

# Complex Query Answering with Neural Link Predictors

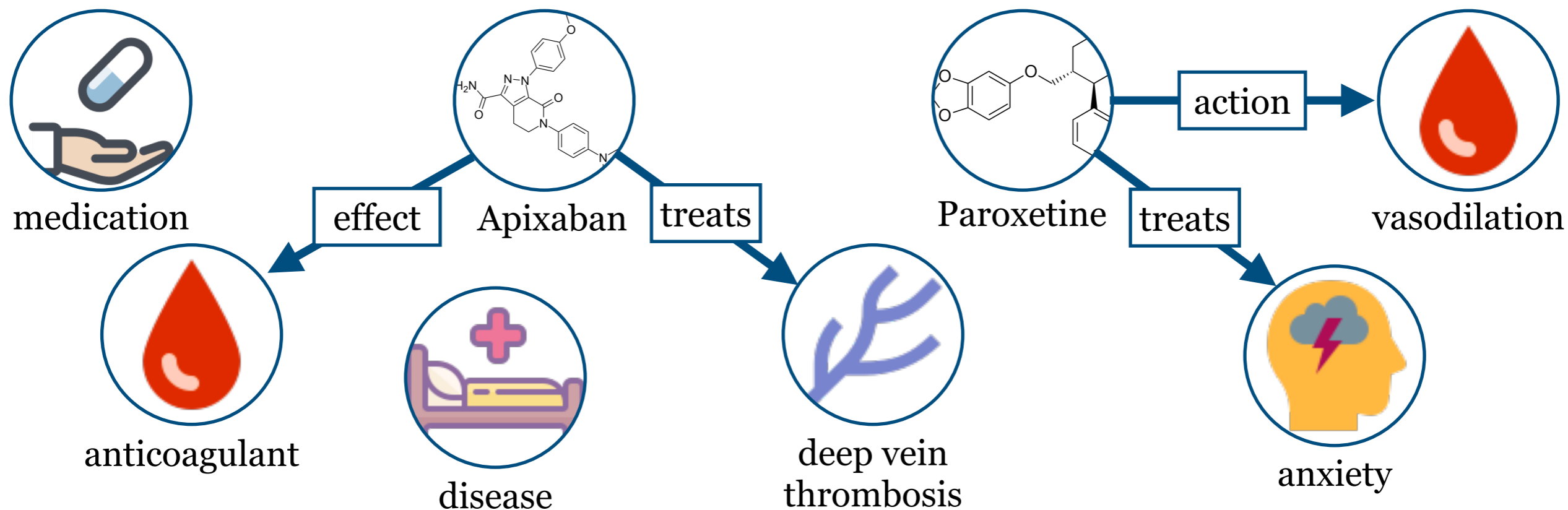
Erik Arakelyan\* Daniel Daza\* Pasquale Minervini\* Michael Cochez



