



Prediction of Anti *P. acnes* peptides from various proteases hydrolyzed Riceberry rice bran

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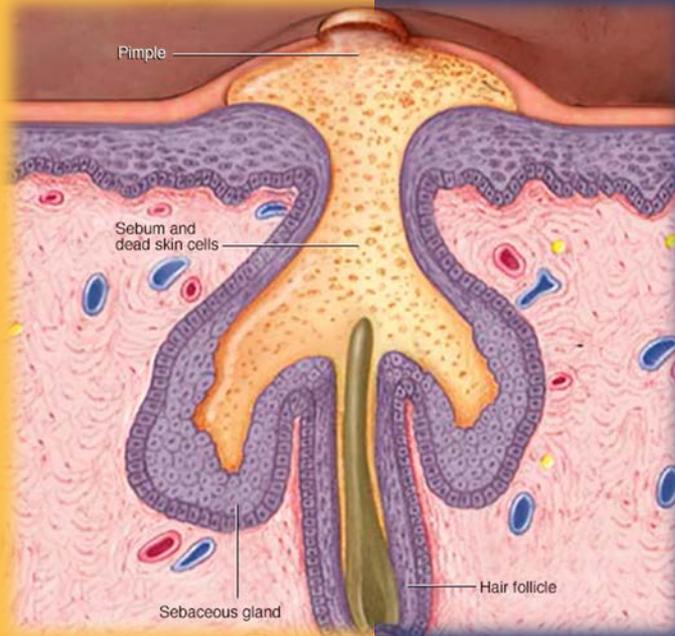
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INTRODUCTION



Acne vulgaris, caused by *P. acnes* infection, is one of the biggest problems in teenagers.



<https://www.mayoclinic.org/diseases-conditions/acne/symptoms-causes/syc-20368047>

<https://www.thailandmedical.news/pages/health/adult-acne---skin-disorders>



INTRODUCTION



<https://www.livescience.com/42400-clindamycin-uses-side-effects.html>



<https://www.pharmaceutical-technology.com/comment/acne-treatment-doxycyclines-side-effects-outweigh-benefits/>

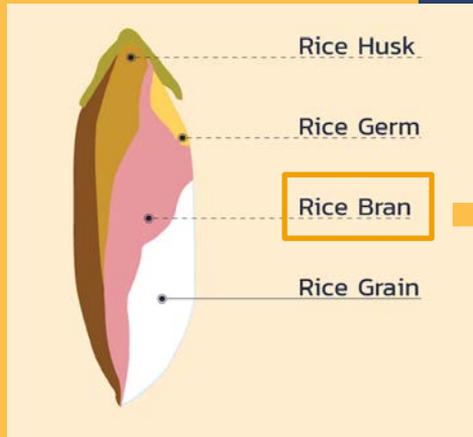
Nowadays, there are some reported cases of drug allergies and drug-resistant pathogenic microbes from chemicals and antibiotics, the major treatment drugs.



INTRODUCTION

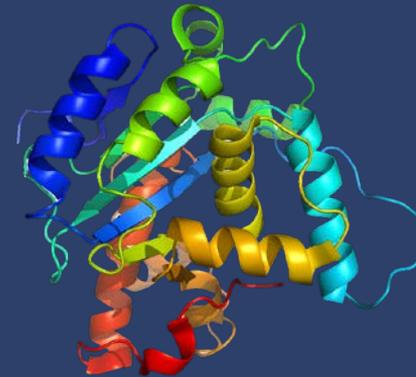


<https://th-test-11slaticnet/shop/a8eab45f2d42569fb35a67ba0266a5f6jpeg>



<https://www.wonnapob.com/images/factory/input-process/rice-anatomy-en.png>

Instead of acne drugs, natural compound and biomimetic molecules is required. The rice bran protein consists of Albumin, Glutelin, Globulin, Prolamin. (Wang & Xu & Li & Zhang, 2015).



<https://www.pngegg.com/en/png-bdnqz>



OBJECTIVES



To predict antibacterial peptides
from various proteases
hydrolyzed riceberry rice bran
using bioinformatics method





METHOD OUTLINE

Start

Protein sequences
Albumin/Globulin/Glutelin/Prolamin

In silico digest with Proteases
(Trypsin/Pepsin/Chymotrypsin)

Remove repeated sequences and
Screen for proper size (> 4 amino acid residues)
Size S (5-20), M (21-35), L (36-50)

