### **BATTLE-AMP**

#### Benchmarking Assessment Tests for The Leading Efficacy of Antimicrobial Peptides

Wojciech Zarzecki

P. Szymczak, **W. Zarzecki**, A. Bukała, R. Olayo, C,Müller J. Borišek, P. Setny, J. Szkóp, E. Szczurek





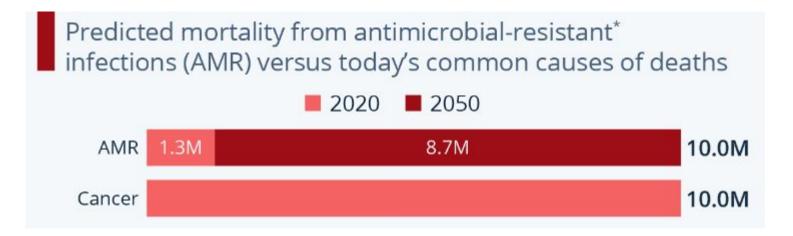
Warsaw University of Technology





UDWIG-MAXIMILIANS JNIVERSITÄT MÜNCHEN







#### Lack of standardization



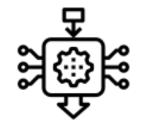
datasets



state of the art

Low reproducibility and reusability

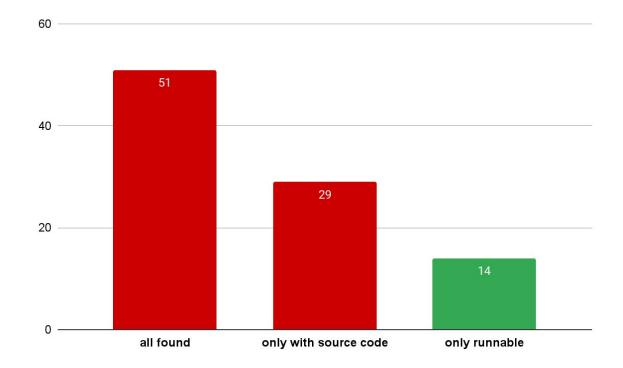


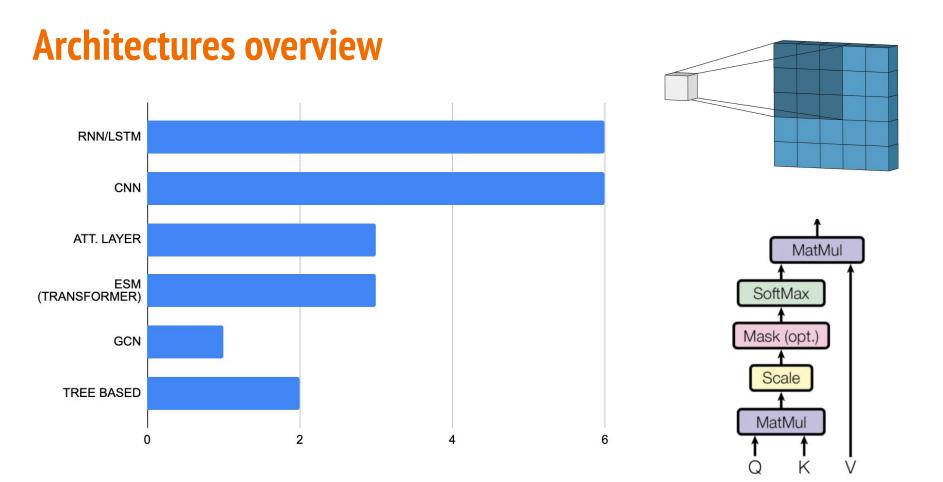


dependencies

inference

### **Models availability**



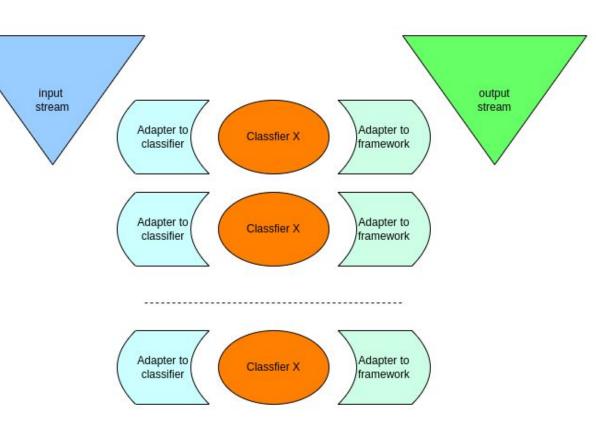


### **Our benchmark**

## Wrapping model

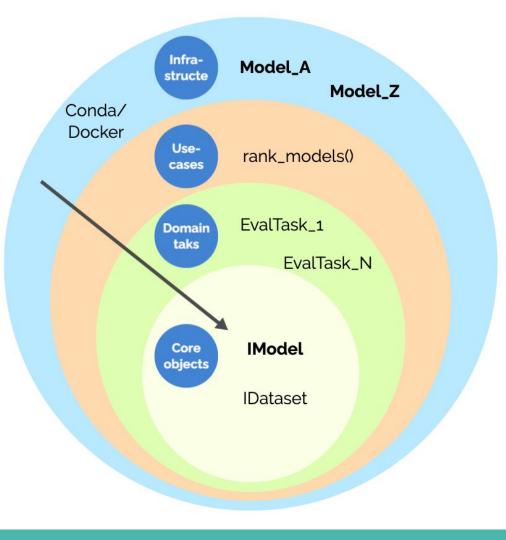
#### model's responsibility inference

- 1. prepare environment
- 2. inference with common format



