

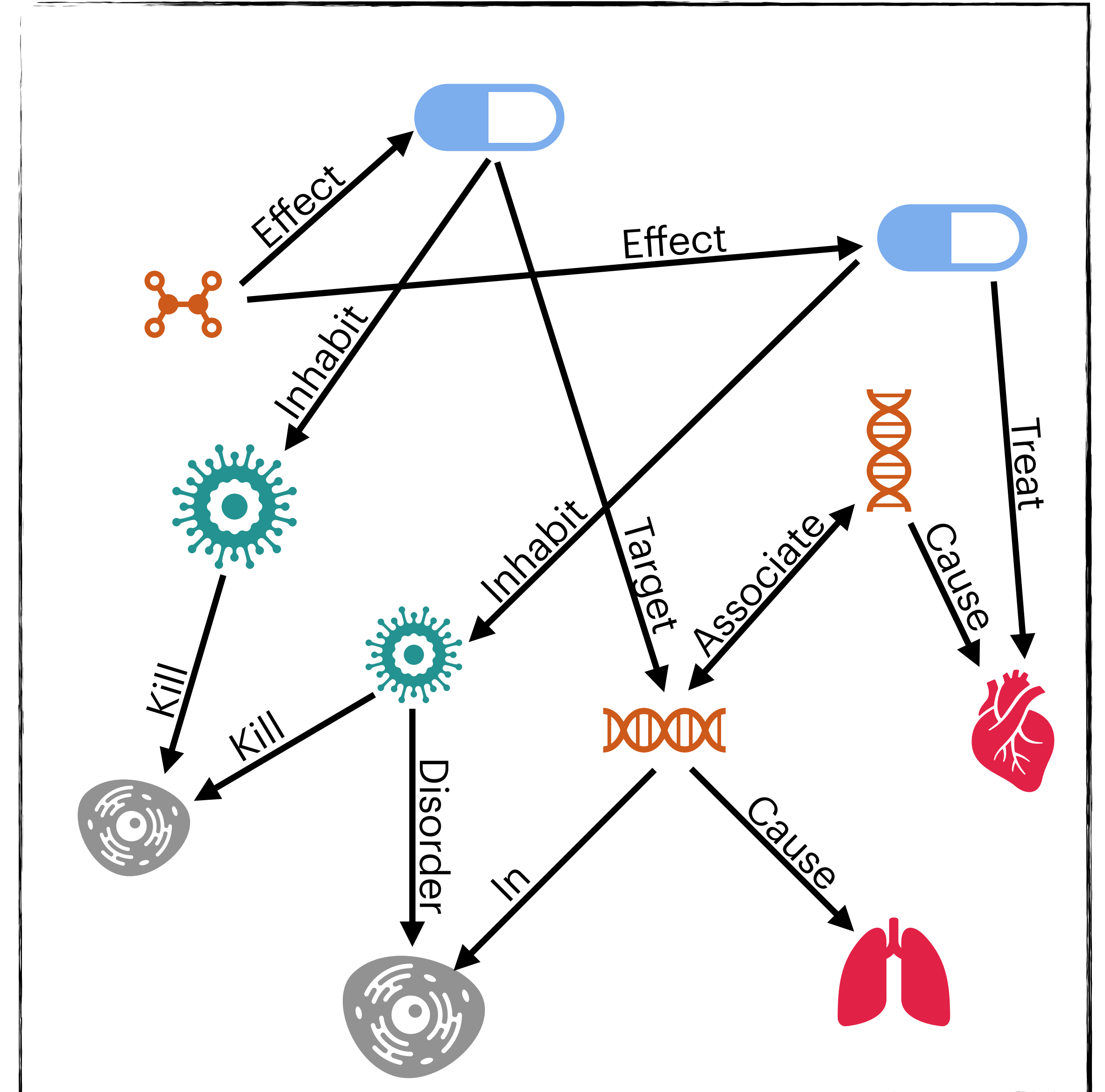
Drug Discovery

With Knowledge Graph

Hao Xu, 2020/05/05