Predict Antibacterial Activity and Toxicity

iAMP

DBAASP

ToxinPred



Predict Mode of Action

CellIPPD

QSPpred

dPABBs

Multifunctional Analysis

Venn diagram

Composition analysis
and Secondary structure prediction

COPID

PEP-FOLD3.5

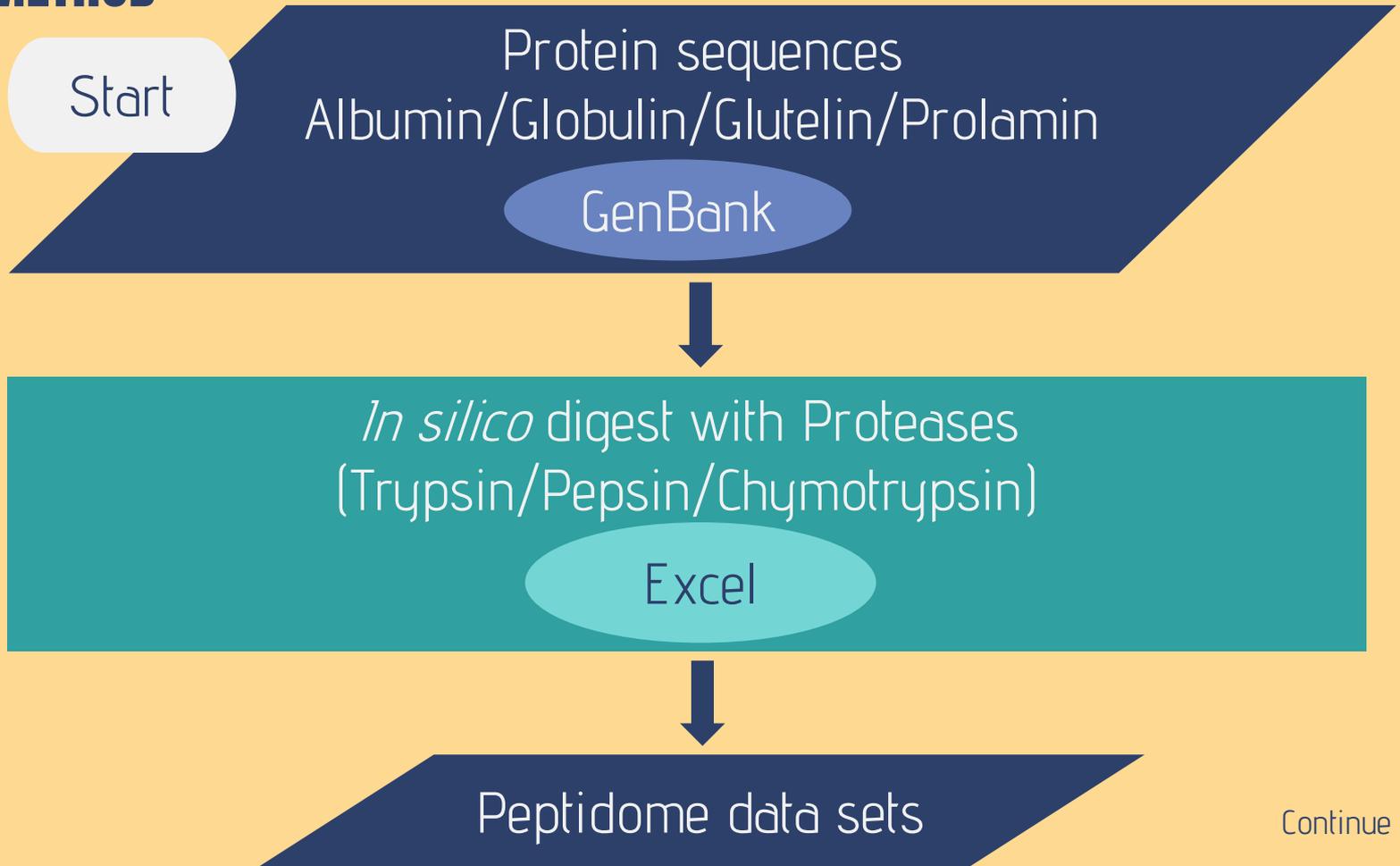
The best peptides