UNIVERSITY  
OF AMSTERDAM

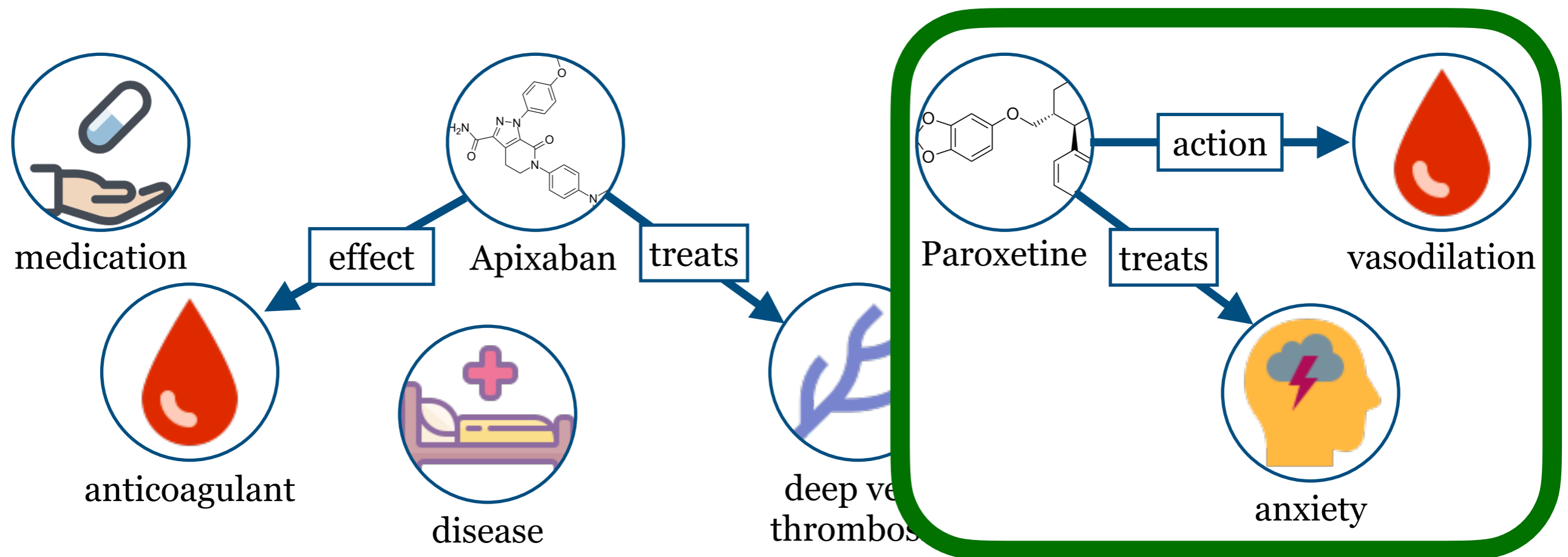
# Knowledge Graphs

**Knowledge Graph** — graph-structured Knowledge Base, where knowledge about the world is encoded in the form of *relationships between entities*



