Prediction of T-cell and B-cell epitopes for merozoites surface protein ($MSP1_{19}$) for *Plasmodium yeolii* using computational techniques

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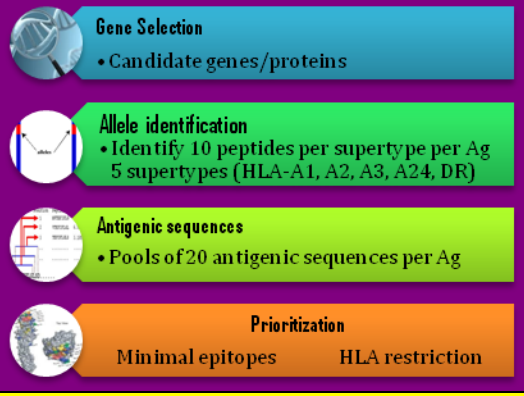
INTRODUCTION

Malaria disease is caused by the transmission of *Plasmodium*, through the bit of a female A*nopheles* mosquito. Although the *Plasmodium* life-cycle has been extensively characterized, relatively little is known about sporozoite interaction with host organelles and proteins. Individuals that survive continuous exposure to infection do eventually develop clinical immunity, suggesting that a vaccine against the asexual blood stage of the parasite is achievable. The merozoite surface protein ($MSP1_{19}$) of *Plasmodium yoelii* was considered for epitope prediction in present work. The T-cell and B-cell epitopes for $MSP1_{19}$ were predicted followed by docking studies using a variety of computational tools.

METHODOLOGY



CONCLUSION

The present research work was conducted to predict epitopes for B-cell and T-cell respectively, and to find the most efficient epitope(s) with highest binding affinity for $MSP1_{19}$ of *Plasmodium yoelii*. After protein-protein docking studies, it was found that epitope 'IYQAMYNVIF' was having the lowest energy score (-579.41 KJ/mole) for MHC-I. For the MHC-II receptors, epitope 'YVLLQNSTI' has shown lowest energy score (-424.77 KJ/mole) which reveals highest binding affinity toward the receptor. The small peptide 'QPTET' was found to be most probable epitope for the B-cell. In future above predicted epitopes can be synthesized in wet laboratory and might become most promising candidate(s) for malarial vaccine development.

RESULTS

Five T-cell epitope prediction algorithms and three B-cell epitope prediction methods were used on IEDB analysis tool. The candidate T-cell and B-cell epitopes and their binding free energy scores with MHC class-I and class-II molecules were identified and used for docking. These docked products were obtained with the Patch dock server and the complexes with finest energy scores are shown in figure 1 and 2 respectively.

Table: Predicted B-cell epitopes with position and residue length

RESULT OF B-CELL EPITOPE PREDICTION				
RANK	START POSITION	END POSITION	EPITOPE	SIZE
1	57	61	QPTET	5
2	152	157	SEEETE	6
3	220	228	SOKYNKKKP	9
4	398	403	KEKKKE	6
5	412	417	CKKNKA	6
6	458	463	THPDNT	6

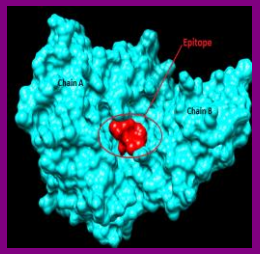


Fig 1: Docked complex of T-cell epitope and human MHC-1 receptor (2XPG)

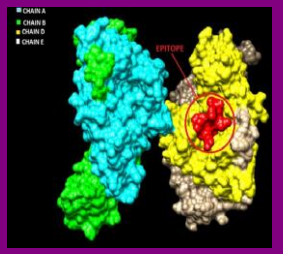


Fig 2: docked complex of T-cell epitope and human MHC-II receptor

The table here represents the common epitopes among all three methods of B-cell epitope prediction. QPTET proved to be the best epitope on the grounds of ranking and scores.

References

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