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Predicting Minimum Energy Structure of a Peptide via a Modified Potential Smoothing Kernel

Leong Wah June and Malik Abu Hassan
Institute for Mathematical Research
and Department of Mathematics,
Universiti Putra Malaysia,
UPM 43400 Serdang, Selangor

ABSTRACT

A global optimization approach is proposed for finding the global minimum energy configuration of a peptide. First, the original nonsmooth total potential energy function of a peptide, composed using the AMBER model, is transformed to a smoother function (shifted-impulsive transformation) via a procedure performed for each pair potential that constitute the total potential energy function. Then, the Potential Smoothing and Search (PSS) procedure is used to provide the global minimum. Based on this procedure global optimum solution is generated for a synthesis peptide named Compstatin.