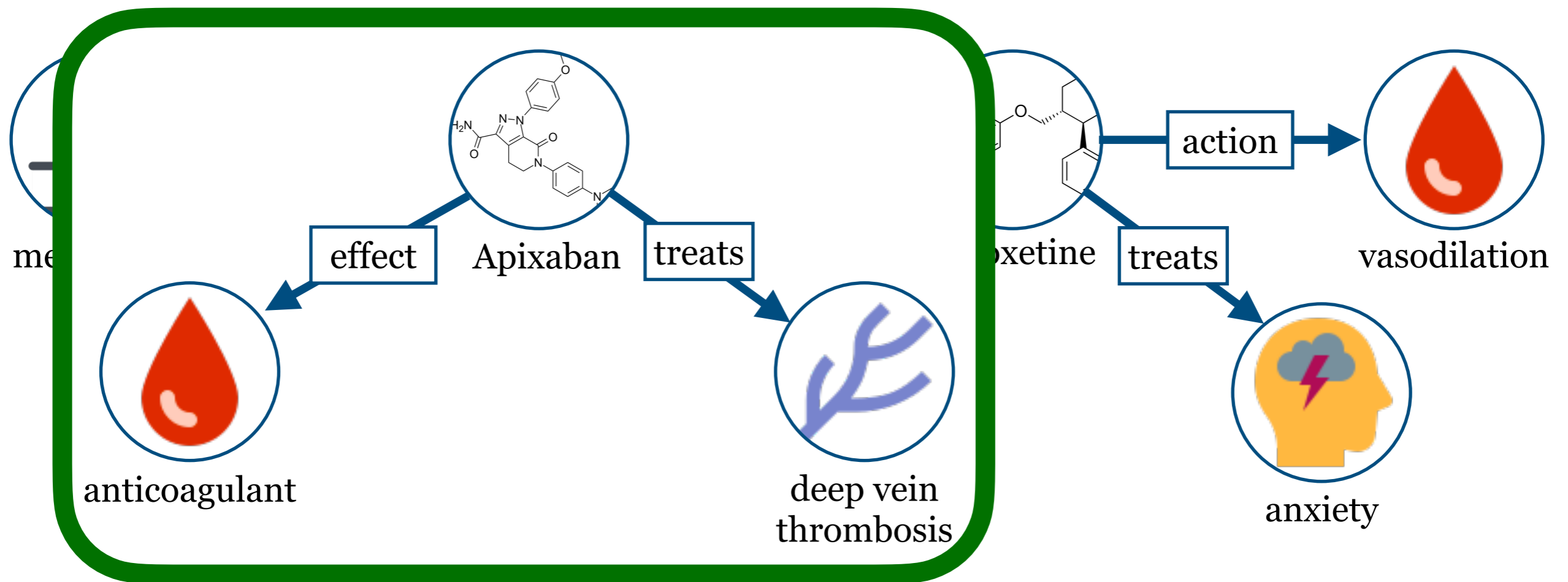
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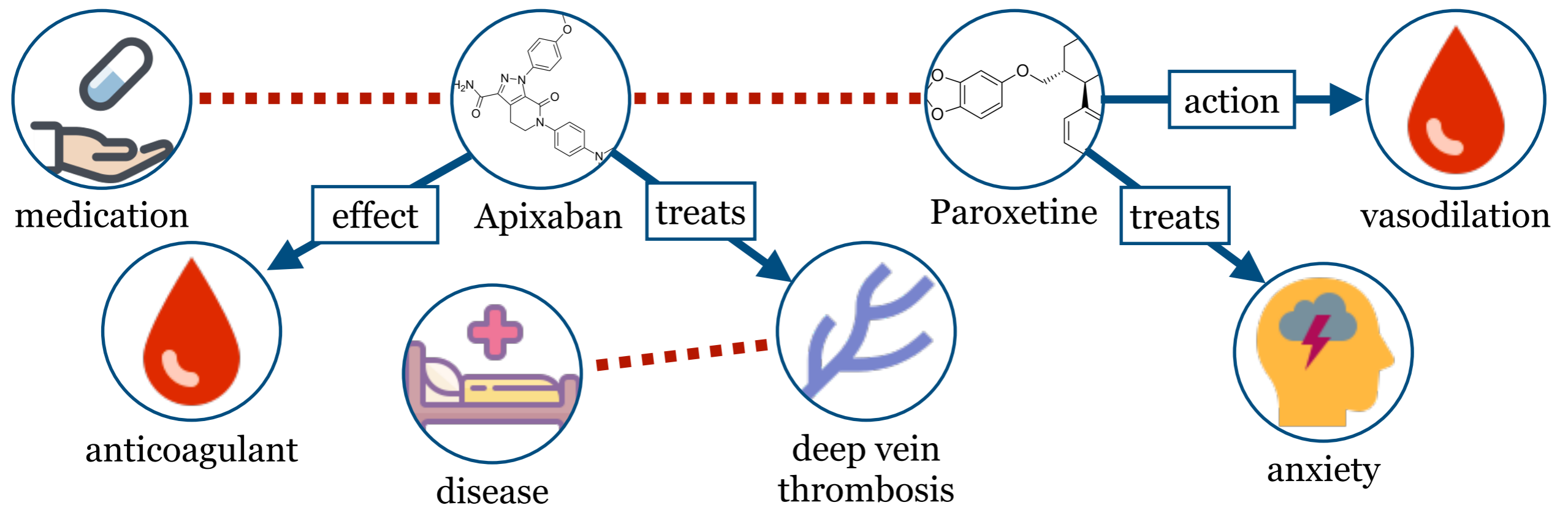
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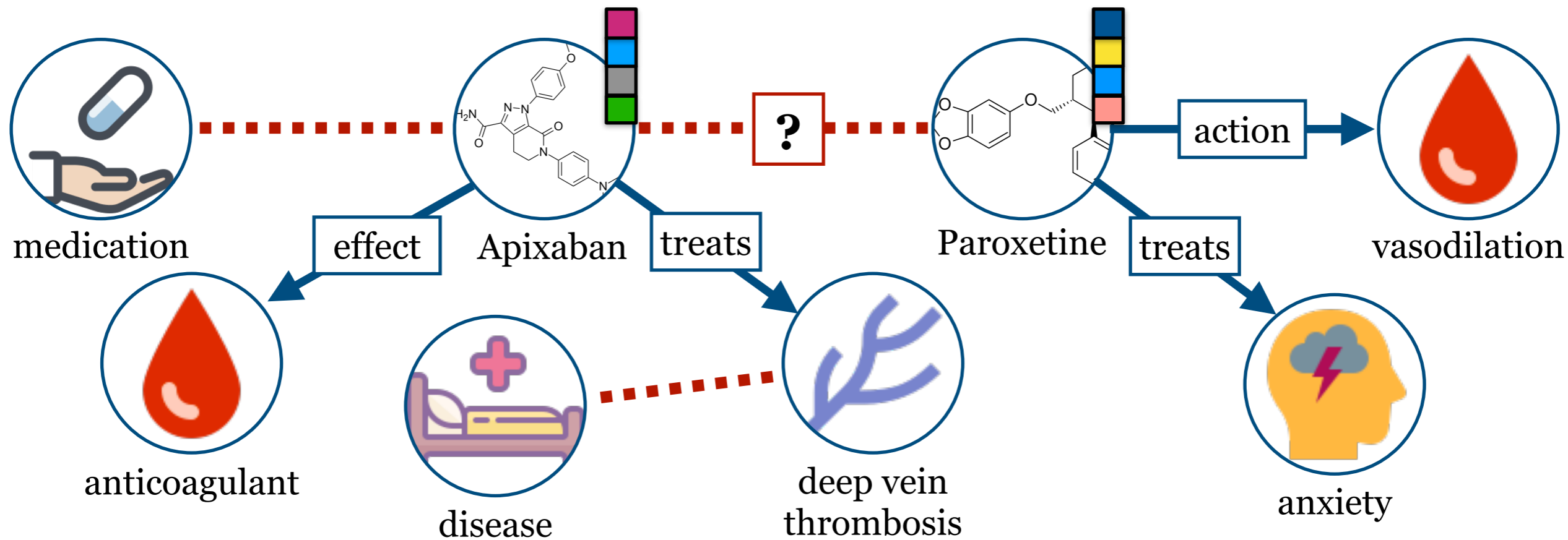


