

DATABASE OF ANTIMICROBIAL ACTIVITY AND STRUCTURE OF PEPTIDES (DBAASP) – FINDING A WAY OUT OF MICROBIAL RESISTANCE

Presenter: Evgenia Alimbarashvili

Co-authors: N. Samsonidze, M. Grigolava, M. Pirtskhalava

Affiliation: Ivane Beritashvili Center of Experimental Biomedicine, Tbilisi, Georgia

TOPICS



Microbial resistance



Antimicrobial peptides



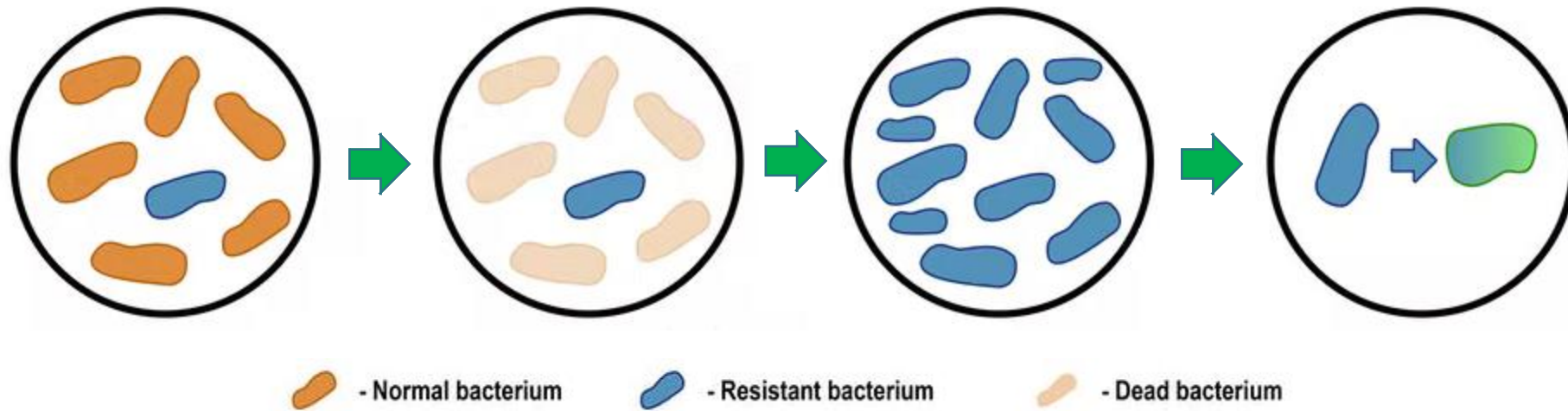
DBAASP



Synergy

MICROBIAL RESISTANCE

Microorganisms are becoming unresponsive to conventional antimicrobial agents

