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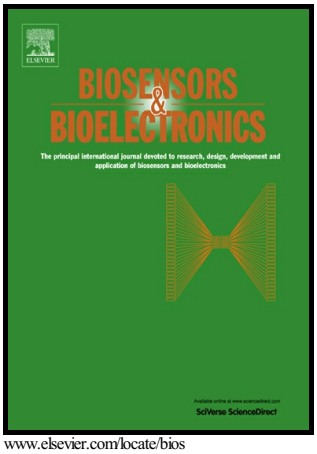

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Aptasensor designed via the stochastic tunneling-basin hopping method for biosensing of vascular endothelial growth factor

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Abstract

The Systematic Evolution Ligands by Exponential Enrichment (SELEX) is common used for selection of high affinity single-stranded DNA (ssDNA) aptamer with target protein. However, we do not know what the most stable configuration of the selected aptamer bound with target protein is. Therefore, a systematic search process using the stochastic tunneling-basin hopping (STUN-BH) method is proposed to find the most stable configuration of the ssDNA aptamer specific for vascular endothelial growth factor (VEGF) capture (Apt_{VEGF}; 5′-TGTGGGGGTGGACGGGCCGGGTAGA-3′). After the most stable configuration was obtained by the STUN-BH method, molecular dynamics (MD) simulation was carried out to investigate the