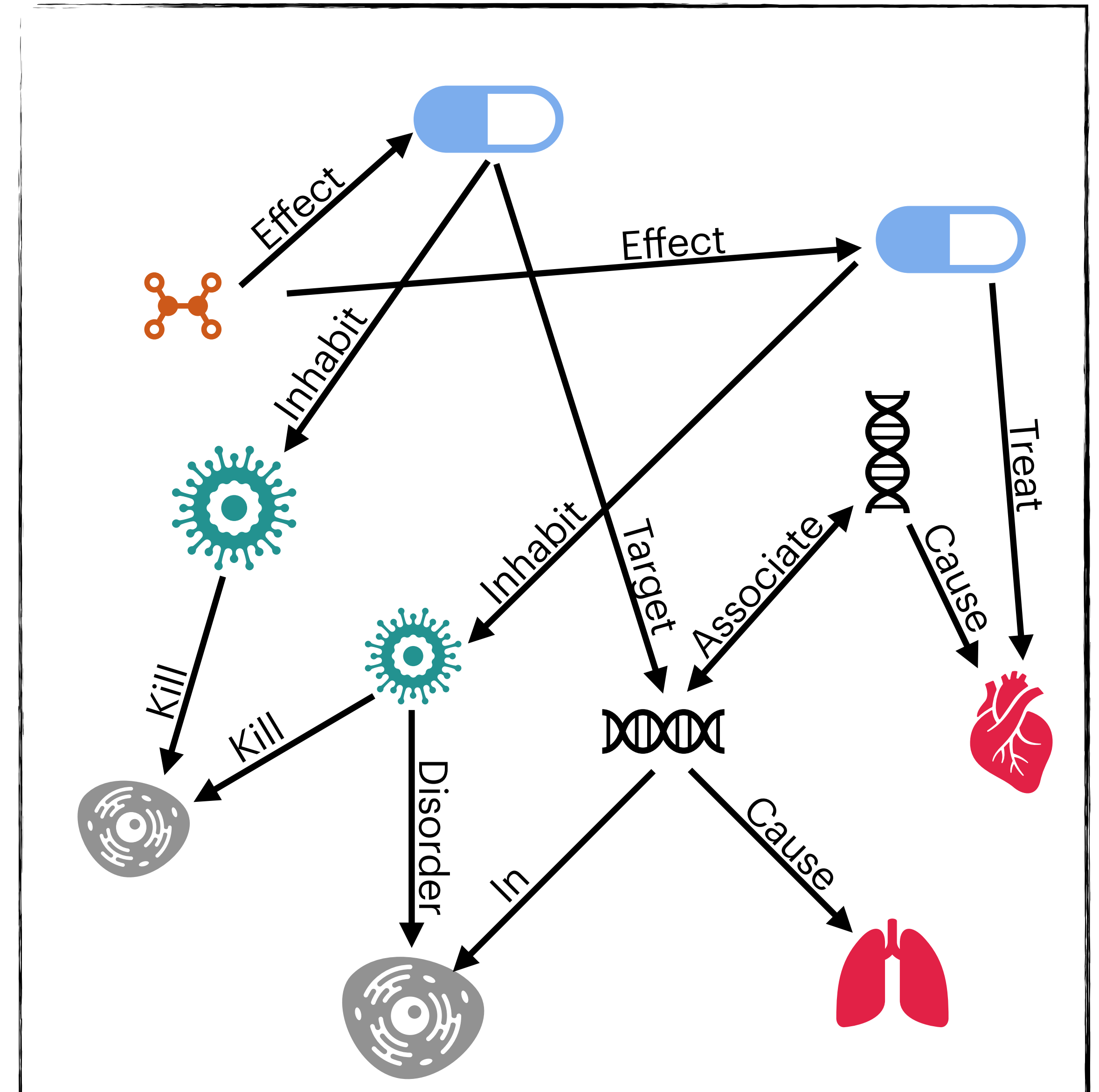
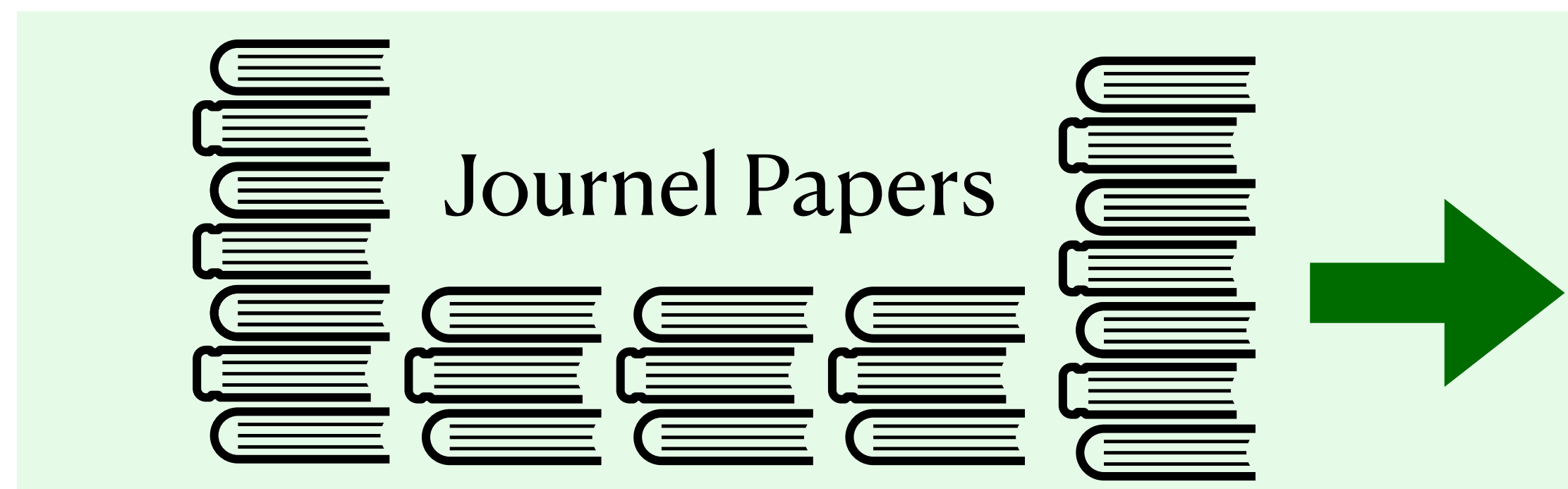
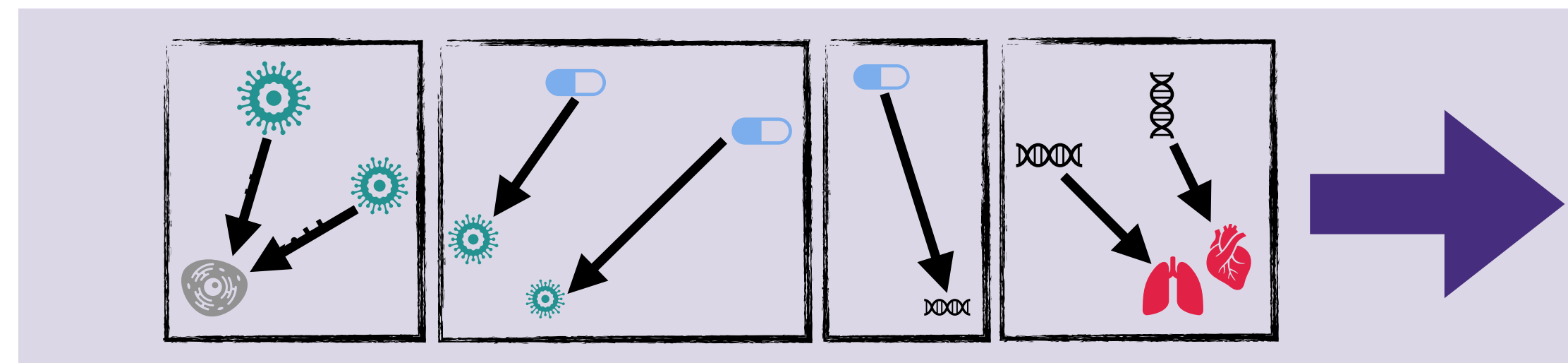
Knowledge Graph

