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A New Method for Evaluation of the Coefficient Vectors in Protein Docking

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We present a new computational method for computing the coefficient vectors in docking problems by using orthonormal spherical polar radial basis functions. This computational technique arises from the modeling of the molecule. Representing the molecules as three-dimensional functions in terms of orthonormal spherical polar radial expansion provides a straightforward way of computing the correlation between pairs of these functions. After rotating and translating the original functions, the correlation has the form of scalar products of suitably rotated and translated coefficient vectors. In this work we explain our algorithem for computing these coefficients.

Keywords: shape complementarity; electrostatics complementarity; Laguerre polynomials; spherical harmonics; spherical polar radial Fourier coefficients, I-coefficients

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