

LAMPIRAN

Lampiran 1. Epitop MHC-II.

Epitop	Alel	Antigenitas	Energi Ikatan (kcal/mol)
MFIFLLFLTLTSGSD	HLA-DPA1*01, DPB1*04:01, DPA1*01:03, DPB1*02:01, DPA1*02:01, DPB1*05:01, DPA1*03:01, DPB1*04:02, DRB1*04:01, HLA-DRB1*04:05, DRB1*11:01	0,6167	-264,53
AYFVGYLKPTTFMLK	HLA-DPA1*02:01, DPB1*01:01, DPA1*02:01, DPB1*05:01	0,7088	-258,58
LYLTQDLFLPFYSNV	HLA-DPA1*01:03, DPB1*02:01, DPA1*02:01, DPB1*05:01	0,4189	-257,25
GYQPYRVVLSFELL	HLA-DPA1*01, DPB1*04:01, DPA1*01:03, DPB1*02:01, DPA1*02:01, DPB1*01:01	1,0740	-219,76
RVVLSFELLNAPAT	HLA-DPA1*01, DPB1*04:01, DPA1*01:03, DPB1*02:01, DPA1*02:01, DPB1*01:01, DPA1*02:01, DPB1*05:01, DRB1*01:0	0,7089	-216,39
DEIFRSDTLYLTQDL	HLA-DRB1*04:01, HLA- DRB3*01:01, HLA-DPA1*02:01, DPB1*01:01	0,3818	-210,94

Lampiran 2. Gambaran Penambatan Molekuler Epitop MHC-I dan alel HLA.



QYIKWPWYV



AEIRASANL



QIAPGQTGV

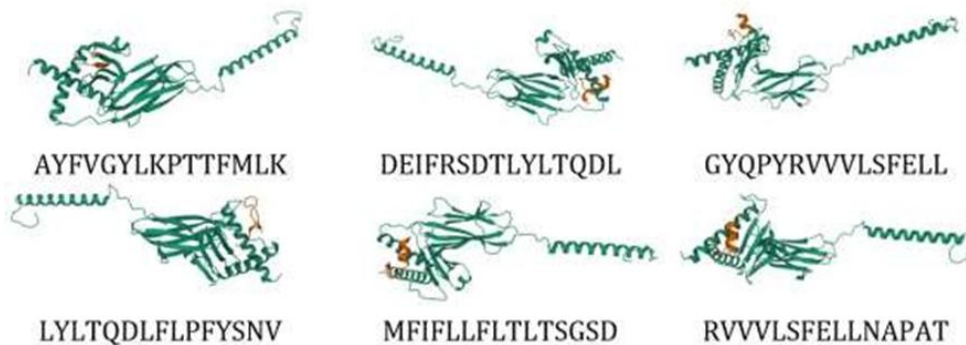


GQTGVIADY



GVIADYNYK

Lampiran 3. Gambaran Penambatan Molekuler Epitop MHC-II dan alel HLA.



Lampiran 4. Hasil Sel B

Epitop	Antigenitas	Toksitas	Alerginitas
PIDVRDLPSGFN	1,5139	Non Toksik	Non Alergen
RNFFSPQITTD	0,2816	Non Toksik	Non Alergen
TLIHAEQLTPAW	0,6664	Non Toksik	Non Alergen
TGVIADYNYKLP	0,9990	Non Toksik	Non Alergen
VSATKLNLCFS	2,2210	Non Toksik	Non Alergen

Lampiran 5. Hasil ProtParam

Formula: $C_{1945}H_{2958}N_{496}O_{557}$

Total number of atoms: 5966

Extinction coefficients:

Extinction coefficients are in units of $M^{-1} cm^{-1}$, at 280 nm measured in water.

Ext. coefficient 62020

Abs 0.1% (=1 g/l) 1.459, assuming all pairs of Cys residues form cystines

Ext. coefficient 61770

Abs 0.1% (=1 g/l) 1.453, assuming all Cys residues are reduced

Estimated half-life:

The N-terminal of the sequence considered is M (Met).

<https://web.expasy.org/cgi-bin/protparam/protparam>

4/26/22, 5:01 AM

ExPASy ProtParam tool

The estimated half-life is: 30 hours (mammalian reticulocytes, in vitro).
>20 hours (yeast, in vivo).
>10 hours (Escherichia coli, in vivo).

Instability index:

The instability index (II) is computed to be 34.28
This classifies the protein as stable.