BEST

End



METHOD



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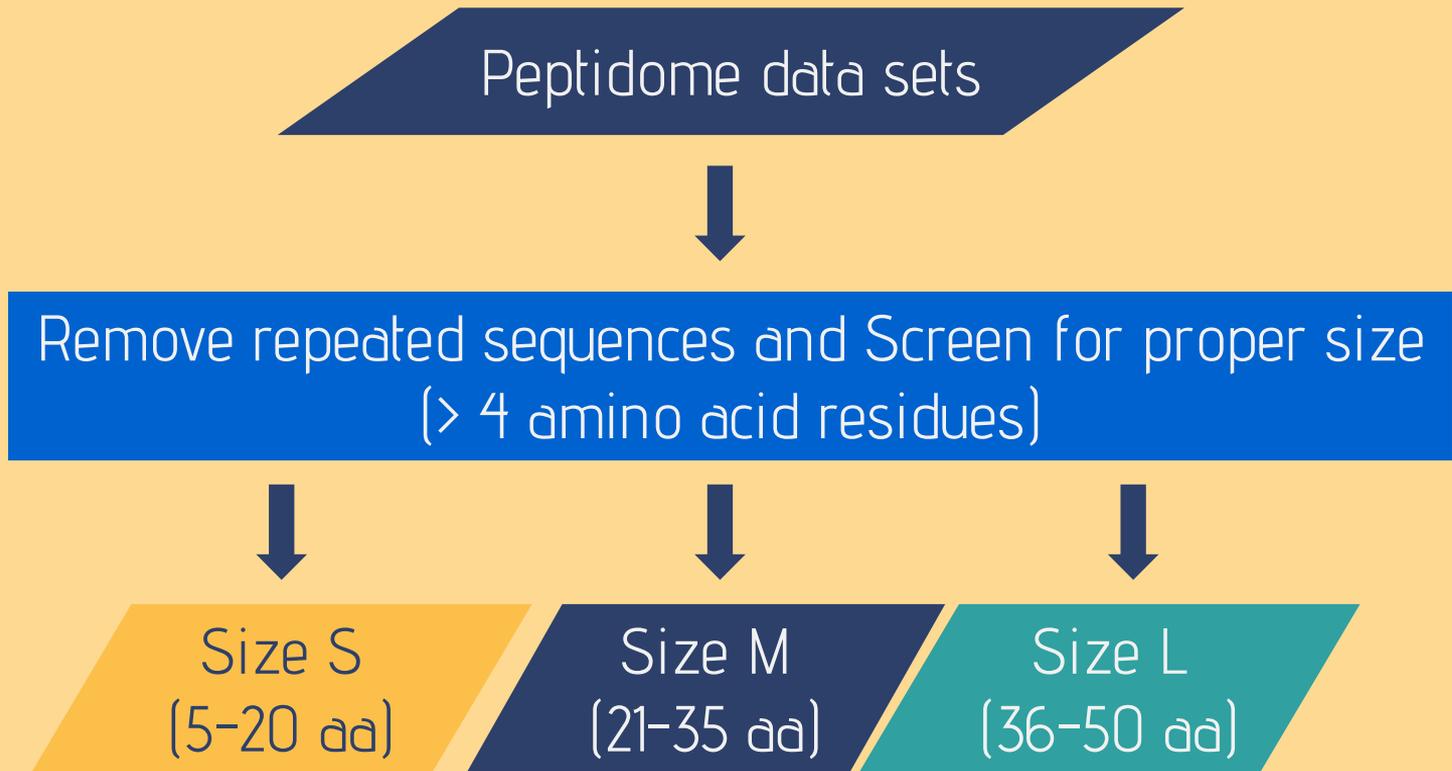
RESULTS

Number of peptidome in each data set (peptide sequences)

Protein Protease	Albumin	Glutelin	Globulin	Prolamin
Pepsin	24	74	83	16
Trypsin	16	49	67	7
Chymotrypsin	22	72	58	27