contains different types of bio-entities, such as **drugs**, **diseases**, **virus**, **genes**, and **cells**, and their relations.



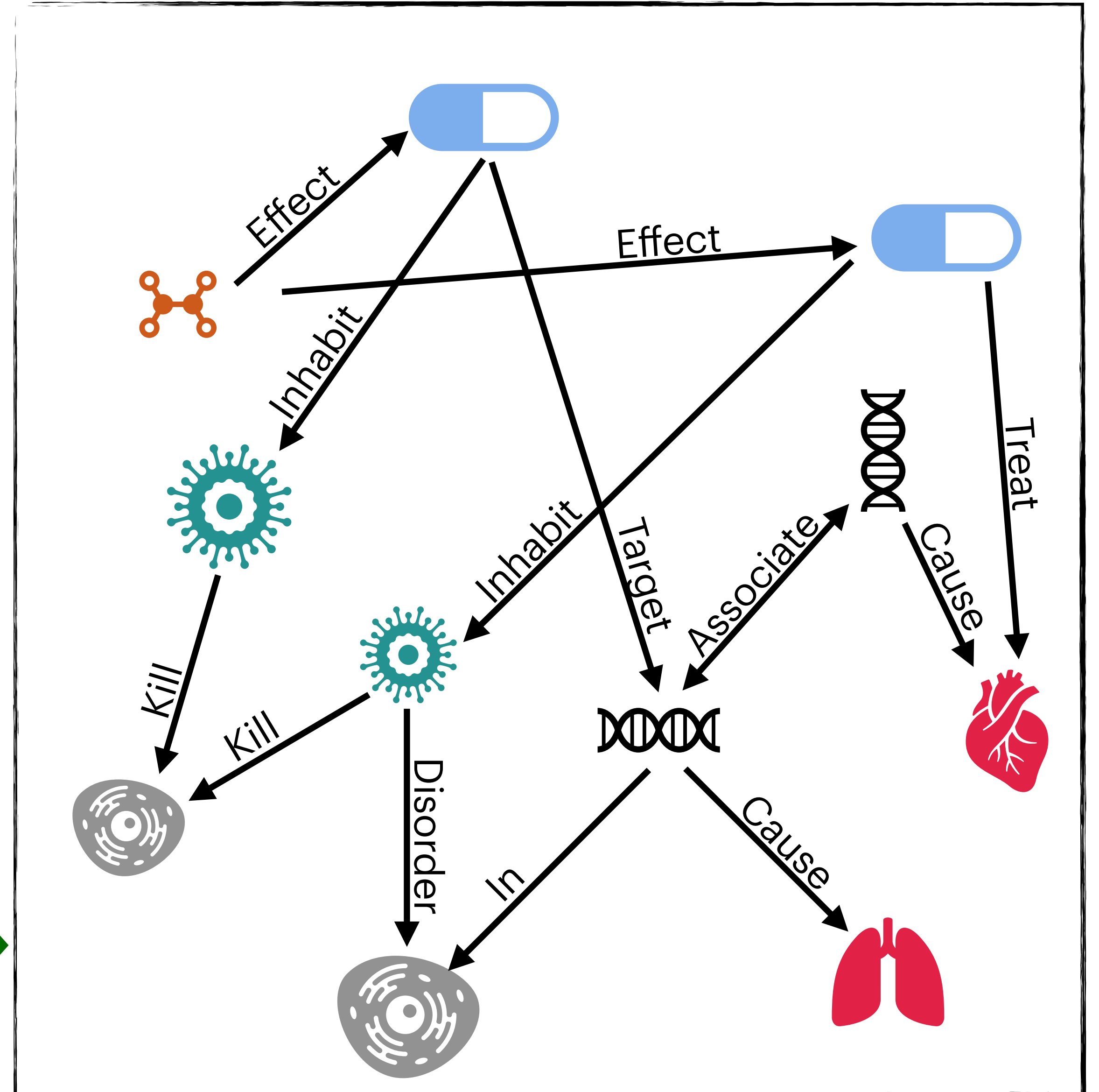
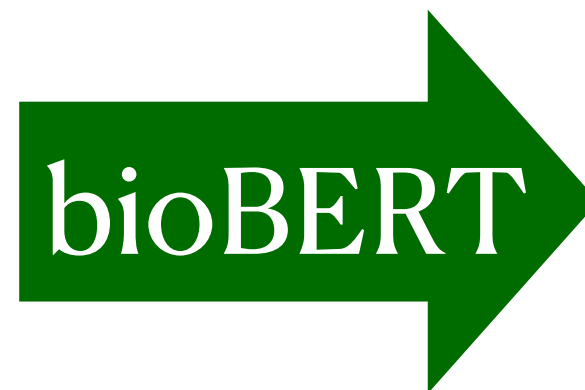
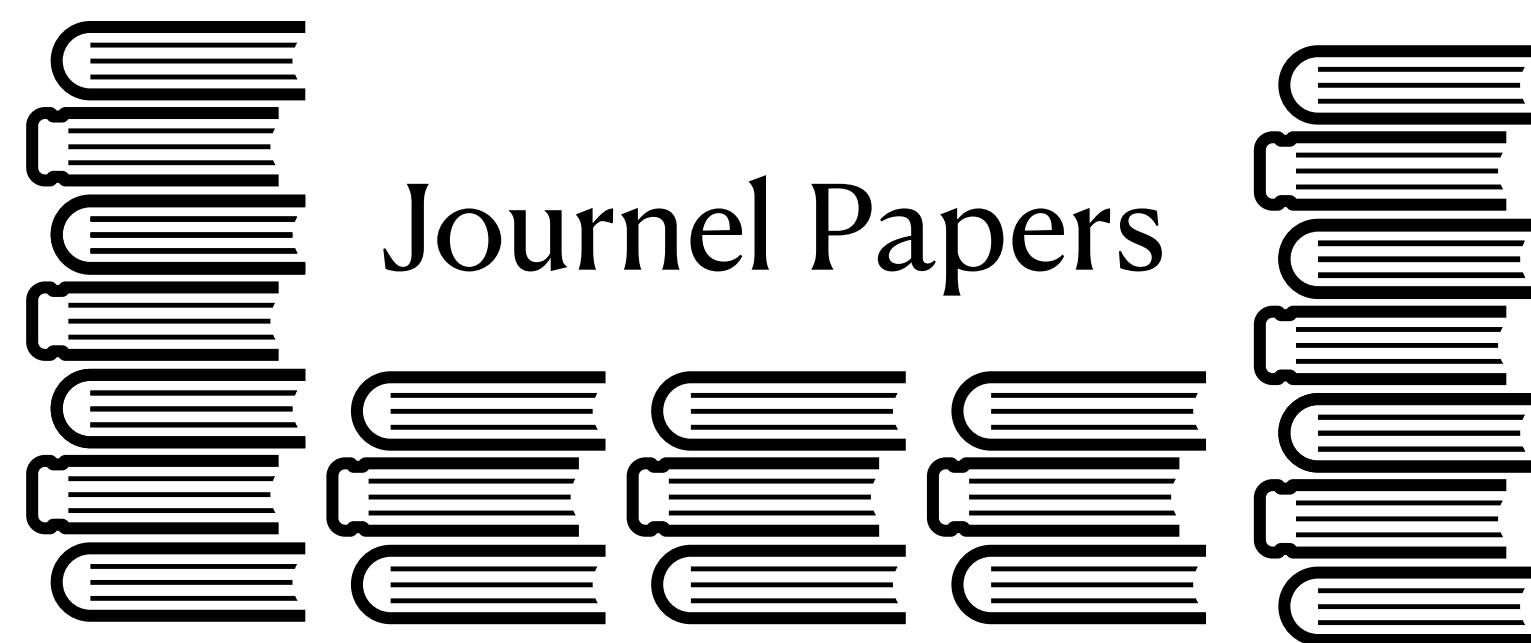
Knowledge Graph