Aliphatic index: 88.79

Grand average of hydropathicity (GRAVY): -0.056


Lampiran 6. Hasil Alerginitas.

Bioinformatics tool for allergenicity prediction.

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Data sets
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AllerTOP v. 2.0

Bioinformatics tool for allergenicity prediction



Your sequence is:

PROBABLE NON-ALLERGEN

The nearest protein is:

[UniProtKB accession number O9HCU4](#)

defined as non-allergen

Lampiran 7. Hasil Antigenitas

VaxiJen3

Model selected: virus

Threshold for this model: 0.4

Your Sequence:

```

MTETIKVSESLHVAESHVTPLYQLICKN
KTWLQQSLNWPQFVQSEEDTRKTVQGNVMLH
QRGYAKFMIFKEDELIGVISFNRIEPLNKT
AETGYWLDESHQGGIISQALQALIHYYAQS
GELRRFVIRCRVDNPPQSNQVALRNGFILEGC
LKQAEFLNDAYDDVNLYARIIDSEAAAKQYI
KWPWYVAAYAEIRASANLAAYQIAPGQTGVA
AYGQTGVIADYAAAGVIADYNYKPGPGPMFI
FLLFLTSTSGSDGPGPGAYFVGYLKPTTFML
GPGGLYLTQDLFLPFYSNVGPGGGYQPYR
VVVLSFELLGPGPGRVVVLSPELLNAPATGP
GPGVSATKLNLDLCFSGPGPGPIDVRDLPSGF

```

#vaxijen/scripts/VaxiJen_scripts/VaxiJen3.pl 1/2

VaxiJen - predicting protective antigens

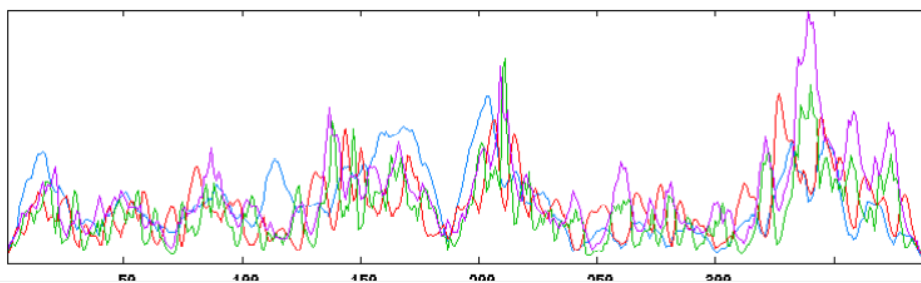
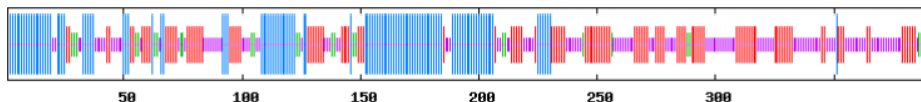
NGPGPGTGVADYNYKLP

Overall Prediction for the Protective Antigen = **0.5114** (Probable **ANTIGEN**).

Lampiran 8. Hasil SOPMA.

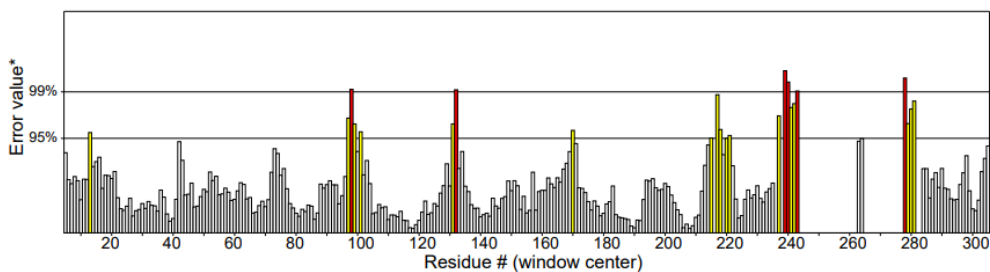
SOPMA :

Alpha helix (Hh) :	114 is	29.23%
3 ₁₀ helix (Gg) :	0 is	0.00%
Pi helix (Ti) :	0 is	0.00%
Beta bridge (Bb) :	0 is	0.00%
Extended strand (Ee) :	116 is	29.74%
Beta turn (Tt) :	25 is	6.41%
Bend region (Ss) :	0 is	0.00%
Random coil (Cc) :	135 is	34.62%
Ambiguous states (?) :	0 is	0.00%
Other states :	0 is	0.00%



Lampiran 9. Hasil ERRAT

Program: ERRAT2
 File: model1.pdb
 Chain#:A
 Overall quality factor**: 86.154



*On the error axis, two lines are drawn to indicate the confidence with which it is possible to reject regions that exceed that error value.

