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Short Communication

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Alpha fold 3D boltz 2 protenix chai discovery systems: reliable results? When concerning sea star antibody- HRP antigen complex study

Abstract

Recently, we have presented the first 3D images of the sea star Antibody (anti-HRP) - HRP Antigen complex in Alpha Fold 3, with minor details. In the present study, we used 4 systems of 3D representation, which are all issued from Alpha Fold, to illustrate this same complex. It appears clearly that these models, by using the ITPM parameter give contradictory results. Nevertheless, we start from the principle that in Science, we must be transparent. Nevertheless, it's the first time, we present such models concerning an invertebrate primitive antibody: you understand that comparisons with other antibody 3D models seem difficult to establish, in the present time.

Keywords: sea star antibody, anti-HRP antibody, HRP antigen, alphafold 3, antigen–antibody complex, 3D molecular modeling, invertebrate immunity, protein–protein interactions

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Introduction

The sea star Asterias rubens possesses lymphocytes, an adaptative immunity towards various antigens and immune genes, CDR1 , CDR2 determining regions. We work especially on the anti-HRP (Horse-radish peroxydase) sea star antibody). Recent modelizations, between the Ab and the Ag HRP have been performed in Alpha Fold.[1]

Material and methods

Alpha Fold 3, Protenix, Chai Discovery and Boltz 3 systems were used. In the same way pTm index and iptm one were performed.[2-6] Iptm measures the accuracy of the predicted relative positions of the subunits forming the protein-protein complex. Values higher than 0.8 are valid and in a weaker way between : 0.6 to 0.8 where it is spoken of grey area.

Results

Results are given according 3 sequences of HRP complexed to SSA (sea star Ab : anti-HRP). Different sequences in Amino-Acids of HRP were given in Reference 1.

1) Neutral HRP

2) HRP-C1A

3) HRP-A2

Modelizations of the different complex are summarized in the following figures with their pTm index and iptm index

We retain mainly that Alpha Fold 3 gives a positive result with Neutral HRP complexed to sea star Ab and Boltz 3 confirms another positive result with HRP-C1A. The other results seem negative as shown below in Figure 1, Figure 2 and Figure 3.

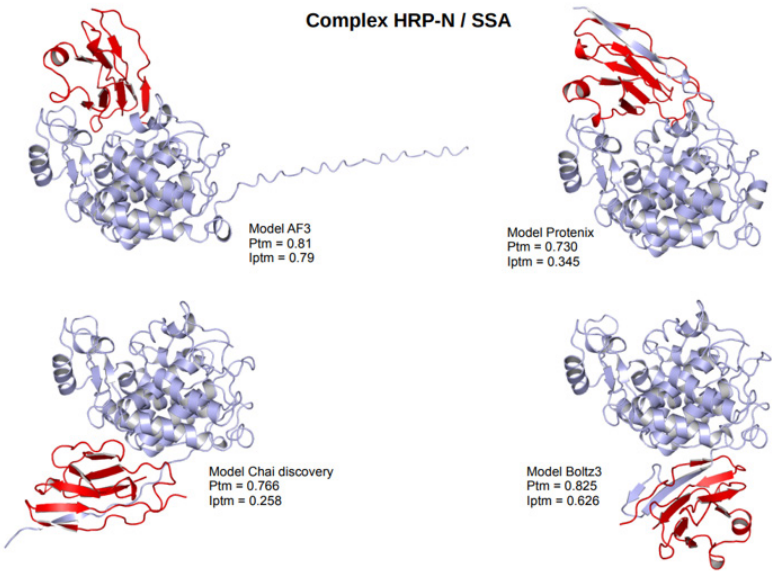

Figure 1 The Ag (HRP) is colored in purple, the Ab in brown. It is the same in Figure 2 &3.

