

## SOFTWARE LICENCE

*deepFPlearn -- Link molecular structures of chemicals (in form of topological fingerprints) with multiple targets.*

*The deepFPlearn package is a program that uses deep learning to associate the molecular structure of chemicals with biological targets on the gene/pathway level. It implements a deep autoencoder for feature compression and a subsequent deep feed forward network for the classification.*

*The aim of this program is to enable the identification of chemicals with potential risk to interfere with biomolecules on a large scale. It is implemented in Python, runs under GNU/Linux and can be controlled from the command-line interface. Although it has been trained on chemicals associated or not to endocrine disruption, the tool is flexible and can be easily retrained to any type of association between chemical structures and effects.*

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