Research Article

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Invertebrate Primitive Antibody Anti-HRP-HRP Complex. Modelisations by Alpha Fold 3: Parameters

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ABSTRACT

Recently, we have shown a modelisation of the Invertebrate sea star Asterias rubens HRP-anti HRP complex. Now, by the use of Alpha Fold 3 model, we present some parameters which characterise the interaction of the sea star Ab-Ag complex when compared to Vertebrates.

Keywords: Alpha Fold 3 Modelisations, IPA, Parameters.

INTRODUCTION

Introducing Alpha Fold 3 a new Al model developed by Google and Deep Mind and Isomorphic Labs. By accurately predicting the structure of proteins, DNA, RNA, ligands and more, and how they interact [1].

In 2009, the used HRP (Horse-Radish Peroydase) as antigen in sea star Asterias rubens (Goteborg University, Sweden) was not clearly identified. We have been obliged, 16 years later to modelise this HRP antigen, according 3 Protein sequences, separately, and, which are repertoried in Uniprot. In these conditione we hoped to find the appropriate one. But other sequences can be used for our work next.

As for the sea star antibody, we have performed the better sequence, in view to obtain a pTM superior to 0.8, as it is asked for Vertebrate antibodies.

RESULTS

The first Protein Alpha Fold 3 analysis of the sea star Ab sequence shows that it contains a N-ter part that Alpha Fold 3 doesn't know how to model

Thus, the sequence for modelisation will be:

>>SSA

IYTFREQPSDTSALQGSTVVLHCSVEQYINTTAIVWWSRDSVISHNKDLK-LSSLNTDQLQRYSISGDASRGEFNLKIVNFTATDAASYRCQM

Effectively, it is of better quality, with a pTM of 0.88, when compared to Vertebrates.The 3D modelisation of the corresponding sequence is given below (Figure 1) :

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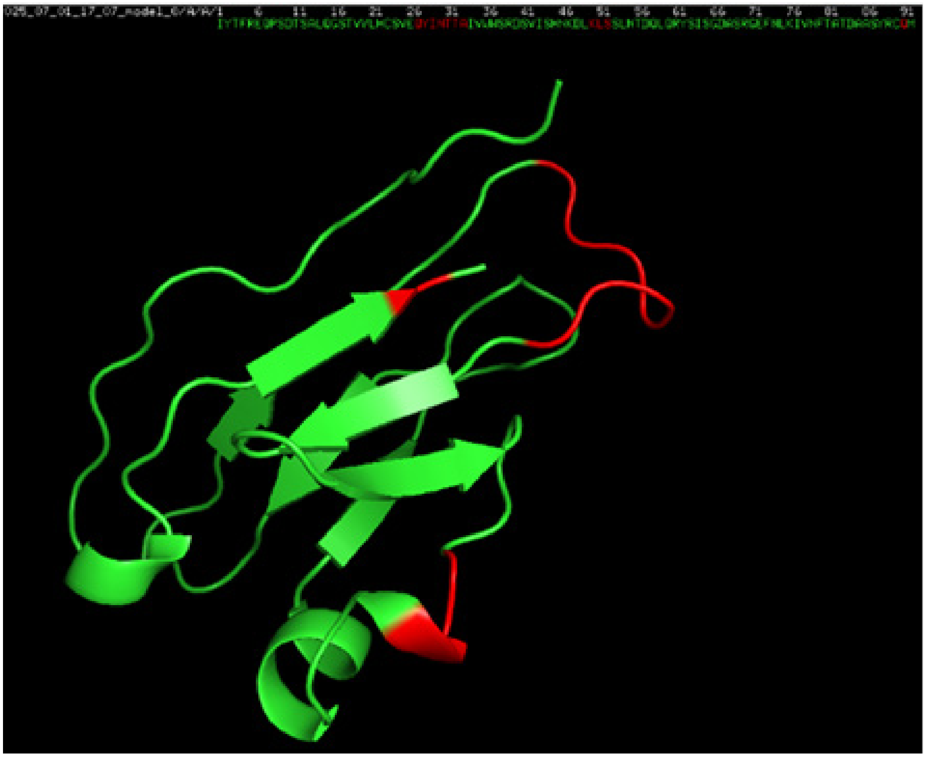


Figure 1. Modelisation of sea star anti-HRP antibody with CDR regions in red.

As for the antigens, we have tested, first (1) protein sequence of HRP neutral, secondly (2) HRP C1A one, thirdly (3) HRP C1A variant one

1. La HRP-Neutral: https://www.uniprot.org/uniprotkb/Q42517/entry

>HRP-N (327 AA, incorporated peptid below in red)

MKTQTKVMGGHVLLTVFTLCMLCSAVRAQLSPDIYAKSCPNLLQIVRDQVKIALKAEIRMAASLIRLHFHDCFVNGCDASVLLDGTNSEKLAIPNVNSVRGFEVIDTIKAAVENACPGVVSCADILTLAARDSVYLSGGPQWRVALGRKDGLVANQSSANNLPSPFEPLDAIIAKFAAVGLNVTDVVALSGAHTFGQAKCDLFSNRLFNFTGAGTPDSTLETTLLSDLQTVCPIGGNGNKTAPLDRNSTDAFDNNYFKNLLEGKGLLSSDQILFSSDLAVNTTKRLVEAYSRSQYLFFRDFTCSMIRMGSLVNGASGEVRTNCRVIN