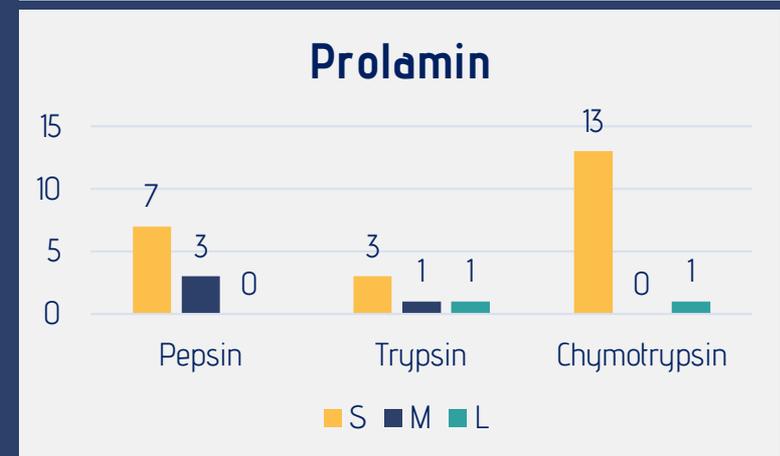
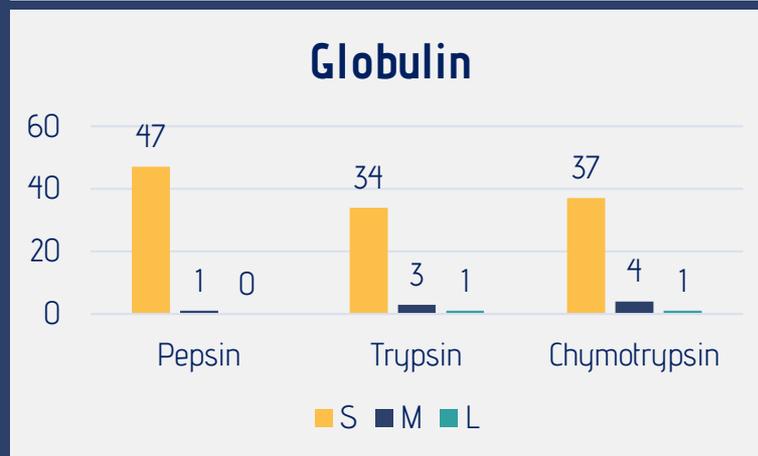
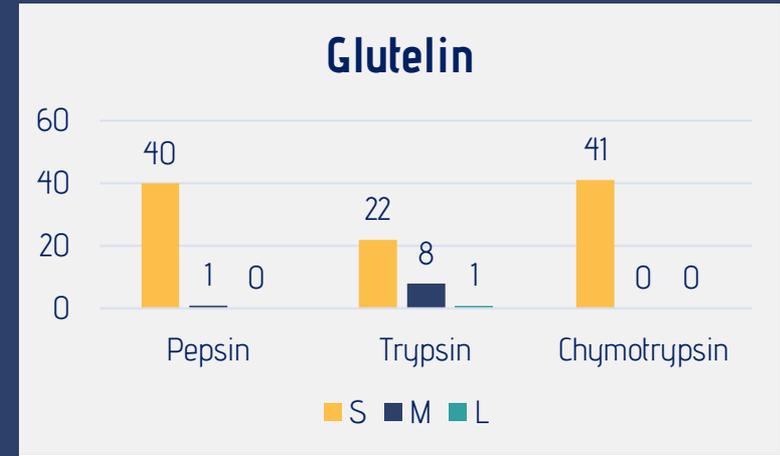
