

## A neuro-reasoning architecture for solving (serious) puzzles - Thomas Schiex

Designing new effective molecules requires to blend in various sources of information: the laws of physics, specific targeted properties and a long history of past successful designs. Originally, the protein design problem has been described as a pure NP-hard discrete constrained energy optimization problem. It is now increasingly solved using pure deep learning architectures.

In our architecture, deep learning is used to extract knowledge from Nature's designs in a format that is amenable to multi-criteria optimization. It can be described as an hybrid auto-encoder where a deep neural net encodes data in a pairwise discrete graphical model latent layer which is then decoded by a discrete optimizer over graphical models. With an enhanced loss (IJCAI 2023), a polytime convex-relaxation based discrete optimization tool (ICML 2022) and better algorithms to deal with design constraints (CPAIOR 22), our architecture preserves the ability of pure deep learning architectures to sample high-quality designs. Its ability to constrain and optimize its output also enables the fruitful exploration of out-of-distribution areas, where current deep learning methods show their limits. For amateurs of less serious puzzles, the same hybrid architecture can be used to simultaneously learn how to decode handwritten digit images and play the Sudoku, perfectly.