimensional structure of protein conformations can provide insightful ways to detect and manipulate global features and those local to contiguous segments of the chain. Discrete cosine transforms have proven to be very useful in the past, and now wavelet transforms appear to have additional advantages. Here the emphasis is on a new generalization of the discrete Haar transform for chains of arbitrary length, as opposed to the customary powers of 2. This can be used to define a true, concrete conformation space, where different conformations correspond to points in the space, and a measure of distance between points corresponds to the customary root-mean-square deviation after optimal pairwise superposition (rmsd). Examples are given of how to do this to high accuracy. The key is to devise a rule for placing individual conformers in a standard position relative to the coordinate system, rather than superimposing them on a pairwise basis.

Keywords: Wavelets; Structural superposition; Conformational similarity

The paper by Gordon M. Crippen was submitted to this special issue of Polymer on protein conformational computations, but was erroneously published in the regular issue: *Polymer* **44**, (2003) 4373–4379.

We would like to apologize for this unfortunate mistake. Because the paper belongs to this special issue we reprint the abstract of the paper and refer all readers to the regular issue of *Polymer* with this interesting article.

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