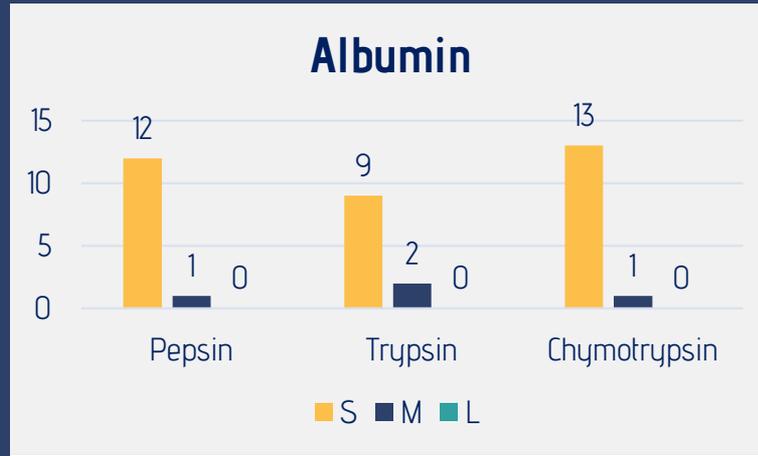
METHOD



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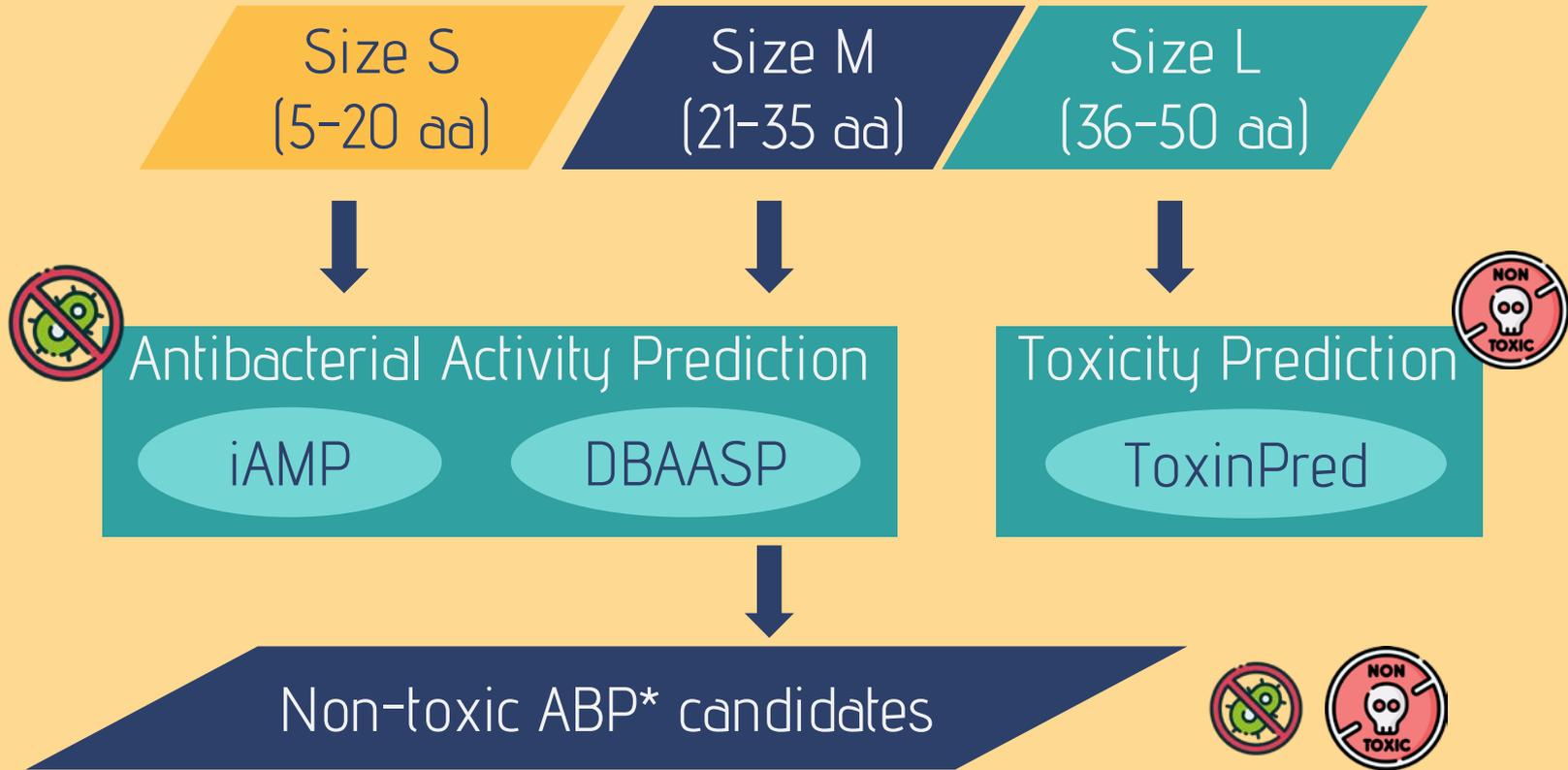


