Data collection for machine design of novel antibiotics against ESKAPE bacteria

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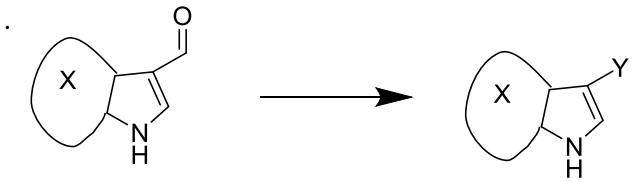
Main Goal

Development of effective machine learning network for the prediction of biological activities indole based antibiotics.

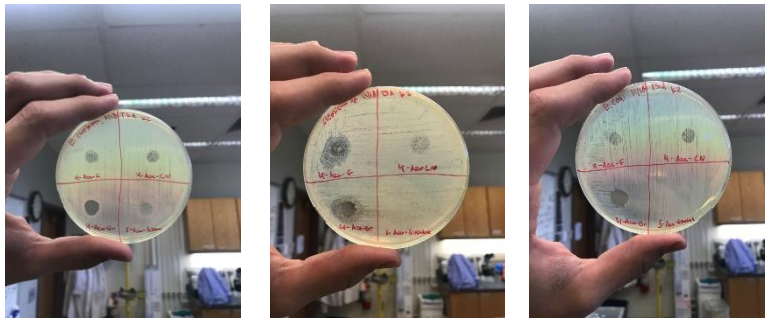
Abstract

Data about biological activity of several dozens of indole derivatives were collected from the literature. Drug-like parameters for those molecules were calculated using ChemDraw Professional Program. The first set of possible antibiotics based on indole core were synthesized and tested against gram-positive and gram-negative strains represented ESKAPE bacteria pathogens. Several compounds with activities were identified.

General Scheme of Synthesis



Using two steps synthesis 16 novel compounds were synthesized, characterized, and tested against ESKAPE bacteria pathogens. Several of them showed some activity against gram-positive and gram-negative strains.



A **B** **C**

Fig. 1. Agar plates with different strains of ESKAPE bacteria treated by novel compounds. **A** - *E. carotovora;* **B** - *Klebsiella sp.*; **C** - *E. coli.*

Results

	Name of new compound					
Strain of bacteria	4-Aza-H	5-Aza-CN	5-Aza-Br	7-Aza-Gu	7-Aza-F	7-Aza-Br
E. coli	+	-	+	-	-	-
E. carotovora	+	+	+	+	+	-
Klebsiella sp.	+	-	+	-	-	-
S. epidermidis	-	-	+	-	-	-
P. aeruginosa	+	-	+	+	+	+
B. subtilis	+	-	+	-	-	-

Conclusions

Based on literature biological data and calculations of drug-like parameters for different indole core molecules, several potential antibacterial scaffolds were synthesized and tested. Some of them showed promising activities against gram-negative bacteria. Further optimization of scaffolds using machine learning technic are highly desired. The collection of data for the training of machine learning network is in the progress.

Acknowledgments

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