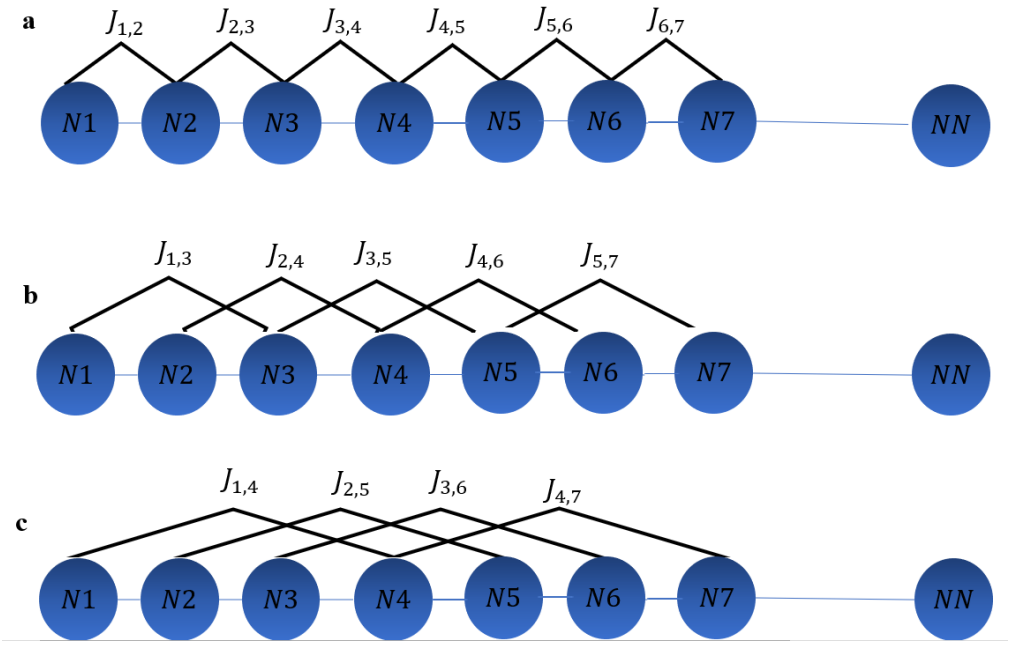
Supplementary Information

Amino acid groups and distributions based on charge, hydrophobicity, normalized van der Waals volume, polarity, polarizability, secondary structure, and solvent accessibility are presented in Appendix 1.

Appendix 1. Division of amino acids in to three groups based on their physicochemical properties

Property	**Class 1**	**Class 2**	**Class 3**
Charge	**Neutral**	**Negatively charged**	**Positively charged**
Residues	*A, C, F, G, H, I, L, M, N, P, Q, S, T, V, W, Y*	*D, E*	*K, R*
Hydrophobicity	**Hydrophobic**	**Neutral**	**Polar**
Residues	*C, F, I, L, M, V, W*	*A, G, H, P, S, T, Y*	*D, E, K, N, Q, R*
Normalized van der Waals volume	**Volume range: 0-2.78**	**Volume range: 2.95-4.0**	**Volume range: 4.03-8.08**
Residues	*A, C, D, G, P, S, T*	*E, I, L, N, Q, V*	*F, H, K, M, R, W, Y*
Polarity	**Polarity range: 4.9-6.2**	**Polarity range: 8.0-9.2**	**Polarity range: 10.4-13.0**
Residues	*C, F, I, L, M, V, W, Y*	*A, G, P, S, T*	*D, E, H, K, N, Q, R*
Polarizability	**Polarizability range: 0 - .108**	**Polarizability range 0.128-0.186**	**Polarizability range 0.219-0.409**
Residues	*A, D, G, S, T*	*C, E, I, L, N, P, Q, V*	*F, H, K, M, R, W, Y*
Secondary Structure	**Coil**	**Helix**	**Strand**
Residues	*D, G, N, P, S*	*A, E, H, K, L, M, Q, R*	*C, F, I, T, V, W, Y*
Solvent Accessibility	**Buried**	**Intermediate**	**Exposed**
Residues	*A, C, F, G, I, L, V, W*	*H, M, P, S, T, Y*	*D, E, K, N, R, Q*



Appendix 2. Schematic presentation of the a) first-ranked, all the most contiguous residues, b) second-ranked, the second most contiguous residues, and c) third-ranked, the third most contiguous residues sequence-order-coupling model in peptide sequences with length equal to N.

A list of global and peptide descriptors and their definitions are summarized in Appendix 3.

