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Topological analysis of the three dimensional structure of antibody

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In silico prediction of the relationships between the protein structure and its physiological activity is an important research topic for drug design. Broad picture of my research is to construct a topological model to clarify the antibody-antigen recognition system, since immunotherapy is applied to wide range of severe diseases such as cancer [1].

To achieve the goal, we focus on a topological method called "Fatgraph models of proteins" [2]. Fatgraph models of proteins are topological two-manifold with boundary components (surface) which have one to one correspondence with three-dimensional protein structures listed on Protein Data Bank (PDB) [3] with only a few exceptions. The traits of each surface for each protein are described by the following invariants; Euler characteristics, number of boundary components, and genus. Fatgraph is also called ribbon graph and has already proven their utility in theoretical physics including string theory [4].

In this research, we constructed fatgraph models of antibodies and investigated the traits of antigen-binding fragments (Fab). Then, we topologically examined the transformations of the fatgraphs of the proteins due to the changes of protein sequences or existence of ligands.

[1] Patel, Shetal A. et al. (2018) Combination Cancer Therapy with Immune Checkpoint Blockade: Mechanisms and Strategies, *Immunity*, Volume 48, Issue 3, 417 - 433

[2] R. C. Penner, *et al.*, (2010) Fatgraph models of proteins, *Communications on Pure and Applied Mathematics*. Volume 63 , Issue 10 , 1249 - 1297.

[3] H.M. Berman, *et al.* (2000) The Protein Data Bank, *Nucleic Acids Research*, 28: 235 - 242. http://www.rcsb.org/

[4] R. C. Penner, (2016) Moduli spaces and macromolecules. *Bull. Amer. Math. Soc.* 53, 217 - 268.

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