INTERACTION OF ANTIBODIES WITH AROMATIC LIGANDS: THE ROLE OF pi-STACKING.

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Antibodies are responsible for antigen recognition in vertebrate organisms. Practically any molecule can be bound by antibodies. In this work structures of 73 complexes of antibodies with small antigens were taken from PDB database and compared. The main epitope of studied ligands was an aromatic ring. Antibodies bound it with a deep cavity, lying between complementary determining regions (CDR) H3 and L3 and formed by aromatic residues. In most cases the aromatic ring of ligand was placed parallel to one or two aromatic sidechains of binding site at 3.5-4 Angstrom distance. This disposition of aromatic rings is a sign of the presence of pi-stacking. It was found that small ligands with aromatics area percentage > 36% predominantly form pi-stacking interaction with antibodies. Most often this interaction was observed for residues in positions H33, H95, L32 and L93.


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