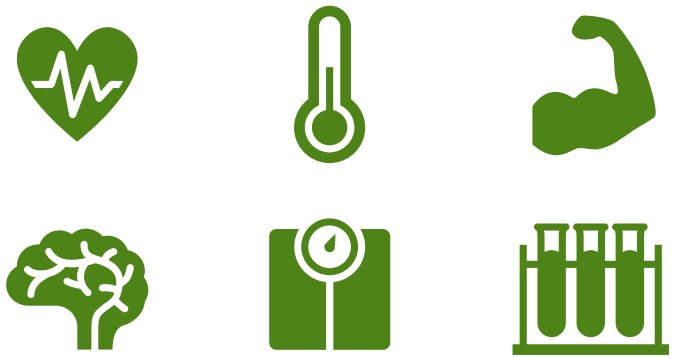
In Silico Models to Predict the Perturbation of Thyroid Homeostasis

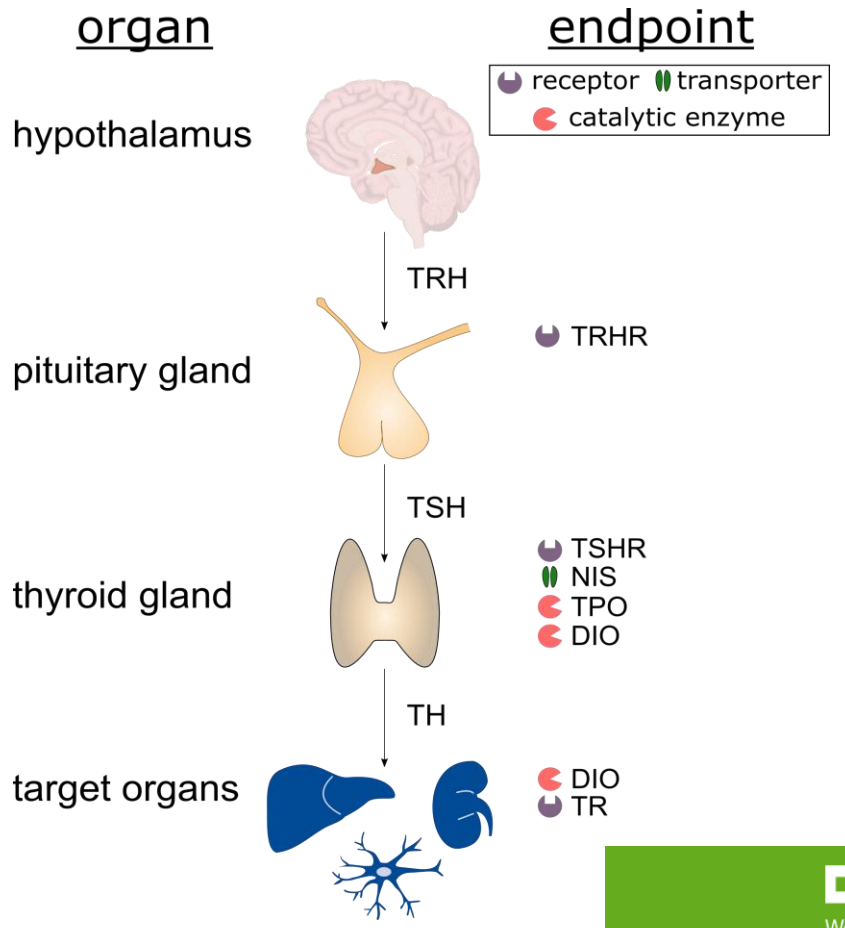
M. Garcia de Lomana, A. G. Weber, B. Birk, R. Landsiedel, K.-J. Schleifer, M. Mathea and J. Kirchmair

Thyroid hormones (TH) are involved in many metabolic and developmental processes



Dysregulation of TH:

- causes hypo- or hyperthyroidism
- shows correlation with cancer, obesity and diabetes