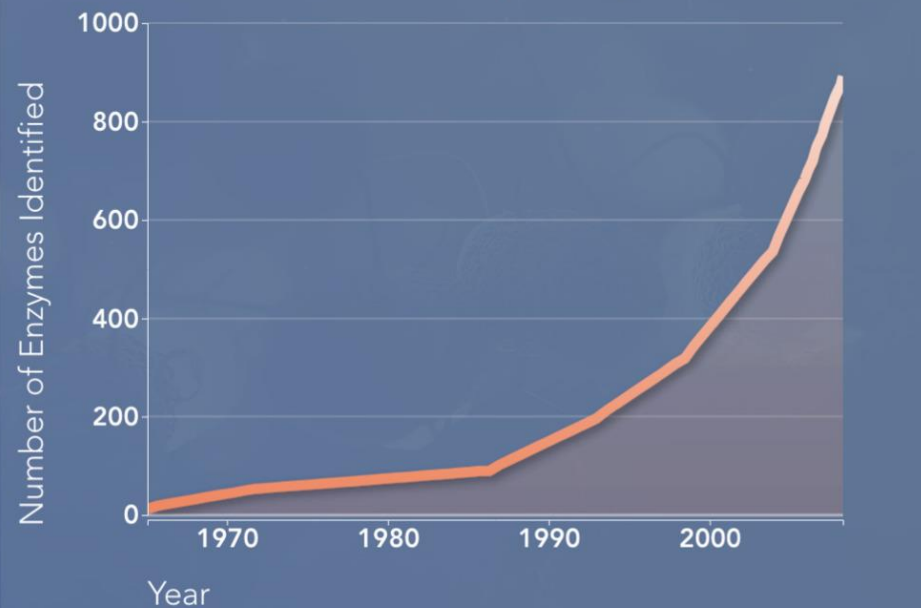


MICROBIAL RESISTANCE

Increasing Antibiotic Resistance

Bacteria have rapidly evolved and developed proteins to resist and destroy antibiotics

Antibiotic Resistance Enzymes (β -lactamase)



Clearvue Health

CDC

New Antibiotic Approvals

While antibiotic resistance rises, fewer new antibiotics are being developed and approved.



Clearvue Health

Ventola et al.

ANTIMICROBIAL PEPTIDES

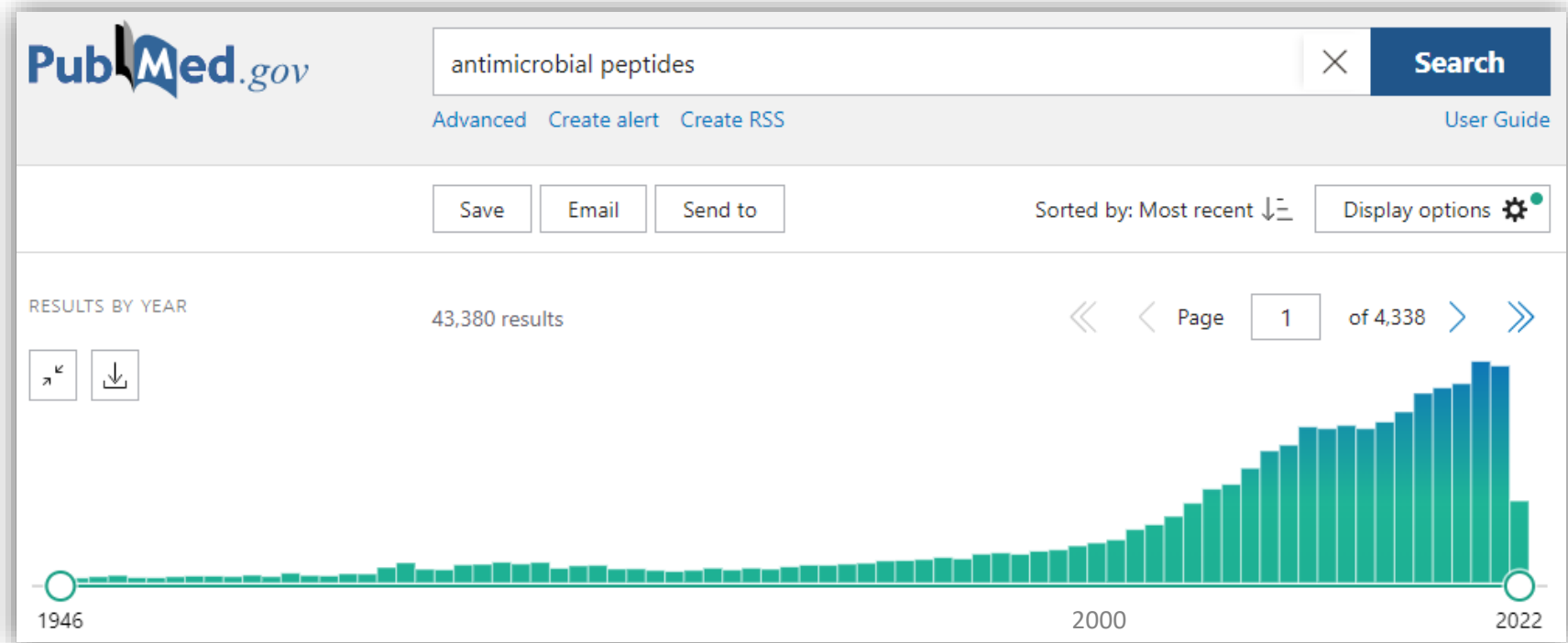
Diverse group of naturally occurring molecules