can be constructed in many ways,
such as **integrating databases** and
information retrieval.



Knowledge Graph

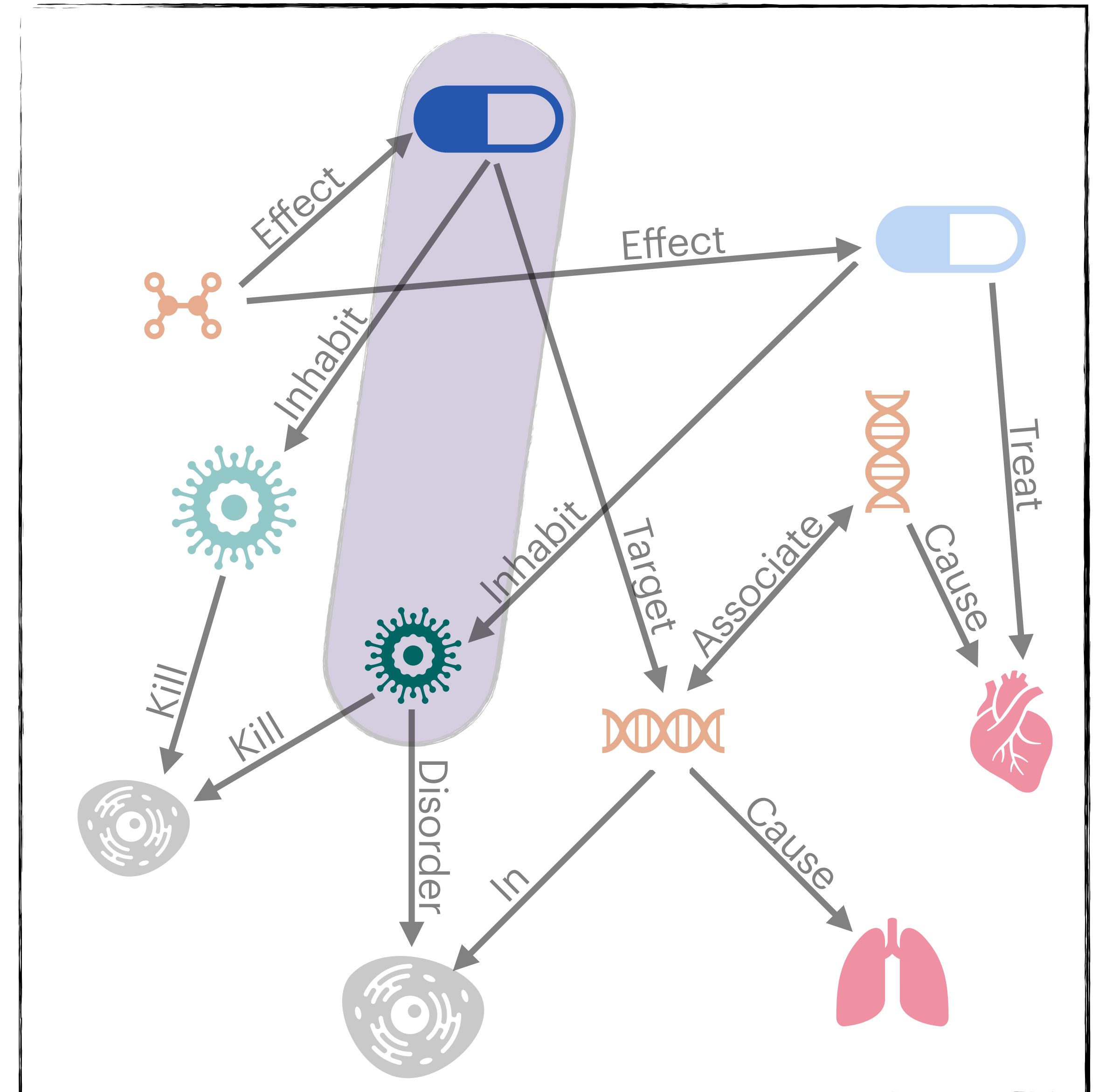
For example, it can be constructed from medical journal papers with **bioBERT**, which can be used to detect bio-entities and their relations.



