# FUNCTIONAL AND BIOINFORMATIC ANALYSIS OF ANTIMICROBIAL PEPTIDE DERIVED FROM LACTIC ACID BACTERIA

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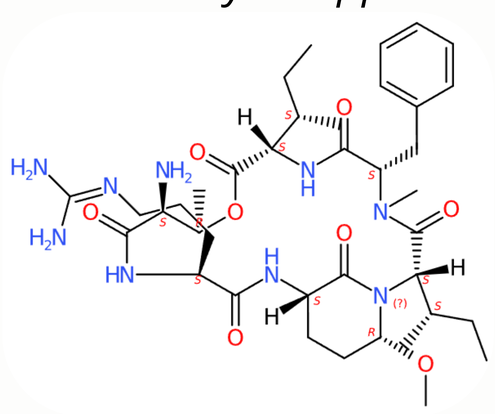
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## Introduction

Lactic acid bacteria (LAB), such as ***Lacticaseibacillus rhamnosus***, are producers of various bioactive compounds. Among them are **antimicrobial peptides (AMPs)**. These natural bioactive molecules play a crucial role in microbial competition and have been widely applied in the food industry as natural preservatives. Due to their broad-spectrum antimicrobial activity, they represent promising tools in the fight against pathogenic microorganisms.

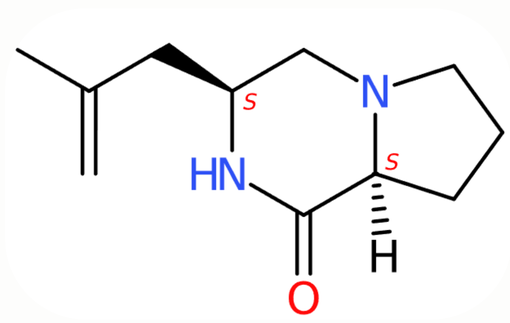
Preliminary analyses of the newly identified *L. rhamnosus* 72 strain (POIR.01.01.01-00-0632/19) demonstrated its antibacterial properties, and cyclic dipeptides were identified within its excretome, suggesting potential application against pathogens.

*Microcystis spp.*



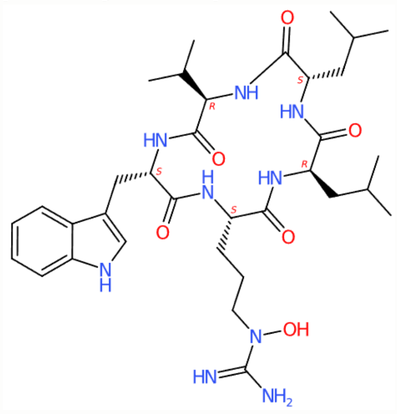
Micropeptin MZ771 ($C_{38}H_{61}N_9O_8$)

*Penicillium purpurogenum G59*



Penicimutide ($C_{11}H_{18}N_2O$)

*Streptomyces sp. RK88-1441*



Pentaminomycin B ($C_{34}H_{53}N_9O_6$)

## *Lacticaseibacillus rhamnosus 72*

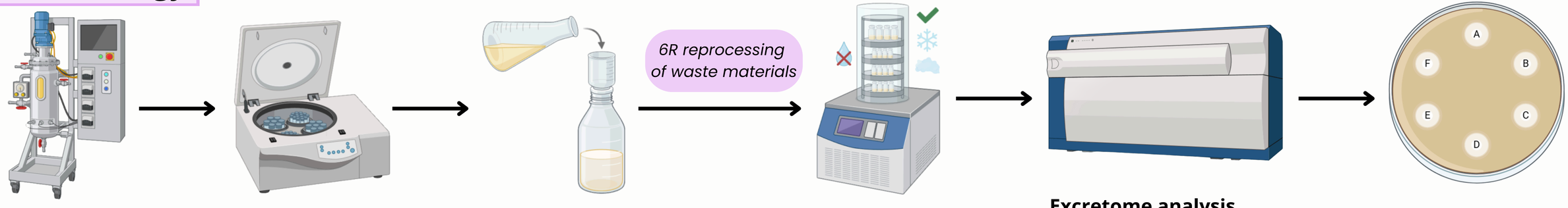
## Aim

This study aimed to evaluate the antibacterial activity of the cell-free culture supernatant using culture-based methods and to assess the therapeutic potential of the main peptide using bioinformatic tools.

***Convergence***

the process by which unrelated organisms living in similar environments develop similar morphological and functional characteristics.