Cecropin (hybrid peptide)



Hyalophora cecropia

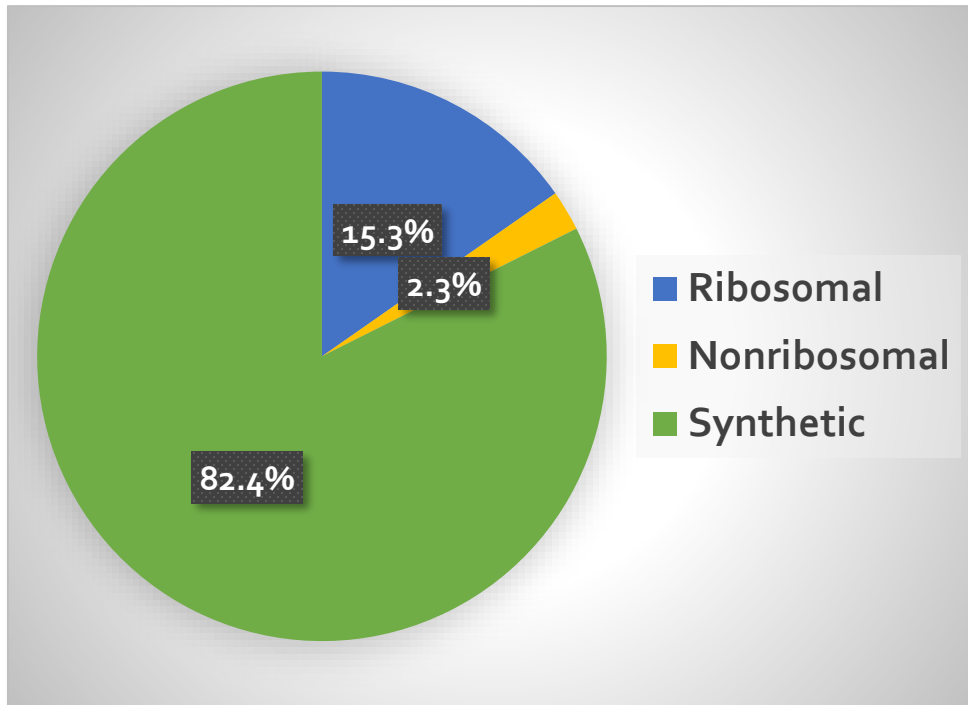


DBAASP

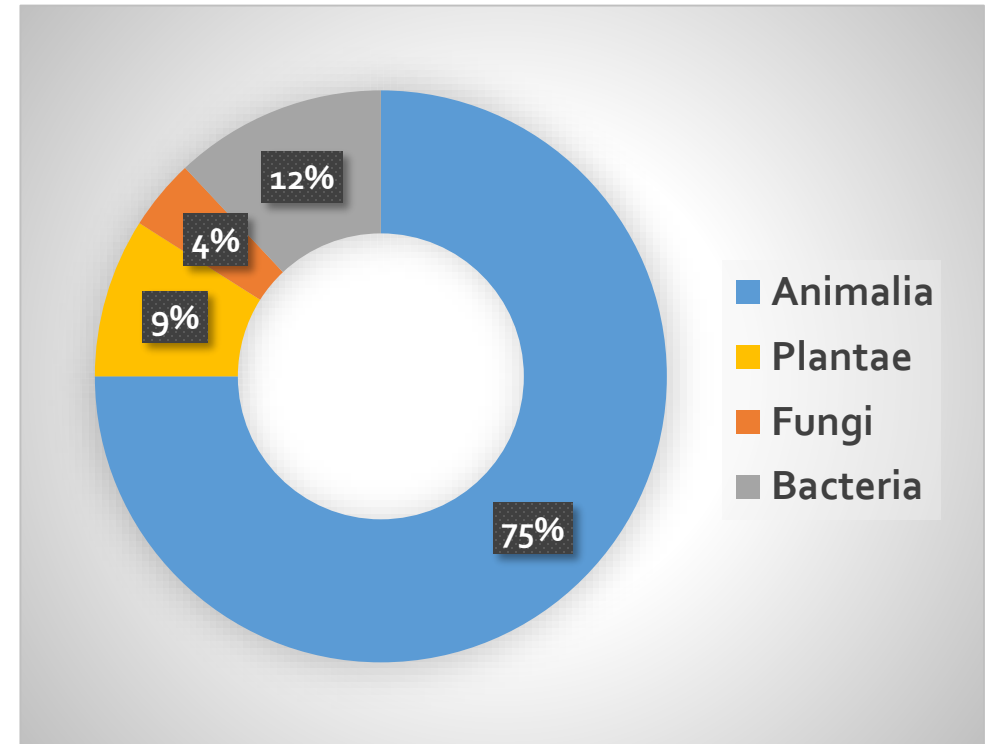
Database of Antimicrobial Activity and Structure of Peptides

