



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

Key words: Alpha Fold 3 modelisations ; IPA ; Parameters

Introduction

Introducing Alpha Fold 3 a new AI 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. (Ref 1)

In 2009, the used HRP (Horse-Radish Peroxidase) 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

IYTFREQPSDTSALQGSTVVLHCSVEQYINTT
AIVWWSRDSVISHNKDLKLSSLNTDQLQRYSI
SGDASRGEFNLKIVNFTATDAASYRCQM

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 (Fig 1) :

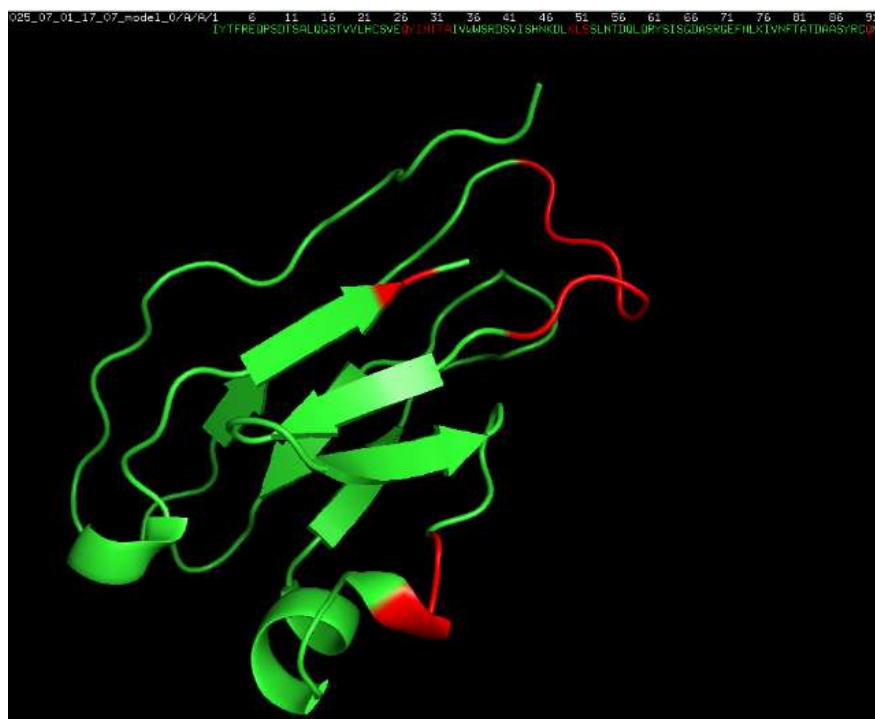


Fig 1 : Modelisation of sea star anti-HRP antibody with CDR regions in red.

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](https://www.uniprot.org/uniprotkb/Q42517/entry)

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

MKTQTKVMGGHVLLTVFTLCMLCSAVRAQL
SPDIYAKSCPNLLQIVRDQVKIALKAEIRMAAS
LIRLHFHDCFVNGCDASVLLDGTNSEKLAIPN
VNSVRGFEVIDTIKAAVENACPGVVSCADILTL
AARDSVYLSGGPQWRVALGRKDGLVANQSSA
NNLPSPFEPLDAIIAKFAAVGL

MKTQTKVMGGHVLLTVFTLCMLCSAVRAQL
SPDIYAKSCPNLLQIVRDQVKIALKAEIRMAAS
LIRLHFHDCFVNGCDASVLLDGTNSEKLAIPN
VNSVRGFEVIDTIKAAVENACPGVVSCADILTL
AARDSVYLSGGPQWRVALGRKDGLVANQSSA
NNLPSPFEPLDAIIAKFAAVGLNVTDVVALSG
AHTFGQAKCDLFSNRLFNFTGAGTPDSTLET
TLLSDLQTVCPIGGNGNKTA PLDRNSTDAFD
NNYFKNLLEGKGLSSDQILFSSDLAVNTTKR
LVEAYSRSQYLFFRDFTCMIRMGSLVNGASG
EVRTNCRVIN

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

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

MHFSSSSTLFTCITLIPLVCLILHASLSDAQLTP
TFYDNSCPNSNIVRDTIVNELRSDPRIAASIL
RLHFHDCFVNGCDASILLDNNTTSFRTEKDAFG
NANSARGFPVIDRMKAAVESACPRTVSCADL
LTIAAQSVTLAGGPSWRVPLGRRDSLQAF
DLANANLPAPFFTLPLQLKDSFRNVGLNRSSD
LVALSGGHTFGKNQCRFIMDRLYNFSNTGLP
DPTLNTTYLQTLRGLCPLNGNLSALVDFDLR
TPTIFDNKYVYNLEEKGLIQSDQELFSSPNA
TDTIPLVRSFANSTQTFNFAVEAMDRMGNI
TPLTGTQGGQIRLNCRVVNSNSLLHDMVEVVD
FVSSM

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

>HRP-A2 (305 AA, no peptid)

QLNATFYSGTCPNASAIVRSTIQQAFQSDTRIG
ASLIRLHFHDCFVDGCDASILLDDSGSIQSEKN
AGPNANSARGFNVDNIKTALENTCPGVVSC
SDILALASEASVSLTGGPSWTVLLGRRDSLTA
NLAGANSAIPSPFEGLSNITSKFSAVGLNTNDL
VALSGAHTFGRARCGVFNNRNFNFSGTNGPD
PTLNSTLLSSLQQLCPQNGSASTITNLDLSTPD
AFDNNYFANLQSNNGLLQSDQELFSTLGSATI
AVVTSFASNQTLFFQAFQASMINMGNISPLTG
SNGEIRLDCKKVDGS

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 inferior to 0.8, 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 (Ref 2 3 4)

References

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Citation: Michel Leclerc, (2025), “ Invertebrate Primitive Antibody Anti-HRP –HRP Complex. Modelisations By Alpha Fold 3: Parameters.”, Arch Health Sci; 9(1): 1-3.

DOI: 10.31829/2641-7456/ahs2025-9(1)-002

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