

Interaction Mechanism of Claudin-4 Receptor and Fab1 Antibody in Pancreatic Cancer Cell Membrane

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Claudin-4 (CLDN4), which belongs to claudin family proteins and tight junction proteins, is overexpressed in pancreatic cancer cell membranes. Due to this overexpression phenomenon, CLDN4 was used to target the protein for pancreatic cancer therapy using antibody interaction. In this study, we investigated detailed interaction mechanism of CLDN4 and Fab1 in cancer cell membrane via coarse grained molecular dynamics (CGMD). CLDN4 was used for the receptor and Fab1 fragment of immunoglobulin G1 (IgG1), which interacted with CLDN4, was used for the antibody for effective calculation. Cancer cell membrane was constructed with neutral dipalmitoylphosphatidylcholine (DPPC) and negatively charged dipalmitoylphosphatidylglycerol (DPPG) to realize the negatively charged state. We revealed that the extracellular loop of receptor and heavy chain of antibody actively participated to antibody-receptor reaction on the cell membrane. These bindings, which were resulted from salt bridge and aromatic interactions, were turned out to be the most important factor for the effective treatment of pancreatic cancer cell.