Knowledge Graph

can suggest undiscovered relations between existing bio-entities by using *KG-embedding* methods.

For example, predicting whether a drug can be used in a new disease (i.e. drug repurposing).

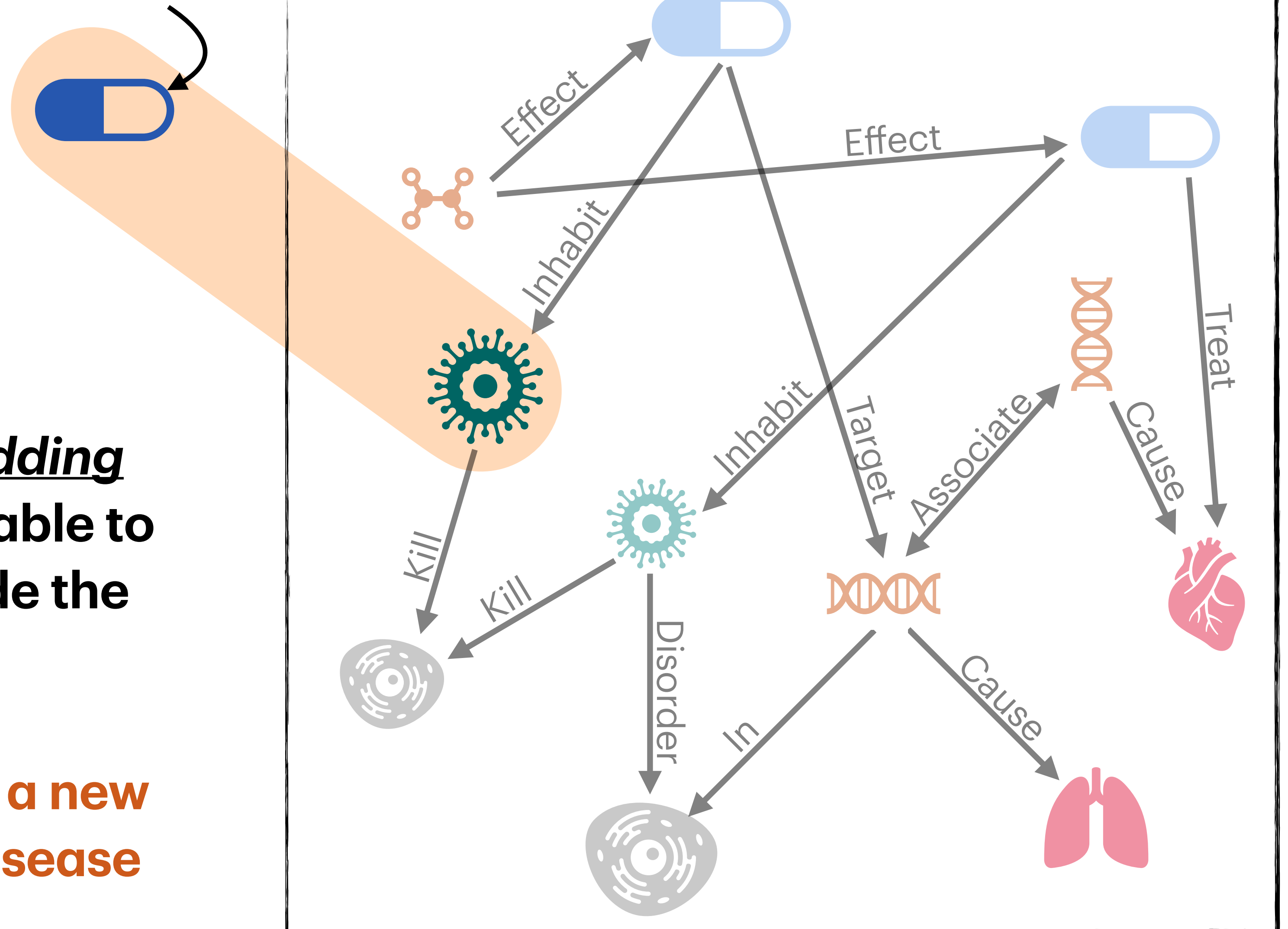


Limitation

of most existing *KG-embedding* methods is that they are unable to predict the relations outside the knowledge base,