BASF
We create chemistry

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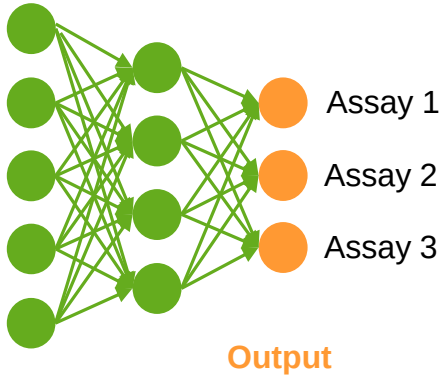
Single-task models

- ML methods
  - Random forest
  - Logistic regression
  - Gradient boosting
  - Support vector machine
  - Neural networks
- Class balancing techniques
  - Balanced class weights
  - Oversampling
  - Undersampling

Multi-task models

Single-task model



Multi-task model

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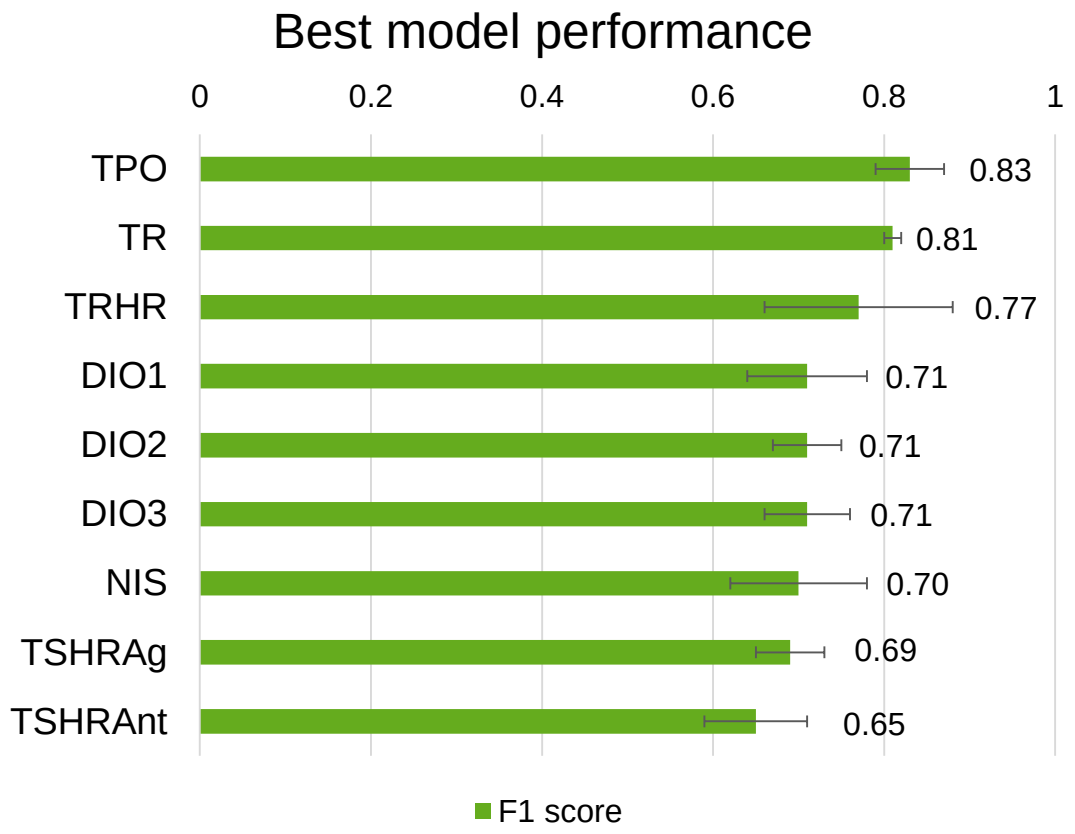

Conclusions

- Explored different single- and multi-task models to optimize the predictivity
- Correlation of confidence of the prediction with:
  - ✓ similarity of compounds to the training set
  - ✓ distance of the prediction to the decision boundary
- Developed models can help to
  - ✓ identify and prioritize compounds with the potential to disturb the TH homeostasis
  - ✓ point-out which key events are affected

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