Number of Peptides: >19 000

Synthesis Type

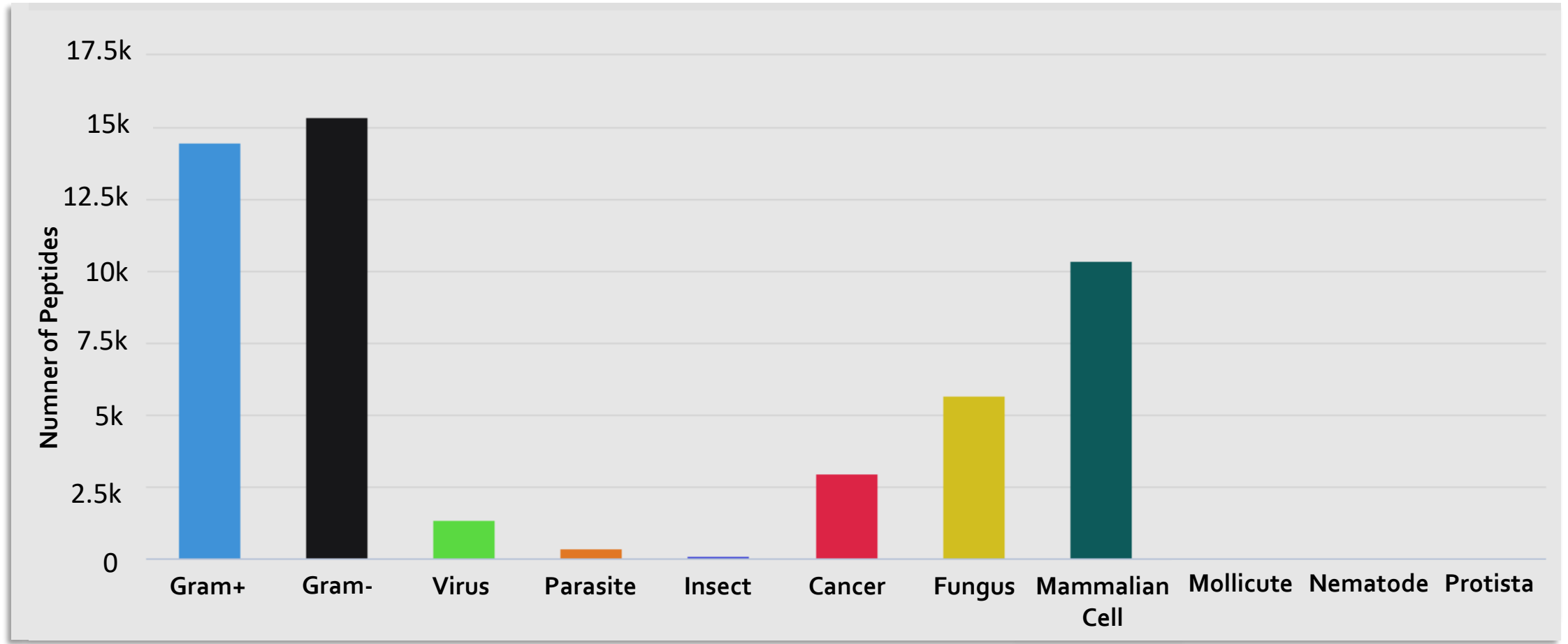


Source Organisms



DBAASP

Target Groups of Organisms



DBAASP PEPTIDE CARD

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General Information

ID : DBAASPR_491

Name : Cathelicidin-4, Indolicidin

Synthesis Type : Ribosomal ?

Complexity : Monomer ?

Target Group : Gram+, Gram-, Virus, Parasite, Cancer, Fungus, Mammalian Cell

Target Object : Lipid Bilayer, Virus Integrase, Virus replication

Note :

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Chemical Structure

Sequence

ID	N terminus	Sequence	C terminus	Length
DBAASPR_491		ILPWKWPWWPWRR	AMD	13

Databases of Chemical structures and Functions

Uniprot

Name	Uniprot ID
Precursor ?	P33046

PubChem - [90478486](#)

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Source ?

Kingdom	Subkingdom	Source	Gene	NCBI	Note
Animalia	Eumetazoa	Bos taurus	CATHL4	NCBI	

DBAASP PEPTIDE CARD

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Physico-Chemical Properties

Normalized Hydrophobicity	Net Charge	Isoelectric Point	Penetration Depth	Tilt Angle	Disordered Conformation Propensity	Linear Moment	Propensity to in vitro Aggregation	Angle Subtended by the Hydrophobic Residues	Amphiphilicity Index	Propensity to PPII coil