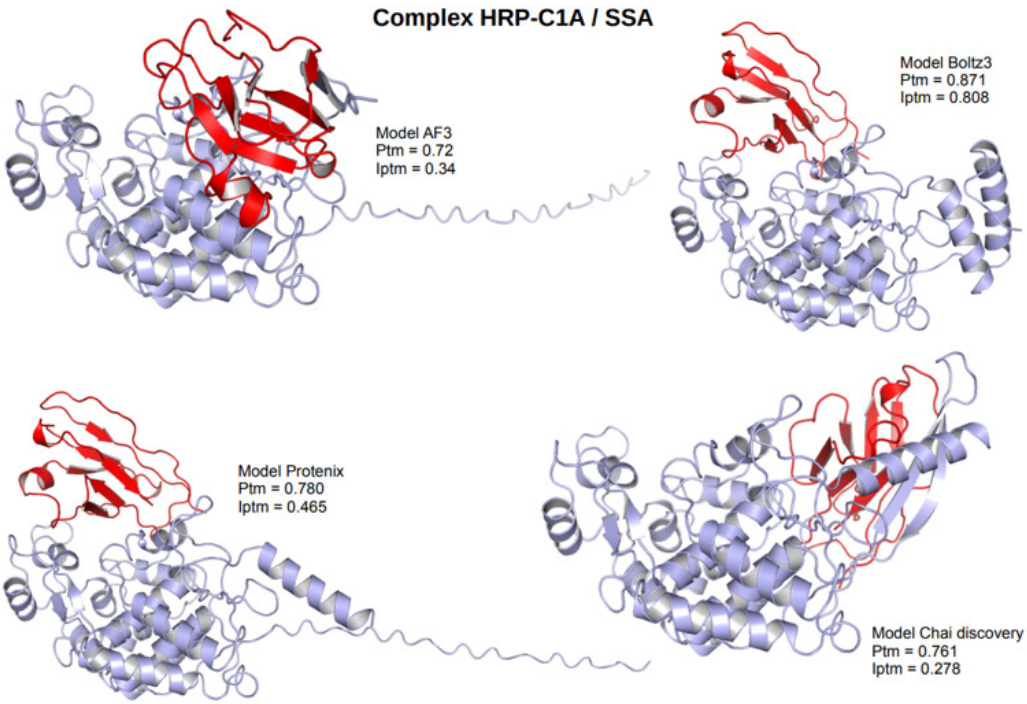

Figure 2 Note the result with Boltz 3(up on the right).

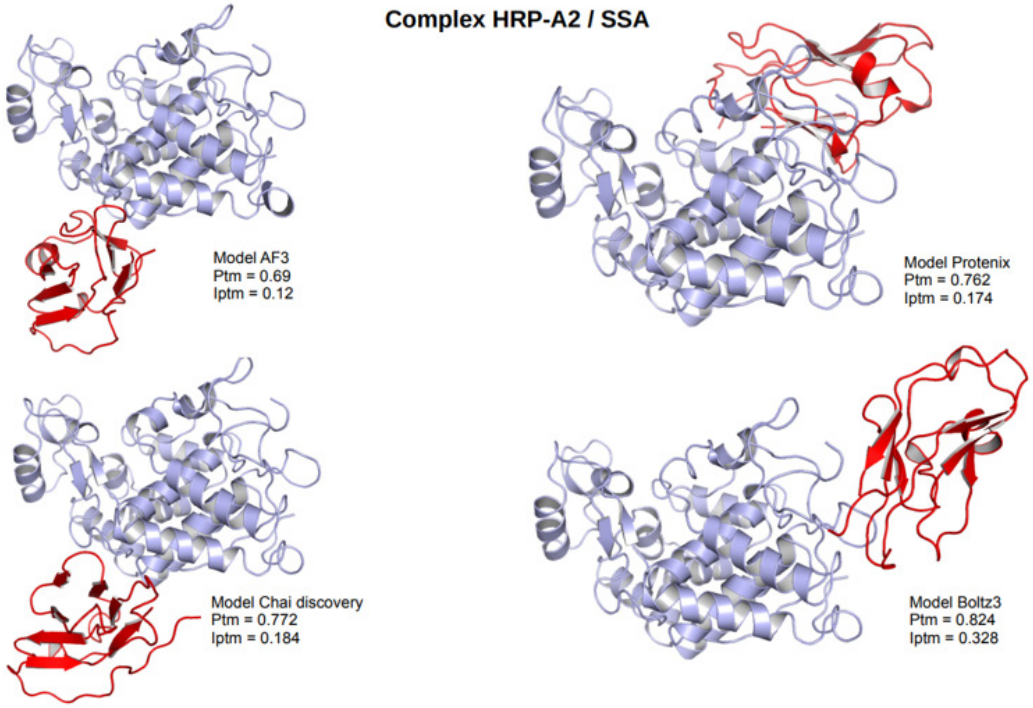

Figure 3 The Ag (HRP) is colored in purple, the Ab in brown.

Conclusion

It appears clearly that these models, by using the iptm parameter, seem , sometimes, contradictory. But we start from the principle that in Science, we must be transparent and we admit also that these studies, based on artificial intelligence, are subject to doubt. Nevertheless, it was necessary to give an overview about. Note also, it is the first time that such models are presened to the scientific communauty.

We will have to wait for a few time to see a « true model » of Ab-Ag complex, in sea star, by the use of crystallization and X-Rays analysis or TEM.

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Conflicts of interest

The author declares that there are no conflicts of interest.

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