

Molecular Modeling for Revealing Cross-Reaction Antibody with *Staphylococcus Aureus* and Human Spermatozoa Protein

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Abstract: Infertile women with non-specific vaginitis due to *Staphylococcus aureus* (*S. aureus*) will develop antibodies that cross-react with human spermatozoa, causing infertility. This study aim is to evaluate the homology of *S. aureus* and spermatozoa proteins based on sequences and structural model through computational approach. All proteins of human spermatozoa were retrieved from UNIPROT. Modeling protein was constructed based on threading modeling using I-TASSER. Sequence homology analysis was evaluated using BLASTP and structural comparison was done by Superpose v.1.0. Antigenicity and epitope mapping of homolog proteins were conducted using IEDB webservices for comparing the potential cross-reaction antibody. The result of sequence comparison showed that there are 5 homolog proteins from human spermatozoa and *S. aureus*. Based on structural analysis, antigenicity and epitope mapping, potential candidate protein that have cross-reaction with human antibody are protein deglycase DJ-1, Sperm acrosome membrane-associated protein 4, UDP-N-acetylhexosamine pyrophosphorylase. These proteins have similar structure and similar position of epitope that locate on surface protein. In addition the protein have high antigenicity profile. It can be concluded that the similar properties of sequence, structure, antigenicity and epitope from those proteins are possible if human antibody can cross-react with human spermatozoa protein after infecting by *S. aureus*. This mechanism may have role in infertile woman.

Keyword : Antigenicity, infertile woman, *S.aureus*, spermatozoa protein.