Kinetics and thermodynamics characterization of the interactions between kynurenic acid and human glutamate receptor fragments by surface plasmon resonance studies

Ádám Juhász, Edit Csapó, Hajnalka Szokolai, Ditta Ungor, Imre Dékány

MTA-SZTE Supramolecular and Nanostructured Materials Research Group, University of Szeged, Dóm Sqr. 8, Szeged, Hungary, e-mail: juhaszadam79@gmail.com

Investigation of receptor – ligand interactions play a determinant role in molecular life science. Detailed quantitative, kinetic and thermodynamic characterization of these biomolecular interactions may decisively contribute to the modern pharmaceutical developments. Surface plasmon resonance spectroscopy is capable of real-time monitoring of these interactions without use of labels via immobilization one of the binding partners (protein or small biomolecule) onto the sensor surface. Understanding the exact molecular mechanism of the action of kynurenic acid on Human Glutamate Receptor (GluR1) peptide fragments might promote future drug development for the therapeutic management of neurological disorders. In our study reversible bonded amount of kynurenic acid have been measured on different peptide-modified gold surface at different temperatures under physiological conditions. Besides the experimental characterization of the receptor-ligand systems the underlying molecular mechanism can be investigated using the methods of computational molecular modelling. The binding mode and structural properties of a peptide or protein adsorbed on a surface can be elucidated using molecular dynamics (MD) simulations. The main object of our SPR experiments is to provide important parameters (quantitative data of bounded amount of drug molecule on different protein-covered solid support; kinetic (rate of association and dissociation) and thermodynamic (ΔG, ΔH, ΔS) data for better understanding of the mechanism of protein-drug molecule bindings.

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References