Appendix 3. Summary of Global and pepdescriptors

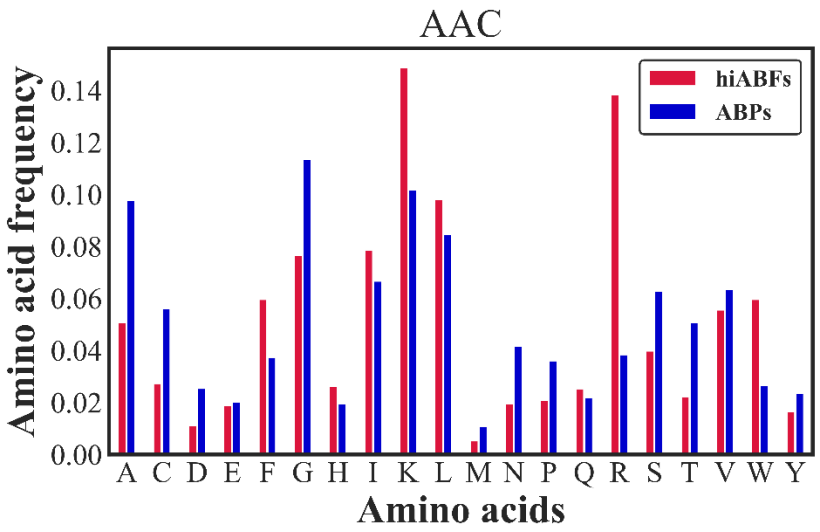
Features	Description
Aromaticity	This feature is calculated based on the relative frequency of amino acids with aromatic R groups; Phenylalanine+Tyrosine+Tryptophan (1).
Aliphatic Index	Aliphatic index is based on the correlation between thermal stability and the aliphatic index of a protein. This descriptor is calculated based on the frequency of the alanine, Valine, Leucine and Isoleucine. Aliphatic index = X(Ala)+a X(Val)+b X(Ile)+X(Leu), where X represents the molar percentage of these amino acids, a and b is the side chain volume of the Valine, Leucine and Isoleucine. For Val a = 2.9 and for Leu and Ile b = 3.9 (2).
Boman Index	This index is based on protein-protein interaction. Indeed, high Boman index indicates that the peptide has a high potential for interaction with other proteins (3).
Hydrophobic Ratio	This feature is calculated based on the relative frequency of Ala, Cys, Phe, Ile, Leu, Met, Val (4).
Hydrophobicity	This descriptor is calculated based on Argos, Hopp-woods, Janin, Gravy, Kyte-Doolittle, and Eisenberg hydrophobicity scale (5–9).
Instability Index	By studying several stable and unstable proteins, Guruprasad *et al*. found that some dipeptides in unstable proteins are significantly different from stable proteins. Based on their effects on protein instability, an instability index is assigned for each. Summation of these indexes normalized on the protein sequences and used as a benchmark for a protein or peptide instability (10).
Length	Peptide sequences length
Molecular weight	MW of peptide sequences
Charge	NetCharge, Calculates charge of peptides sequence at pH 7.4, charge_pysc and charge_acid calculates amino acid charge at pH 7 and acidic pH respectively (11).

Charge density	Calculated by dividing charge by molecular weight
Isoelectric point	A pH of a solution that a net charge of a peptide sequence is zero
Bulkiness	This feature is calculated based on amino acid side chain bulkiness (12)
Insertion	E(z) is a residue-based potential for calculating the amino acid side chain insertion propensity into the lipid bilayer (13)
α-helix propensity	This descriptor is obtained based on Levitt amino acid alpha helix propensity. Statistical studies of proteins of the known structure have shown that amino acids have clear conformational preferences for one type of secondary structure (14).
Flexibility	Amino acid side chain flexibility scale (11).
Side chain composition, polarity, molecular volume	Mainly two methods are used to calculate these features: The Grantham method that analyzed amino acid formulation to explain protein evolution, and a PCA-derived scale based on amino acid side chain that uses six different probes from GRID program (15,16).
Isotropic surface area (ISA) Electronic charge index (ECI)	ISA and ECI are used as descriptor for amino acids side chains. ISA is the molecule's surface accessible to nonspecific interactions with the solvent; the molecule's surface involved in specific hydrogen bonding with water is not considered. ECI is a measure of molecular polarity (17).
Polarity	This feature is based on amino acid polarity scale (11).
Refractivity	The refractive index of each amino acid was calculated by McMeekin *et al*. For each protein or peptide, their refractivity is estimated based on the refractive index of each amino acid (11,18).
Selectivity	In modlamp, this feature is calculated based on Juretic *et al*.'s method. Their study has been done on antimicrobial peptides' data and assessing their selectivity (19).
Topology	The topological shape and size of the amino acid side chain are calculated based on graph theory and weighted connected graph model of amino acid side chain (20).
Side chain conformation and rotamer	This descriptor is derived from principal component analysis (PCA) applied to MS-WHIM 3D-description matrices. MS-WHIM indexes are a collection of 36 statistical indexes to extract a molecule's steric and electrostatic 3D properties. Zaliani *et al*. extended MS-WHIM to natural amino acid's side-chain conformation and the rotamer library. Modlamp calculates this feature with MSW function(11,21).
Transmembrane propensity	TM propensity is based on hydrophobicity analysis of transmembrane proteins of known structure (22).
Z-Scale	These features are based on PCA on 26 peptide descriptors, including NMR, TLC, formation heat, absolute electronegativity, etc. Principal properties were calculated and mainly reflected lipophilicity, steric and electrostatic properties. In modlamp, these descriptors are calculated by Z-Scale function (23).
Pharmacophoric features	PepArc is pharmacophoric feature based on hydrophobicity, polarity, positive charge, negative charge and proline. PPCALI is a descriptor obtained by PCA on 143 amino acids physicochemical properties and pepCAT is based on pharmacophoric features of side chains (24).

