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P2057 *In silico* discovery of antibiotic resistance patterns and artificial intelligence-based decision support systems for rational drug use

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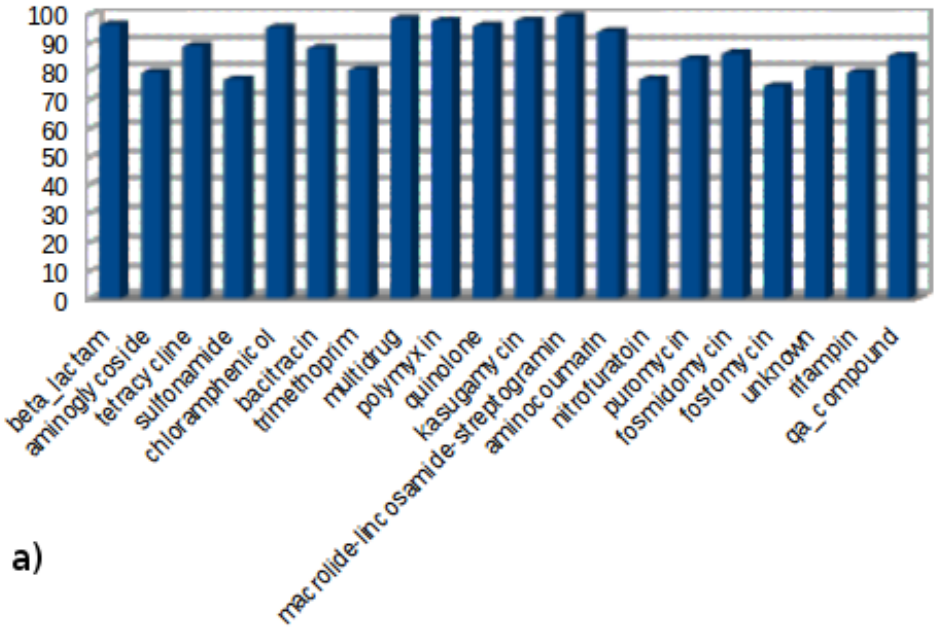
Background:t is known that an important part of antibiotic resistance mechanisms emerge as functionally convergent evolution or as resistance islands acquired via horizontal gene transfers although bacterial species are capable of developing independent mechanisms. Therefore, the resistance mechanisms are expected to correlate and exhibit certain occurrence patterns. It should be possible, to a certain extent, to predict the existence of a resistance element given the context of others. This study aims to conduct an *in silico* data mining approach on the sequenced genomes of *Klebsiella pneumoniae* and *Acinetobacter baumannii* to predict the antibiotic resistance profile from partial knowledge.

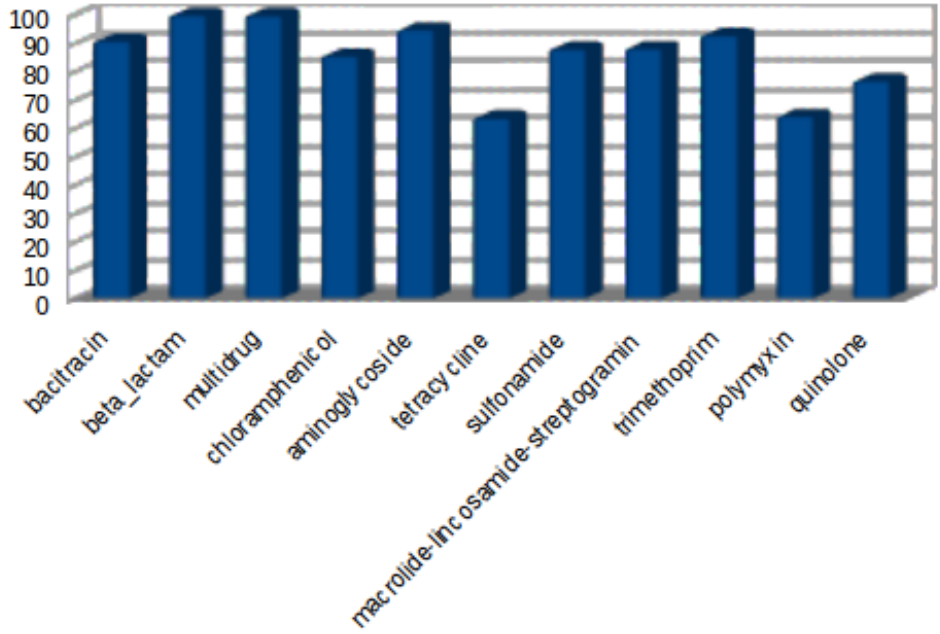
Materials/methods: Whole genome sequences of 3031 *A.baumannii* and 4301 *K.pneumoniae* strains were obtained from molecular databases. Antibiotic resistance genes (ARGs) and drug resistance classes were predicted using DeepARG program. Each resistance element in a strain was predicted from the existence of the others using deep learning models, and a drug resistance cooccurence network was constructed. Network component analyses revealed the correlated resistance clusters. A prediction model was trained using this clustering information to infer the existence of a resistance gene/class using an incomplete information on a small number of resistances for a strain, both for *A.baumannii* or *K.pneumoniae*.

Results: According to the constructed co-occurence network models, resistance to beta-lactam, chloramphenicol, and aminoglycosides tend to coocur ($r=0.75$, $p<0.001$) in *A.baumanni* strains, while tetracycline, polymixin, and macrolide/lincosamide/streptogramin resistance are highly correlated for *K.pneumoniae* ($r=0.79$, $p<0.001$). On the other hand, sulfonamide and trimethoprim resistances were found to be inversely related ($r=-0.4$, $p<0.001$). For those drug classes, the predictions and risk associations were made more confidently (ROC-AUC: 0.81), whereas the weaker correlations resulted in less accurate predictions ROC-AUC: 0.59).

Conclusions: The positive and negative correlation patterns in antimicrobial resistance classes/genes in *A.baumannii* or *K.pneumoniae* allows predicting the resistance of a drug given a few others fairly accurate. The results are encouraging for the possibility of artificial intelligence driven decision support systems for infection treatment.



a)



b)

Figure: Average prediction accuracy for each antimicrobial class for a) *K. pneumoniae* b) *A. baumanni*