such as predicting whether a new drug can be used for any disease

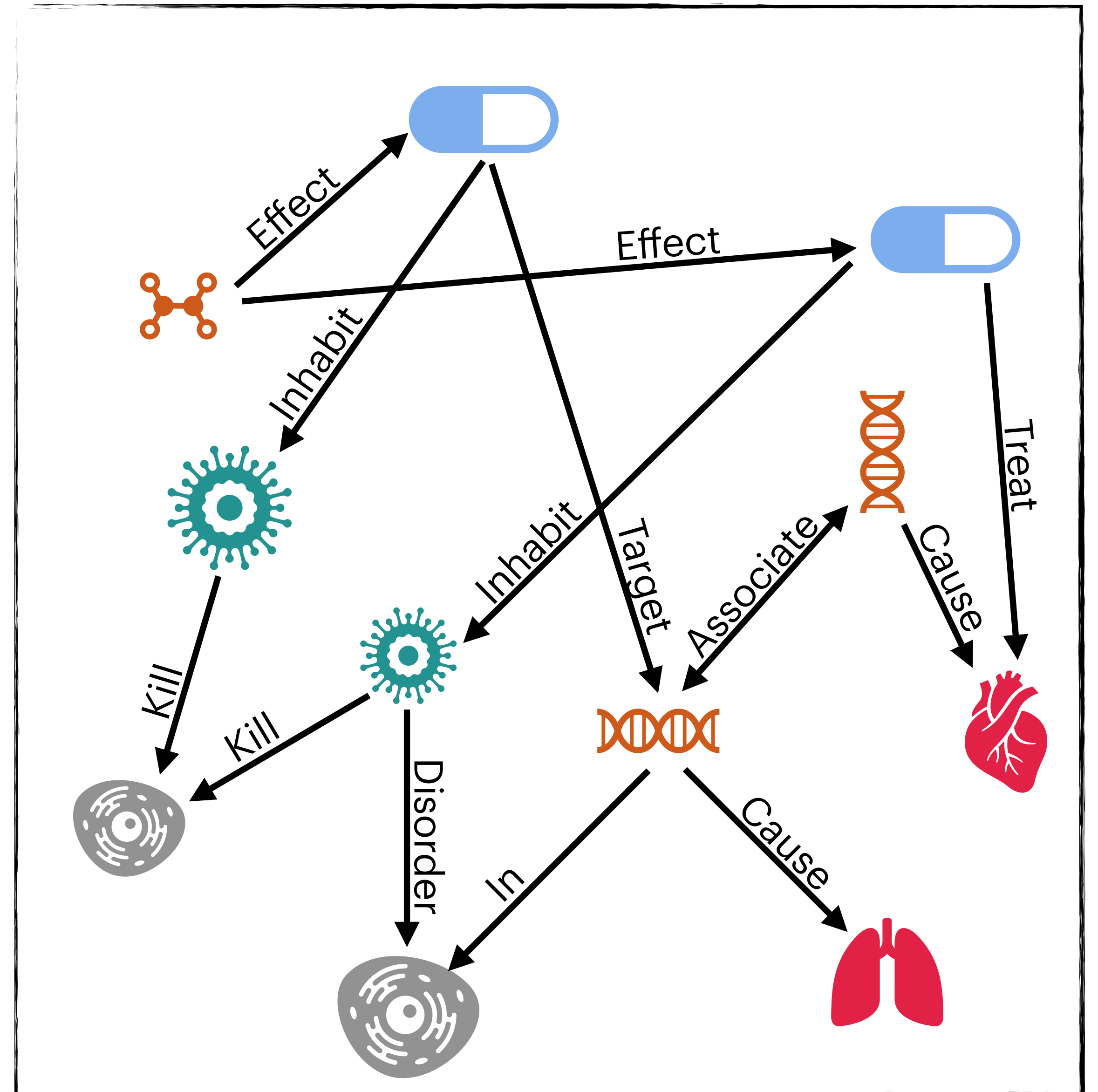
A new drug



The GripNet

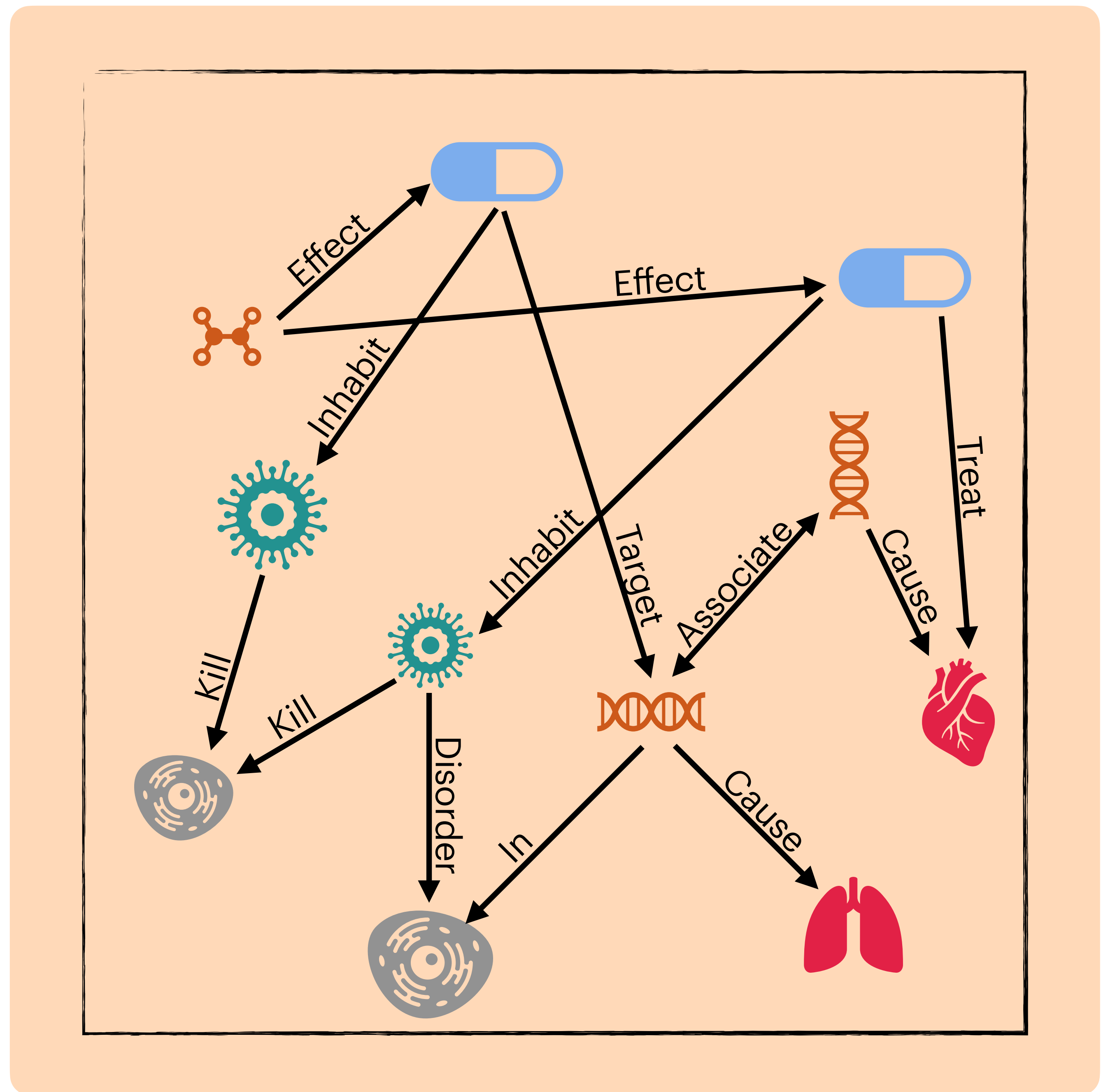
Representation Learning with GripNet

Learn low-dimensional vector representations for each bio-entities