RESULTS No. of peptidome in each data set (peptide sequences)





METHOD

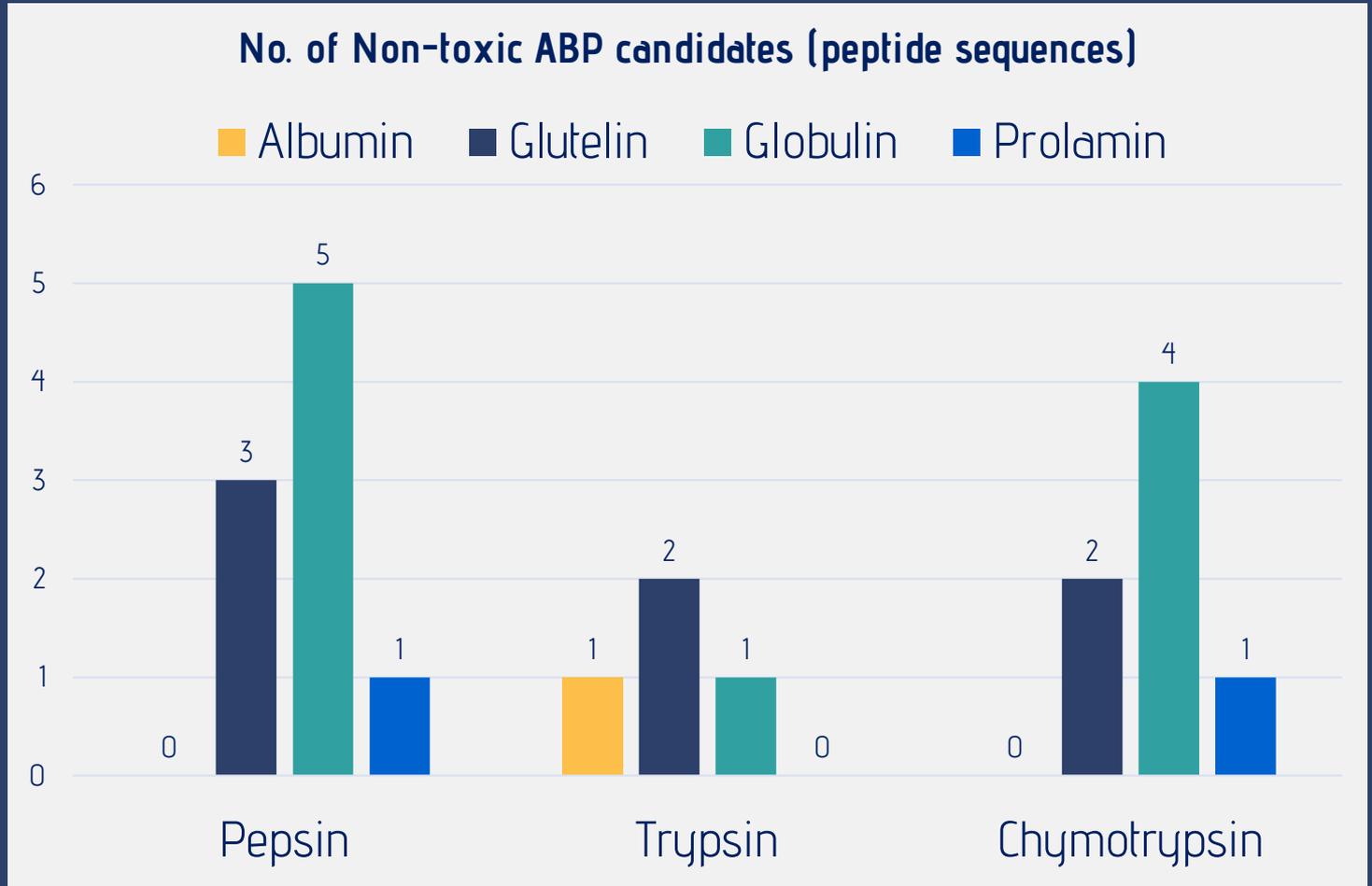


ABP = Antibacterial peptide

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RESULTS & DISCUSSION





METHOD

Non-toxic ABP candidates



Predict
Mode of Action

Anti-biofilm
Activity Prediction

dPABBs

Cell Penetration
Activity Prediction

CellPPD

Anti-Quorum Sensing
Prediction

QSPpred

1

ABP

2

Anti-biofilm

3

Cell
Penetration

4

Anti-Quorum
Sensing

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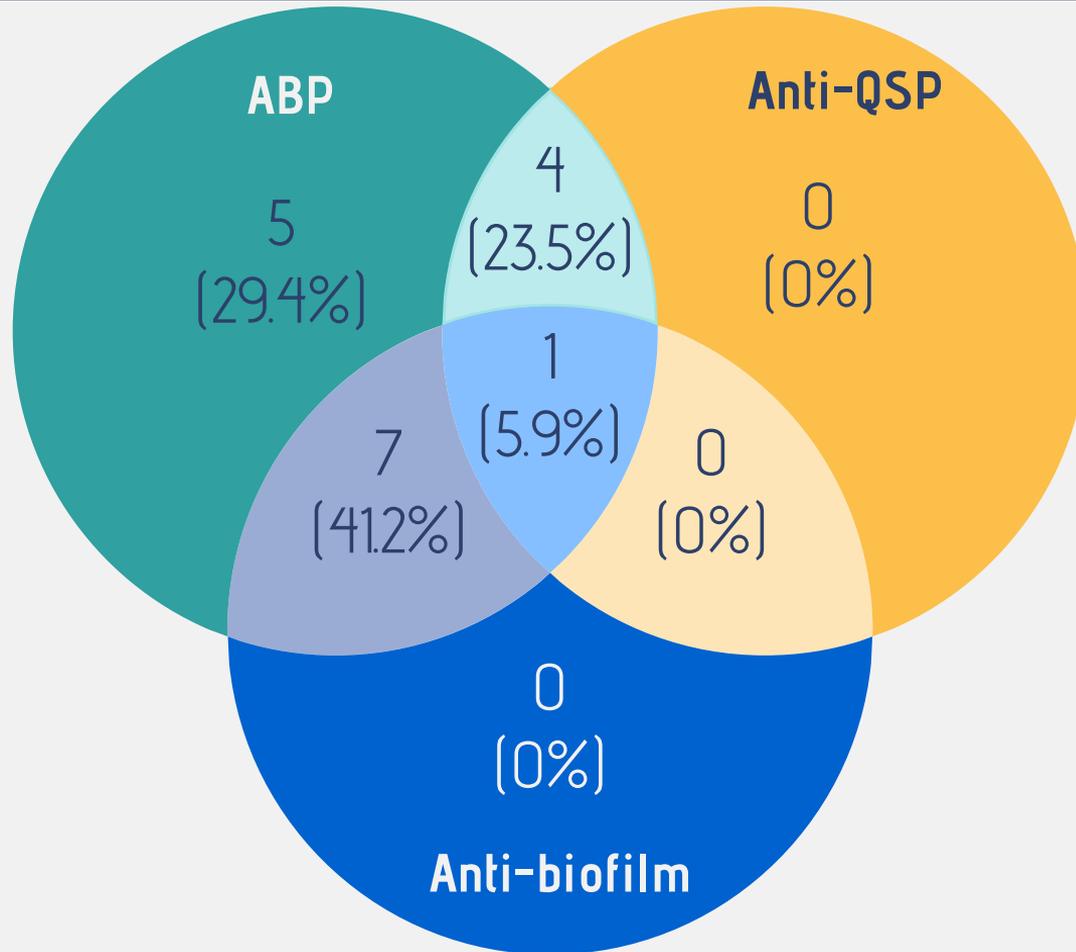