# Extendable benchmark

#### benchmark's responsibility evaluation independ of models



### Labeling methods

AMP vs non-AMP

- if has been reported to AMP database
- binary classification

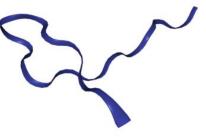
Activity measure

- measure describing inhibition of bacterial growth (the lower, the better)
- regression of continuous value
- classification via regression

### **Robustness evaluation**

**robustness** refers to the ability of a system, model, or entity to maintain stable and reliable performance across a broad spectrum of conditions, variations, or challenges

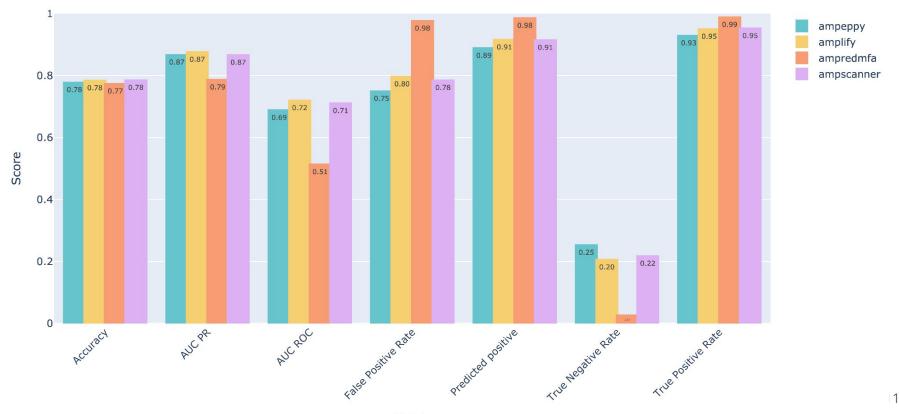
#### FLGVVFK**L**ASKVFPAVF**K**KV - 4 μg/ml FLGVVFK**S**ASKVFPAVF**G**KV - >256 μg/ml



MIC *E. coli* = 256 μg/ml MIC *S. aureus* = 8 μg/ml FLG**V**VFKLASKVF**G**AVFKKV

### **Excessive positive predictions**

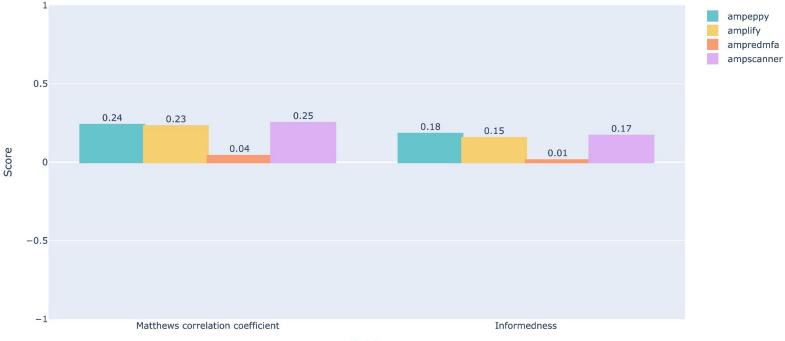
Model performance comparison - BroadActivityTask