## Methodology




**Bacterial culture** → **Centrifugation** → **Filtration** → **Freeze-drying** → **Excretome analysis at IBB in Warsaw** → **Disk-diffusion testing**

## Results

| PATHOGEN | A postbiotic obtained from the result of culturing probiotic bacteria carried out by: 24 h | 48 h | 72 h | 7 days |
|---|---|---|---|---|
| | **A** | **B** | **C** | **D** |
| *Candida albicans (Robin) Berkhout ATCC 10231* | | | L P | G |
| *Streptococcus agalactiae PCM2683* | | L P | L P | G |
| *Proteus mirabilis ATCC 29906* | | P | G P | |
| *Staphylococcus epidermidis* | | | G P | |
| *Streptococcus pyogenes* | | L | G P | |
| *Staphylococcus aureus 6538P* | | | G | G |
| *Escherichia coli ATCC 8739* | | G L P | G L P | |
| *Pseudomonas aeruginosa PAO1* | | L | L G | G |

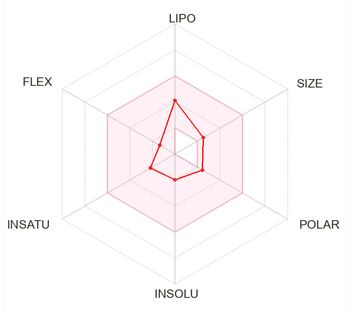
*Legend:* ***L -*** *laboratory medium MRS* ***P*** *- production medium (5% whey + 2% yeast)*
***G*** *- production medium supplemented with 2% glucose*

**MIC**
*7.82 mg/mL*

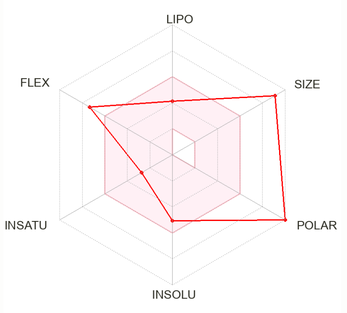
**MBC**
*15.63 mg/mL*

**MBC**
*15.63 mg/mL*

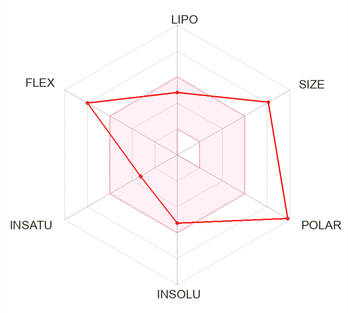
Penicimutide




Micropeptin MZ771




Pentaminomycin B




*Legend:*
***LIPO (LIPOPHILITY):*** *-0.7 < XLOGP3 < +5.0*
***SIZE:*** *150G/MOL < MW < 500G/MOL*
***POLAR (POLARITY):*** *20Å² < TPSA < 130Å²*
***INSOLU (INSOLUBILITY):*** *-6 < LOG S (ESOL) < 0*
***INSATU (INSATURATION):*** *0.25 < FRACTION CSP3 < 1*
***FLEX (Flexibility):*** *0 < Num. rotatable bonds < 9*

Data derived from:

SwissDrugDesign

| Feature | Micropeptin MZ771 | Penicimutide | Pentaminomycin B |
|---|---|---|---|
| **Water Solubility Class** | *Moderately soluble* | *Very soluble* | *Moderately soluble* |
| **GI absorption** | *Low* | *High* | *Low* |
| **BBB permeant** | *No* | *No* | *No* |
| **Log Kp (skin permeation)** | *-9.79 cm/s* | *-6.28 cm/s* | *-8.39 cm/s* |
| **Druglikeness (Lipinski)** | *No; 3 violations* | *Yes; 0 violation* | *No; 3 violations* |
| **Bioavailability Score** | *0.17* | *0.55* | *0.17* |

*Legend:* ***GI*** *- gastrointestinal absorption,* ***BBB*** *- Blood-brain barrier permeant*

## Conclusions

- Biofilm inhibition was additionally confirmed by a reduction in pyoverdine production by *Pseudomonas aeruginosa* PAO1 , which is regulated by the quorum-sensing system. This observation suggests that the mechanism of action of the investigated AMPs may involve membrane interaction or inhibition of pyoverdine recycling.
- The predicted profiles of the AMPs indicated high water solubility, high absorption, good membrane permeability, and gastrointestinal uptake, without the ability to cross the blood–brain barrier.
- The results indicate the investigated peptide's potential therapeutic application.

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Schemes created in BioRender.com