and each relations efficiently and effectively.



Task 0

According to published biomedical *journal papers*, predict undiscovered relations between **existing diseases/genes/drugs/cells...**

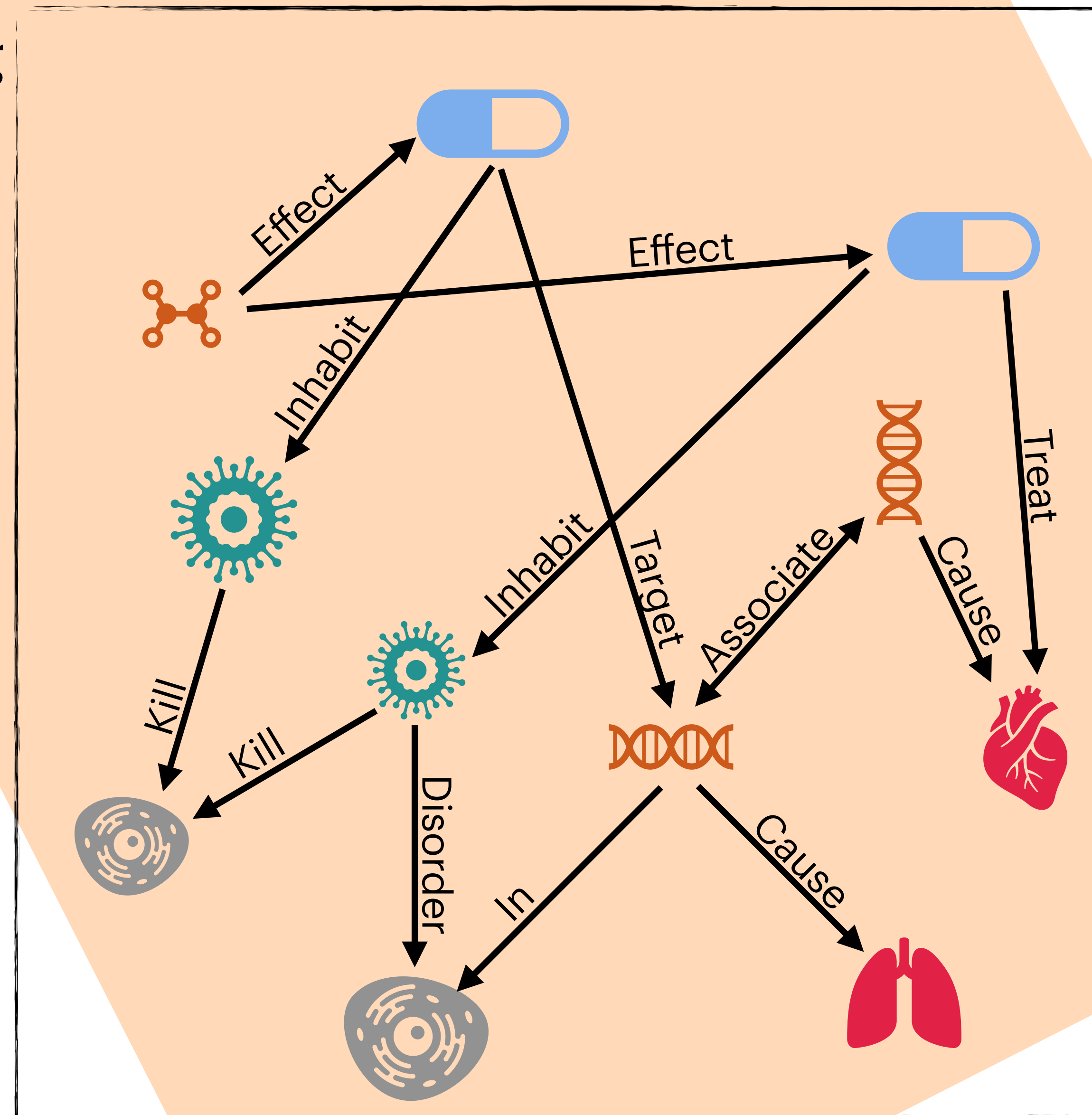
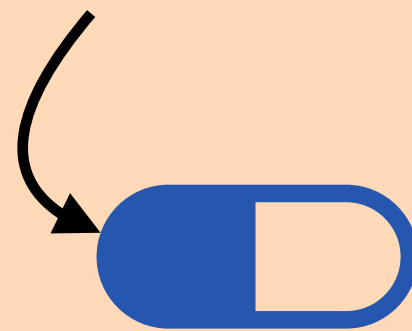