2. La HRP-C1A: https://www.uniprot.org/uniprotkb/P00433/entry

>HRP-C1A (353 AA, incorporated peptid; below in red)

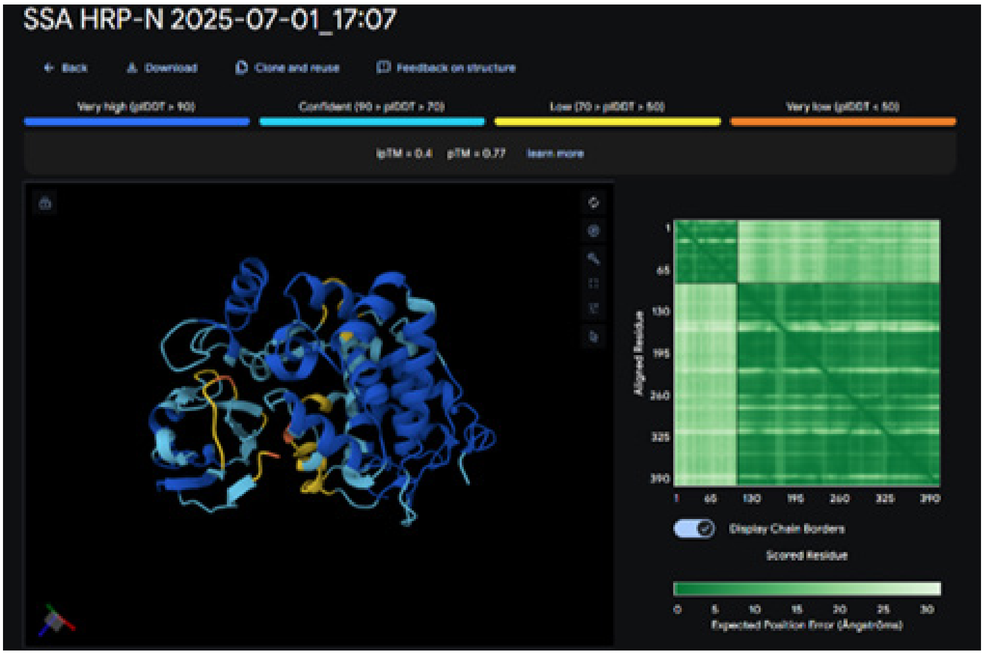
MHFSSSSTLFTCITLIPLVCLILHASLSDAQLTPTFYDNSCPNVSNIVRDTIVNELRSDPRIAASILRLHFHDCFVNGCDASILLDNTTSFRTEKDAFGNANSARGFPVIDRMKAAVESACPRTVSCADLLTIAAQQSVTLAGGPSWRVPLGRRDSLQAFLDLANANLPAPFFTLPQLKDSFRNVGLNRSSDLVALSGGHTFGKNQCRFIMDRLYNFSNTGLPDPTLNTTYLQTLRGLCPLNGNLSALVDFDLRTPTIFDNKYYVNLEEQKGLIQSDQELFSSPNATDTIPLVRSFANSTQTFFNAFVEAMDRMGNITPLTGTQGQIRLNCRVVNSNSLLHDMVEVVDFVSSM

3. La HRP-A2: https://www.uniprot.org/uniprotkb/P80679/entry

>HRP-A2 (305 AA, no peptid)

QLNATFYSGTCPNASAIVRSTIQQAFQSDTRIGASLIRLHFHDCFVDGCDASILLDDSGSIQSEKNAGPNANSARGFNVVDNIKTALENTCPGVVSCSDILALASEASVSLTGGPSWTVLLGRRDSLTANLAGANSAIPSPFEGLSNITSKFSAVGLNTNDLVALSGAHTFGRARCGVFNNRLFNFSGTNGPDPTLNSTLLSSLQQLCPQNGSASTITNLDLSTPDAFDNNYFANLQSNNGLLQSDQELFSTLGSATIAVVTSFASNQTLFFQAFAQSMINMGNISPLTGSNGEIRLDCKKVDGS

We have found, that neutral HRP fixed our antibody in a better way than the 2 other HRP, at 0.77 pTM. For information the Ab-Ag complex, in Alpha Fold 3 is given below, in these conditions:



SEA STAR ANTI-HRP -HRP COMPLEX, AT 0.77 PTM (ALPHA FOLD 3)

CONCLUSION

We retain mainly that the interaction between the IPA (Invertebrate Primitive Antibody) or sea star anti-HRP antibody- HRP antigen, (neutral HRP) culminates at 077 pTM., **which is slightly inferiror to0.8, when compared to Vertebrate Ab-Ag complex.** But, it is a preliminary data for these first results. We have, in the future to compose with other parameters such as new HRP protein sequences to test and a new Alpha Fold model. **As new HRP sequences we 'll try that of HRP Armoracia rusticana: Uniprot K B and PRXC1C HRP one.**

Whatever our IPA resembles in many points to Vertebrate ones [2-4].

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