METHOD





RESULTS - Multifunctional analysis





RESULTS - Multifunctional analysis

- 1 ABP (5 peptides) :
- LLPPFHQASSLLR
 - TNPNSMVSHIAGK
 - ANTDGRRKL
 - SKGVQRAAF
 - TSLRRCLQRCE

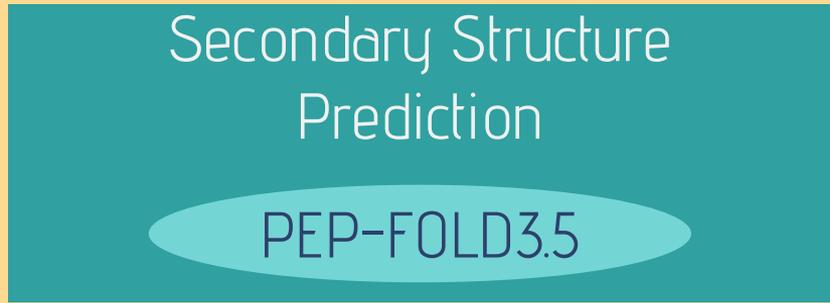
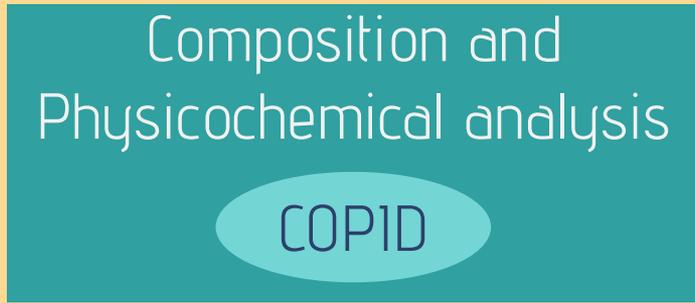
- 3 ABP + Anti-Quorum Sensing (4 peptides) :
- MKIIF • RG1KNY
 - SSIFR • IVTKIL

- 2 ABP + Anti-biofilm (7 peptides) :
- KLLGKQD
 - AVVKKAQRE
 - ITQGRARVQVVNNNGKTVF
 - NPRAGRVTNL
 - CSALNHMVGGIYR
 - GRRKLIVTKILHTISVPGQIQF
 - LAGMNSVLKKLD

- 4 ABP + Anti-biofilm + Anti-Quorum Sensing (1 peptide) :
- HQKIHRF



METHOD





METHOD



The best peptides and
their composition and
physicochemical properties

End



RESULTS - ABP (Helix 4 + Random coil 1)

Helix – 13 aa



LLPPFHQASSLLR
(Globulin cut with Trypsin)

Helix – 13 aa



TNPNSMVSHIAGK
(Glutelin cut with Trypsin)

Random Coil – 9 aa



ANTDGRRL
(Globulin cut with Chymotrypsin)

Helix – 9 aa



SKGVQRAAF
(Globulin cut with
Chymotrypsin or Pepsin)

Helix – 11 aa



TSLRRCLQRCE
(Globulin cut with Pepsin)



RESULTS - ABP + Anti-biofilm (Helix 4 + Random coil 2 + Beta sheet 1)

Random Coil – 19 aa



ITQGRARVQVVNNNGKTVF
(glutelin chymotrypsin pepsin)

Helix – 9 aa



AVVKKAQRE
(glutelin pepsin)

Beta Sheet – 10 aa



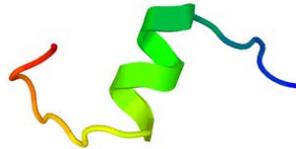
NPRAGRVTNL
(glutelin chymotrypsin)

Helix – 13 aa



CSALNHMVGGI4R
(albumin trypsin)

Helix – 22 aa



GRRKLIVTKILHTISVPGQIQF
(globulin pepsin)

Helix – 12 aa



LAGMNSVLKKLD
(globulin pepsin)

Random Coil – 7 aa



KLLGKQD
(globulin pepsin)



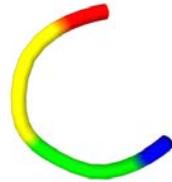
RESULTS & DISCUSSION - ABP + Anti-biofilm (Helix 4 + Random coil 2 + Beta sheet 1)

Peptide sequences	Score	Hydrophobicity	Amphipathicity	Hydrophilicity	Charge
ITQGRARVQVVNNNGKTVF	0.57	-0.22	0.58	-0.08	+3.00
AVVKKAQRE	0.53	-0.41	1.37	0.91	+2.00
NPRAGRVTNL	0.03	-0.36	0.49	0.22	+2.00
CSALNHMVGGI4R	0.30	-0.03	0.30	-0.55	+1.50
 GRRKLIVTKILHTISVPGQIQF	1.20	-0.10	0.74	-0.22	+4.50
LAGMNSVLKKLD	0.17	-0.09	0.61	0.07	+1.00
KLLGKQD	0.31	-0.34	1.23	0.80	+1.00



RESULTS - ABP + Anti-Quorum Sensing (Random coil 4)

Random Coil – 5 aa



MK11F
(prolamin chymotrypsin pepsin)

Random Coil – 5 aa



SS1FR (glutelin trypsin)

Random Coil – 6 aa



RG1KN4
(globulin chymotrypsin)

Random Coil – 6 aa



IVTKIL
(globulin chymotrypsin)