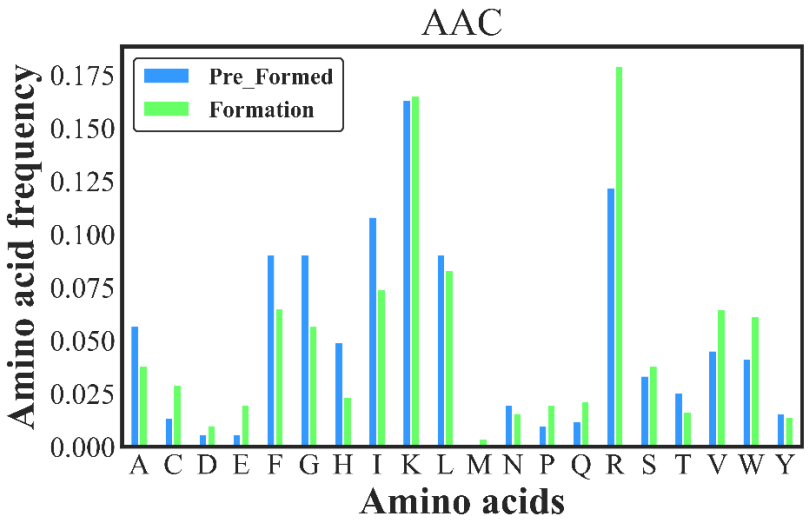
Appendix 4. Amino acids' R-group properties

Amino acids	**Properties**
Glycine (Gly, G)	Nonpolar aliphatic R-group
Alanine (Ala, A)	
Proline (Pro, P)	
Valine (Val, V)	

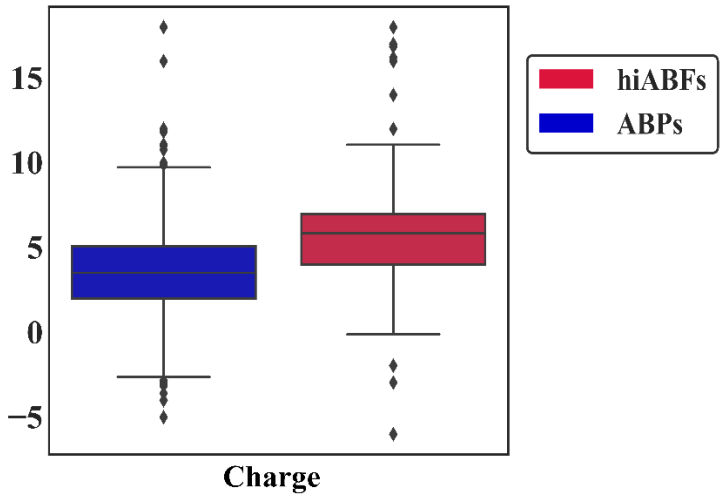
Leucine (Leu, L)	
Isoleucine (Ile, I)	
Methionine (Met, M)	
Lysine (Lys, K)	Positively charged R-group
Arginine (Arg, R)	
Histidine (His, H)	
Phenylalanine (Phe, F)	Aromatic R-group
Tyrosine (Tyr, Y)	
Tryptophan (Trp, W)	
Aspartate (Asp, D)	Negatively charged R-group
Glutamate (Glu, E)	
Serine (Ser, S)	Polar, uncharged R-group
Threonine (Thr, T)	
Cysteine (Cys, C)	
Asparagine (Asn, N)	
Glutamine (Gln, Q)	



Appendix 5. Comparison between amino acid frequencies between hiABFs and ABPs



Appendix 6. Comparison between amino acid frequencies between preformed and Formation group.

