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Determination of surface clefts in human IgG Fab region by computational data analysis

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TYPE OF ARTICLE: CONFERENCE ABSTRACT

ABSTRACT

Introduction: Antibodies (Abs) play a vital role in defense against pathogens and consist of two fragments: fragment of antigen binding (Fab) and fragment of crystalizable (Fc). Immunoglobulin G (IgG) is maximum abundant Abs existing in sera and has an imperative role in infection damage. Amount of serum IgG is dependent on severity of several diseases, including infections. Thus, IgG has special diagnostic worth. Antigenic determinants (epitopes) are mostly located near surface clefts of molecules. Therefore, surface clefts play an important role in epitopes recognition. Computational data analysis models can be useful for better understanding of biological systems such as molecular basis of diseases through different plans, including understanding molecular interactions. The aim of this study is determination of human IgG Fab clefts by computational data analysis.

Methods: The amino acid sequence and third construction of reference human IgG were attained from PDB database. Second IgG structure was defined by Phyre 2 software. The human IgG Fab clefts were determined by Profunc software.

Results: Ten clefts on human IgG were found by Profunc software. The first and second largest and deepest clefts were located on human IgG Fab region.

Conclusion: According to results of present study of the human IgG, the largest and deepest clefts are located in the Fab region. Precise identification of the Fab clefts amino acids would be useful in recognition of most immunogenic epitopes and therefore helpful for designing of more specific elements for optimizing the existing IgG diagnostic assays. Also Profunc software could be a useful tool in the analysis of surface clefts.

KEYWORDS: Computational, Analysis, Surface cleft, IgG