The Dynamic GripNet

Task 1

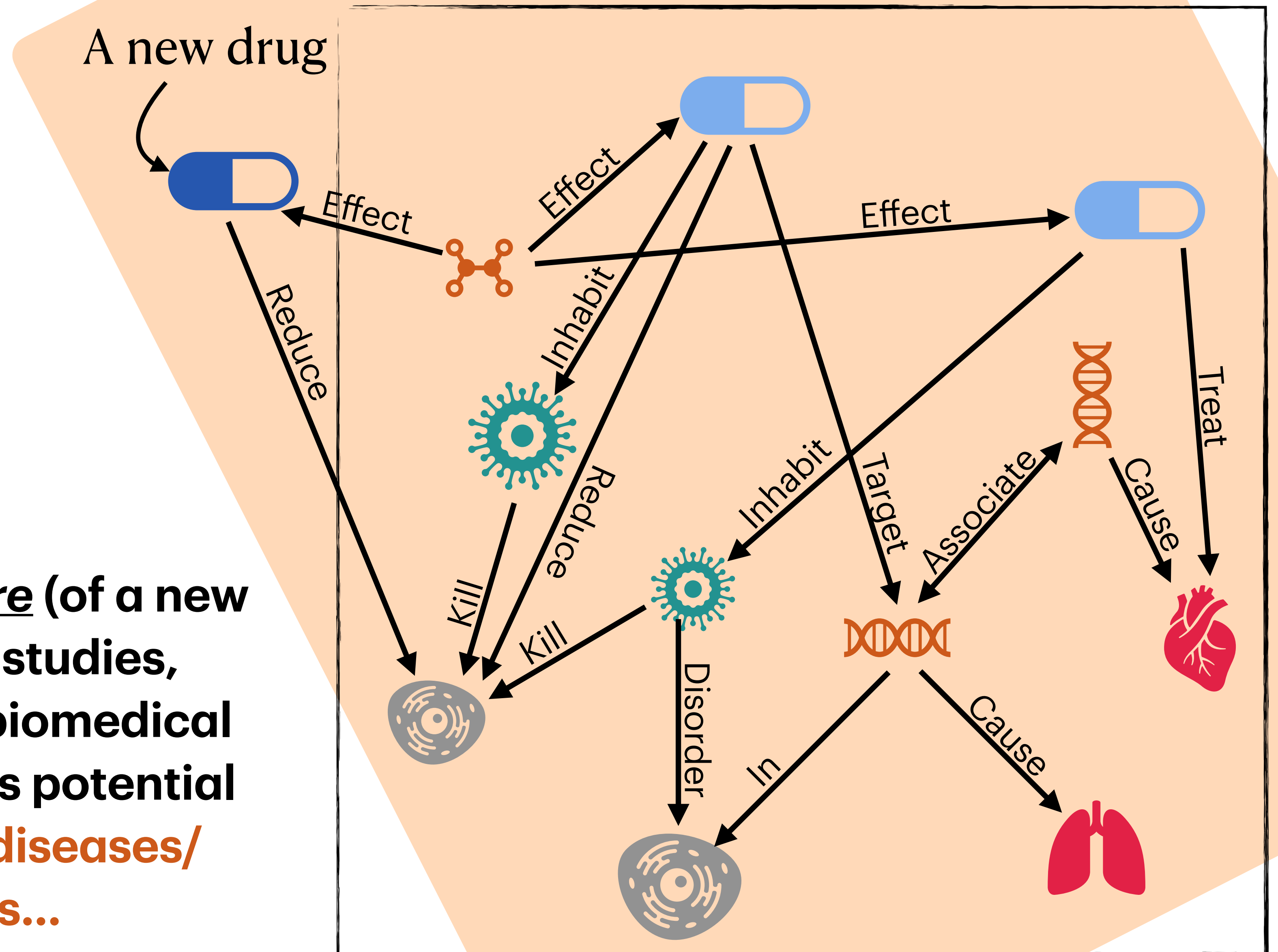
Given a chemical structure (of a new drug), according to published biomedical journal papers, predict its potential **relations with existing diseases/genes/drugs/cells...**

A new drug



Task 2

Given a chemical structure (of a new drug) and preliminary studies, according to published biomedical journal papers, predict its potential relations with existing diseases/genes/drugs/cells...



Beyond Drug Discovery...

- Help to understand the influence of chemical substructures on relations between bio-entities
- ...