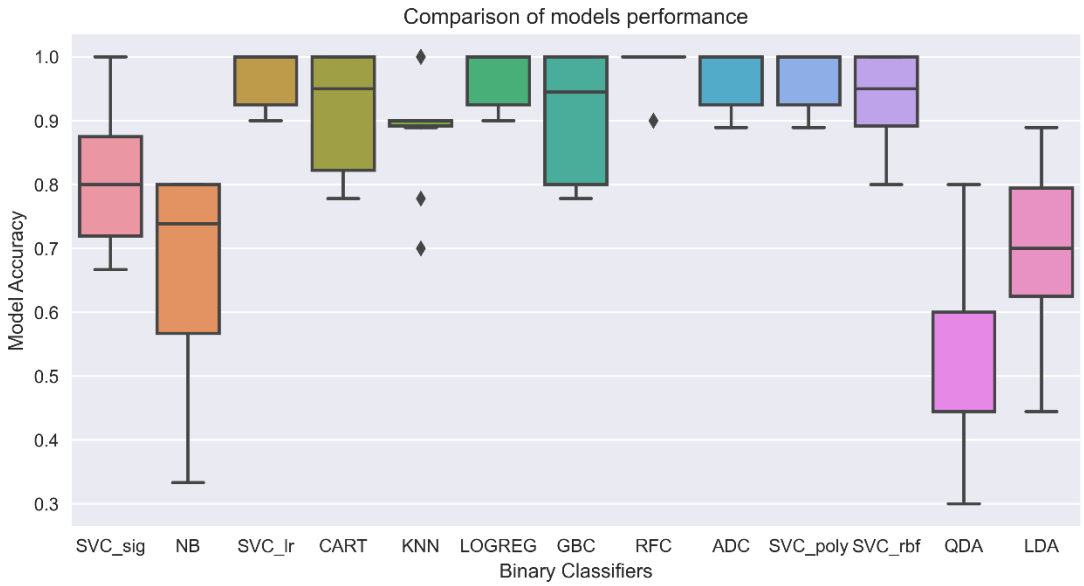


Appendix 7. Comparison of charge between Antibacterial Peptides (ABPs) and Antibiofilm Peptides (ABFs).

The performance metrics of binary classifiers on training and validation data with ten-fold cross-validation are presented in Appendix 8 and Appendix 7.

Appendix 8. Binary classifiers' performance metrics, Based on 10-fold cross validation

Classifier	CV (std)	A	P	R	MCC	CK	ROC-AUC score	F1-score
LOGREG	2.29%	99%	99%	99%	97.18%	97.18%	98.59%	99%
		93%	93%	92%	82.92%	82.61%	90.71%	93%
CART	5.85%	92%	90%	90%	84.31%	83.96%	92.46%	90%
		83.5%	83%	80%	65.47%	65.22%	82.14%	80%
RF	2.07%	99%	99%	99%	98.60%	98.59%	99.21%	99%
		94%	94%	94%	87.13%	87.05%	93.21%	93%
GBC	2.78%	97%	97%	97%	96.47%	96.47%	98.19%	98%
		85%	83%	81%	69.95%	69.34%	83.93%	82%
ADC	3.10%	97%	96%	96%	95.92%	95.92%	96.9%	96%
		91%	92%	91%	80.23%	80.35%	91.43%	92%
LDA	8.31%	75%	70%	71%	51.01%	50.65%	75.71%	74%
		75%	74%	60%	48.08%	46.27%	72.14%	70%
QDA	9.23%	61%	60%	61%	22.53%	22.31%	61.24%	60%
		55%	60%	55%	4.93%	4.83%	52.5%	50%
NB	11.93%	72%	70%	75%	44.60%	43.64%	72.40%	71%
	17.78%	67%	62%	62%	37.14%	35.14%	68.57%	67%
SVC_lr	2.29%	99%*	98%	98%	97.18%	97.18%	98.59%	98%
		93%	93%	93%	82.86%	82.86%	91.43%	93%
SVC_rbf	3.18%	98%*	99%	98%	96.48%	96.48%	98.28%	98%
		93%	94%	95%	88.79%	88.10%	93.21%	92%
SVC_poly	2.29%	99%*	99%	99%	97.18%	97.18%	98.59%	99%
		92%	92%	94%	87.79%	87.60%	92.21%	92%
SVC_sig	3.17%	97%	97%	97%	95.77%	97.88%	97.88%	96%
		85%	82%	82%	70.66%	68.89%	83.21%	80%
KNN	5.37%	90%	90%	90%	83.05%	82.98%	91.27%	91%
		91%	90%	90%	83.67%	82.35%	90%	91%



Appendix 9. Comparison of classifiers' performance based on Accuracy

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