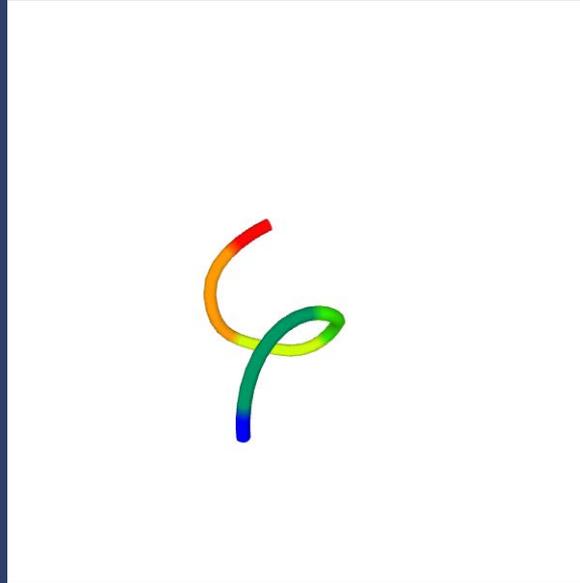


RESULTS & DISCUSSION - ABP + Anti-Quorum Sensing (Random coil 4)

Peptide sequences	Score	Hydrophobicity	Amphipathicity	Hydrophilicity	Charge
 MKIIF	11	0.25	0.73	-0.88	+1.00
SSIFR	9	-0.19	0.49	-0.14	+1.00
RGIKN ₄	9	-0.43	1.02	0.35	+2.00
IVTKIL	8	0.21	0.61	-0.72	+1.00



RESULTS - ABP + Anti-biofilm + Anti-Quorum Sensing



HQKIHRF

(Glutelin cut with Pepsin)

- random coil
- 7 aa sequences (size s)
- Hydrophobicity : -0.43
- Amphipathicity : 1.47
- Hydrophilicity : 0.13
- Charge : 3.00



CONCLUSION

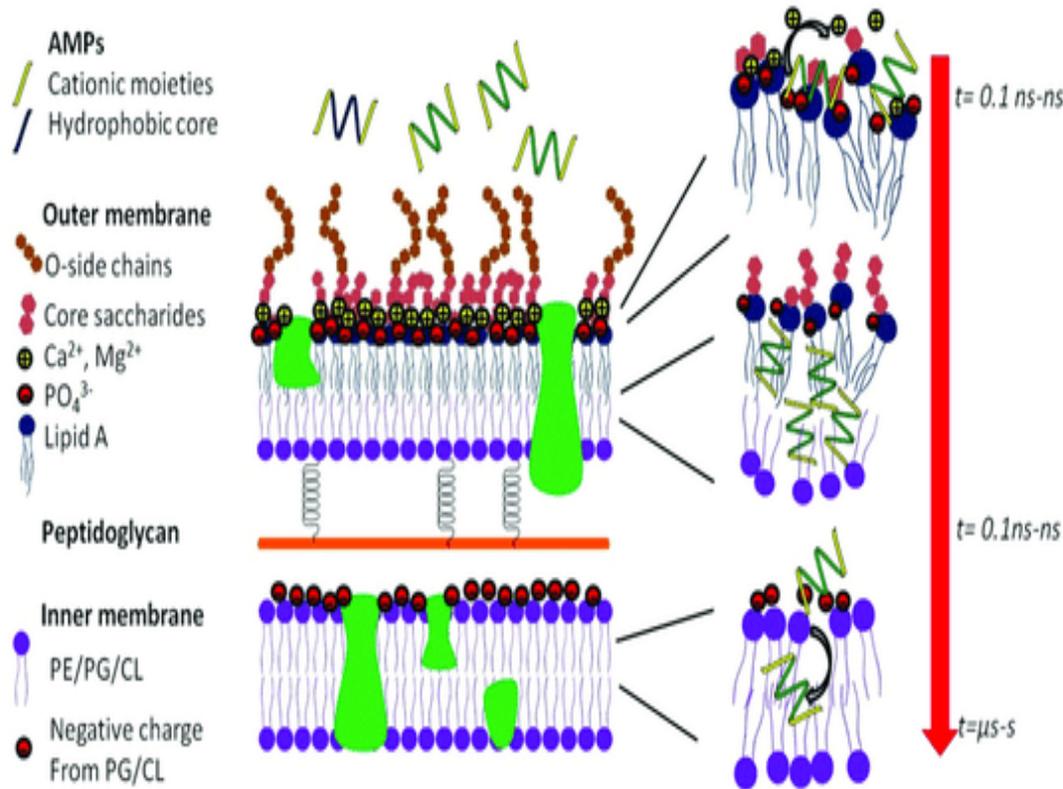
ABP properties

- Net charge is positive
- Helix / Random Coil
- 5-22 aa sequences (size s & m)
- Amino sequences : Isoleucine leucine lysine Arginine
- Most of amino acid are Non-Polar, Positive charge



DISCUSSION

(Malanovicand & Lohner, 2016)

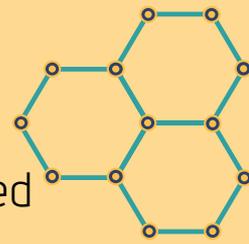


Properties :

- % hydrophobic residues = 31-50
- Positive charge
- 10-50 amino acid



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THANK YOU FOR YOUR ATTENTION