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The analysis of potential binding sites of TiO_2 nanoparticles docked to the extracellular part of $GABA_{B1a}$

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The search and analysis of possible binding sites of titanium dioxide nanoparticles ($npTiO_2$) to the extracellular part of $GABA_{B1a}$ subunit (ECP $GABA_{B1a}$) was conducted using molecular docking method. The spatial structure of the first $npTiO_2$ was constructed using Discovery Studio Visualizer software, versions 2.0 and 2.5. The dimensions of the $npTiO_2$ surface were (18.925 × 3.785 × 19.028) Å. Four potentially possible sites of docking were identified using the algorithm for molecular docking PatchDock. Geometric shape complementarity scores for these sites were 12562, 10746, 10370, and 10204, respectively. The approximate interface areas of the complex of ECP $GABA_{B1a}$ with $npTiO_2$ for obtained sites were 1949.80 $Å^2$, 1273.20 $Å^2$, 1261.10 $Å^2$ and 1170.30 $Å^2$, respectively. The evaluations of atomic contact energy for $npTiO_2$ binding sites were 362.92, 173.93, 340.63 and 224.61.

We have also constructed second $npTiO_2$ using Discovery Studio Visualizer software, versions 2.0 and 2.5. The dimensions of the $npTiO_2$ surface were (19.029 × 17.059 × 18.925) Å. Molecular docking showed that there are two potentially possible binding sites. The geometric shape complementarity scores in these sites demonstrated the following values: 14,746 and 14,228, respectively. The approximate interface area of each of the sites was 1931.40 $Å^2$ and 1816.40 $Å^2$, respectively. The evaluations of atomic contact energy were 121.09 and 208.31.

The nature of connections, stabilizing the sites of $npTiO_2$ docking to the ECP $GABA_{B1a}$ was analyzed in accordance to their amino acid composition. The results of the studies demonstrated that $npTiO_2$ interact with ECP $GABA_{B1a}$ and form a supermolecular structure. It may be assumed that it will be accompanied with modulations of ECP $GABA_{B1a}$ spatial organization.