DEVELOPMENT OF A STANDARDIZED APPROACH FOR TRANSFER LEARNING WITH QSAR MODELS

Luis Felipe de Morais Melo
Federal University of Paraiba, Brazil
INTRODUCTION

• What is transfer learning?
• How are we going to transfer information from the source task to the target task?

• Which targets should we use as source tasks for a particular target task of interest?
OBJECTIVES

• Creating a model capable of predicting the successfulness of a transfer between two datasets

• Creating a standardized transfer learning protocol capable of being implemented in an algorithmic manner
MATERIALS AND METHODS
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RESULTS AND DISCUSSION

• Successful transfers are very rare, with a probability of occurrence of 0.126%.

• The transferability prediction model achieved a precision of 17%, which represents a 127 times increase when compared to random chance.

• The transferability prediction model was capable of identifying the majority of the successful transfers achieving a sensitivity of 92%.

• Out of the 100 targets selected in the applicability subset 17 had at least one significant transfer identified.

• Cell-lines are highly transferable amongst each other.
RESULTS AND DISCUSSION

Single domain transfer

Mean MCC increase: 0.19

Multi domain transfer

Mean MCC increase: 0.44
CONCLUSION

• Successful transfers are very rare

• Transfer learning as limited applicability even when source datasets are available

• Finding a successful transfer in a naive manner is much less efficient than using a transferability prediction model

• Transfer learning can provide considerable performance increases on QSAR models
THANK YOU!

Luis Felipe de Morais Melo
luisfelipe.melo@hotmail.com