Metric

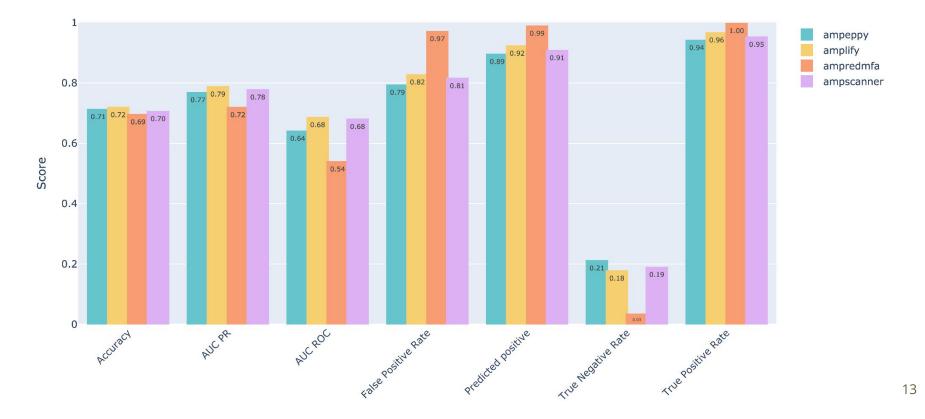
### **Inability to distuigh negatives**

Model performance comparison - BroadActivityTask



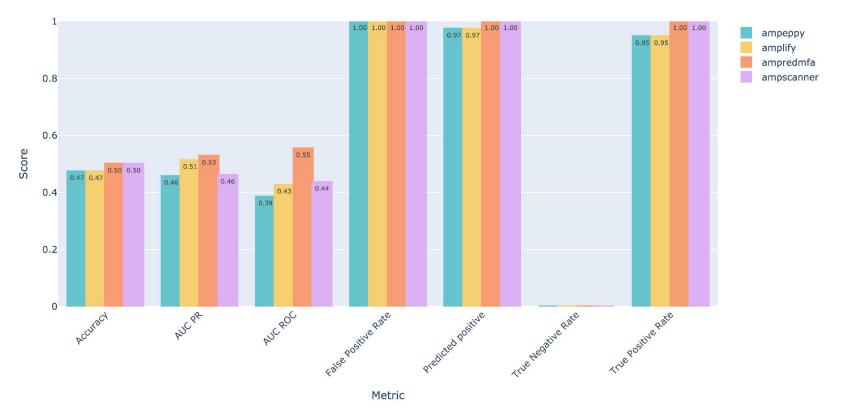
### **Issues with microbe specific predictions**

Model performance comparison - SpeciesActivityTask Ecoli



### Non-distinguishment of highly similar sequences

Model performance comparison - HighSimilarityTask



### **Acknowledgments**



#### Paulina Szymczak



#### Adriana Bukała



#### Ewa Szczurek



#### Roberto Olayo Alarcon



#### Jure Borišek

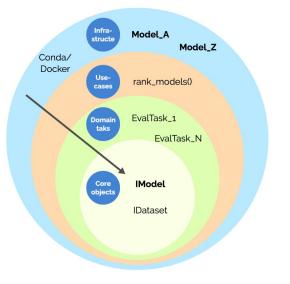
#### Piotr Setny



Julia Szkóp

### **BATTLE-AMP**

- lack of standardization
- thread of AMR
- extendable benchmark



**Poster session:** #62 BATTLE-AMP

🛱 SATURDAY / 9 NOVEMBER

● 10:30 - 12:00 (POSTER SESSION 2)

 $\square$ 

in

wojciechzarzecki5@gmail.com



 $\mathbf{C}$ 

/szczurek-lab/BattleAMP-benchmark