1.07	4.00	14.00	15	72	-0.32	0.57	0.00	20.00	3.32	1.28

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3D Structure

MD Structural Model

MD Structural Model

Representative structure	View	Download
Molecular Dynamics Trajectory	View	Download(DCD) Download(PSF)
Self-consistency	View	Download
Secondary structure	View	Download

Structural Databases

PDB : 1G8C [View](#)

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Family and Domain

Family and Domain Databases

Prosite: [Prosite Results Viewer](#)

DBAASP PEPTIDE CARD

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Activity Against Target Species ?

Target Species	Activity Measure	Activity	Unit	pH	Ionic Strength mM	Salt Type	Medium	CFU	Note	Reference
Staphylococcus aureus ATCC 259 23	MIC	8	µg/ml				LBB	1E5		1
Staphylococcus aureus SAP 0017	MIC	8	µg/ml				LBB	1E5	MRSA clinical isolate	1, 21
Enterococcus faecalis ATCC 2921 2	MIC	>64	µg/ml				LBB	1E5		1
Listeria monocytogenes NCTC 79 73	MIC	4	µg/ml				LBB	1E5		1

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Hemolytic and Cytotoxic Activities ?

Target Cell	Activity Measure for Lysis	Peptide Concentration	Unit	Note	Reference
Human erythrocytes	5% Hemolysis	50	µg/ml		3
Human erythrocytes	50% Hemolysis	254	µg/ml		9