**Expressed as the percentage of the protein for which the calculated error value falls below the 95% rejection limit. Good high resolution structures generally produce values around 95% or higher. For lower resolutions (2.5 to 3Å) the average overall quality factor is around 91%.

Lampiran 10. Hasil Swiss Model

MolProbity Results		
MolProbity Score	2.61	
<input type="checkbox"/> Clash Score	139.06	(A60 MET-A60 MET), (A157 LYS-A157 LYS), (A62 HIS-A68 LYS), (A89 PRO-A92 LYS), (A361 GLY-A362 PRO), (A157 LYS-A168 ASP), (A280 GLY-A281 PRO), (A243 GLY-A244 PRO), (A150

<https://swissmodel.expasy.org/assess/5zyJRA/01>

4/26/22, 8:25 PM

model1.pdb | Structure Assessment

Ramachandran Favoured	98.71%	
Ramachandran Outliers	0.00%	
Rotamer Outliers	0.00%	
C-Beta Deviations	0	
<input type="checkbox"/> Bad Bonds	1 / 3093	A331 PHE
<input type="checkbox"/> Bad Angles	2 / 4217	A84 PHE, A150 PHE

Lampiran 11. Hasil Residu TLR 3



RESULTS from consPPISP job ID=020000200

1 pesan

<pi2pe.fsu@gmail.com>
 Kepada: firmansyahm0@gmail.com

Sel, 8 Mar 2022 pukul 12.03

Submission name: TLR
 Job submitted : Tue Mar 8 04:57:25 UTC 2022
 Job done : Tue Mar 8 05:03:46 UTC 2022

Prediction by cons-PPISP : consensus Protein-Protein Interaction Site Predictor

Column 1: AA (Amino Acid code)

Column 2: Ch (Chain ID)

Column 3: AA# (Amino Acid number)

Column 4: Score (neural network score)

Column 5: Prediction of whether the residue contacts

(P = Positive; N = Negative; - = Burried and not predicted)

```
*****
AA Ch AA# Score Prediction
E X 1 0.036 N
P X 2 0.088 N
C X 3 0.000 -
V X 4 0.878 P
E X 5 0.817 P
V X 6 0.087 N
V X 7 0.005 N
P X 8 0.045 N
N X 9 0.004 N
I X 10 0.005 N
T X 11 0.015 N
Y X 12 0.000 -
Q X 13 0.932 P
*****
```

Lampiran 12. Hasil Residu Desain Vaksin



RESULTS from consPPISP job ID=020000199

1 pesan

<pi2pe.fsu@gmail.com>
Kepada: firmansyahm0@gmail.com

Sel, 8 Mar 2022 pukul 11.44

Submission name: Ribosomal
Job submitted : Tue Mar 8 04:42:00 UTC 2022
Job done : Tue Mar 8 04:44:48 UTC 2022

Prediction by cons-PPISP : consensus Protein-Protein Interaction Site Predictor

Column 1: AA (Amino Acid code)

Column 2: Ch (Chain ID)

Column 3: AA# (Amino Acid number)

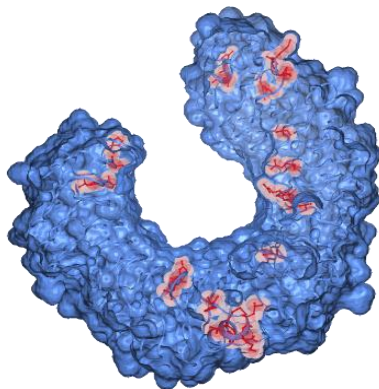
Column 4: Score (neural network score)

Column 5: Prediction of whether the residue contacts

(P = Positive; N = Negative; - = Burried and not predicted)

AA	Ch	AA#	Score	Prediction
M	A	1	0.953	P
T	A	2	0.931	P
E	A	3	0.982	P
T	A	4	0.985	P
I	A	5	0.986	P
K	A	6	0.361	N
V	A	7	0.073	N
S	A	8	0.009	N
E	A	9	0.058	N
S	A	10	0.097	N
L	A	11	0.000	-
E	A	12	0.041	N
L	A	13	0.000	-

Lampiran 13. Gambaran Letak Residu TLR 4



Lampiran 14. Gambaran Letak Residu Desain Vaksin