DBAASP PEPTIDE CARD

9 Synergy Between Current Peptide and Antimicrobials

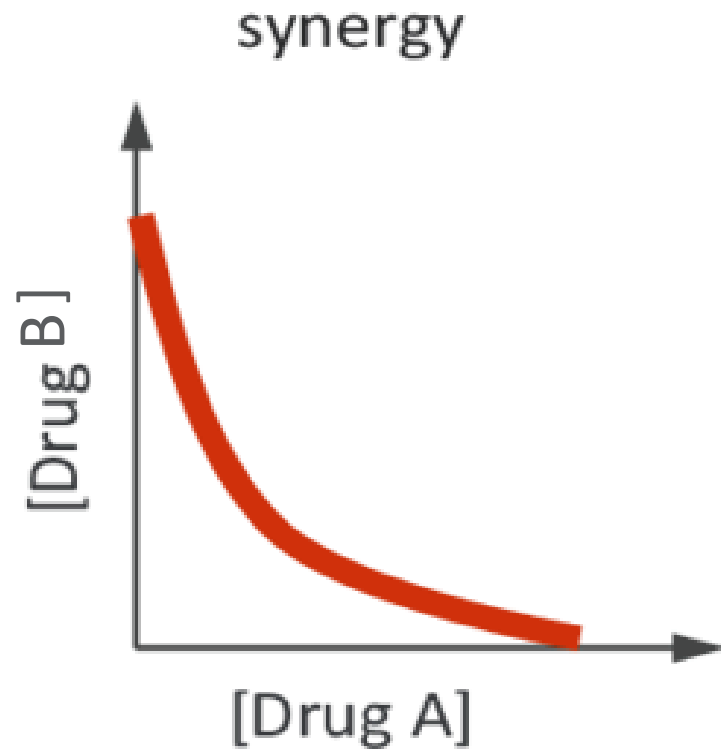
Target Species	Antimicrobial ID/Name	Activity Measure	Unit	Activity of Current Peptide Alone	Activity of Current Peptide in Combination	Activity of Antimicrobial Alone	Activity of Antimicrobial in Combination	FICI	Reference
Staphylococcus aureus SAP 0017	764	MIC	µg/ml	8	32	64	64	1	21
Pseudomonas aeruginosa 910	Polymyxin B	MIC	µM	32		0.13		0.5	23

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References

Article	View Abstract
1 Friedrich CL, Moyles D, Beveridge TJ, Hancock RE Antimicrob Agents Chemother, 2000, 44, 2086-2092 Antibacterial action of structurally diverse cationic peptides on gram-positive bacteria	Pubmed
2 Rathinakumar R, Walkenhorst WF, Wimley WC J Am Chem Soc, 2009, 131, 7609-7617 Broad-spectrum antimicrobial peptides by rational combinatorial design and high-throughput screening: the importance of interfacial activity	Pubmed

SYNERGY



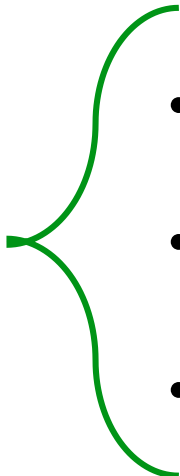
- ➔ New mechanisms of actions
- ➔ New combinations
- ➔ MDR pathogens
- ➔ Way to potentiate antibiotics

CONCLUSION

- Antimicrobial resistance – global public health issue

SOLUTION



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- Antimicrobial peptides as a potential class of new therapeutics
 - DBAASP offers to be one place for comprehensive information on AMPs
 - Synergistic interactions – new perspectives in pharmacology

RESOURCES

- Malak Pirtskhalava, Anthony A Armstrong, Maia Grigolava, Mindia Chubinidze, Evgenia Alimbarashvili, Boris Vishnepolsky, Andrei Gabrielian, Alex Rosenthal, Darrell E Hurt, Michael Tartakovsky, DBAASP v3: database of antimicrobial/cytotoxic activity and structure of peptides as a resource for development of new therapeutics, *Nucleic Acids Research*, Volume 49, Issue D1, 8 January 2021, Pages D288–D297, <https://doi.org/10.1093/nar/gkaa991>.
- Cokol, M. Drugs and their Interactions. *Current Drug Discovery Technologies* 2013 (10): 106-113. doi: 10.2174/1570163811310020003.
- Antibiotic Resistance Research & Statistics | Visualized Health. *Antibiotics* 2019. <https://www.clearvuehealth.com/b/antibiotic-resistance-research-statistics/>
- World Health Organization. Antimicrobial resistance. <https://www.who.int/news-room/fact-sheets/detail/antimicrobial-resistance>
- Public Health Notes. How It Happens. <https://www.publichealthnotes.com/antimicrobial-resistance-amr/how-it-happens/>



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