# Knowledge Graphs

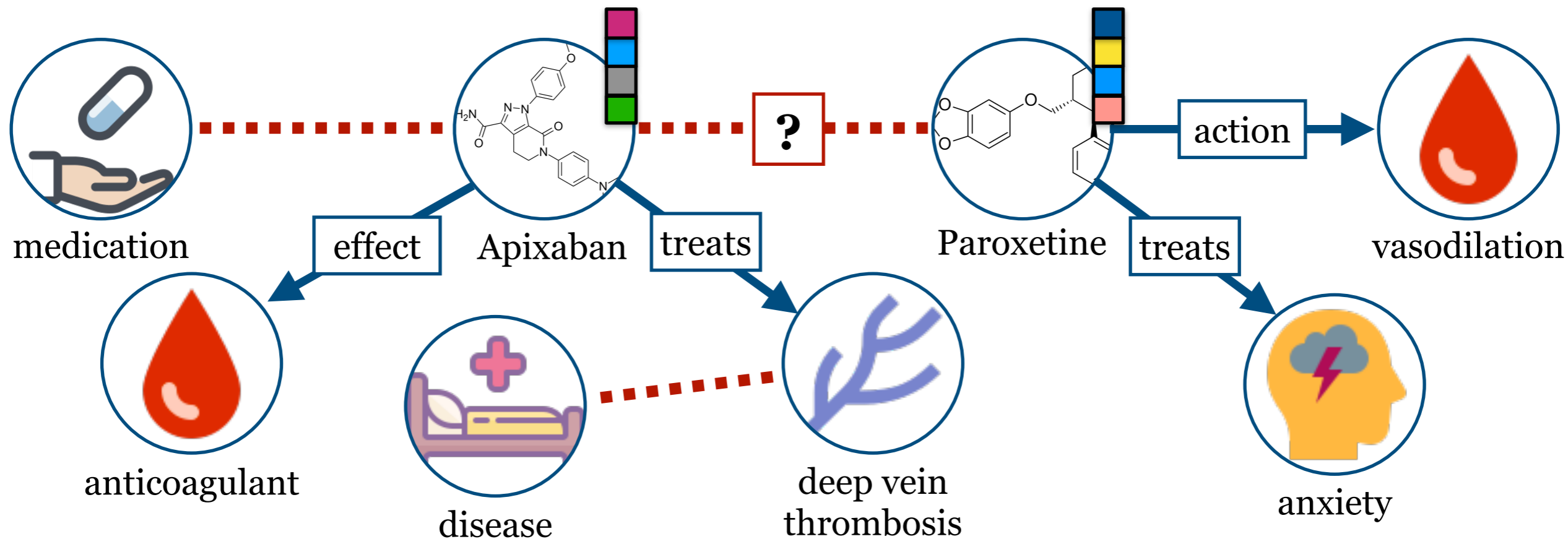
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# Neural Link Prediction

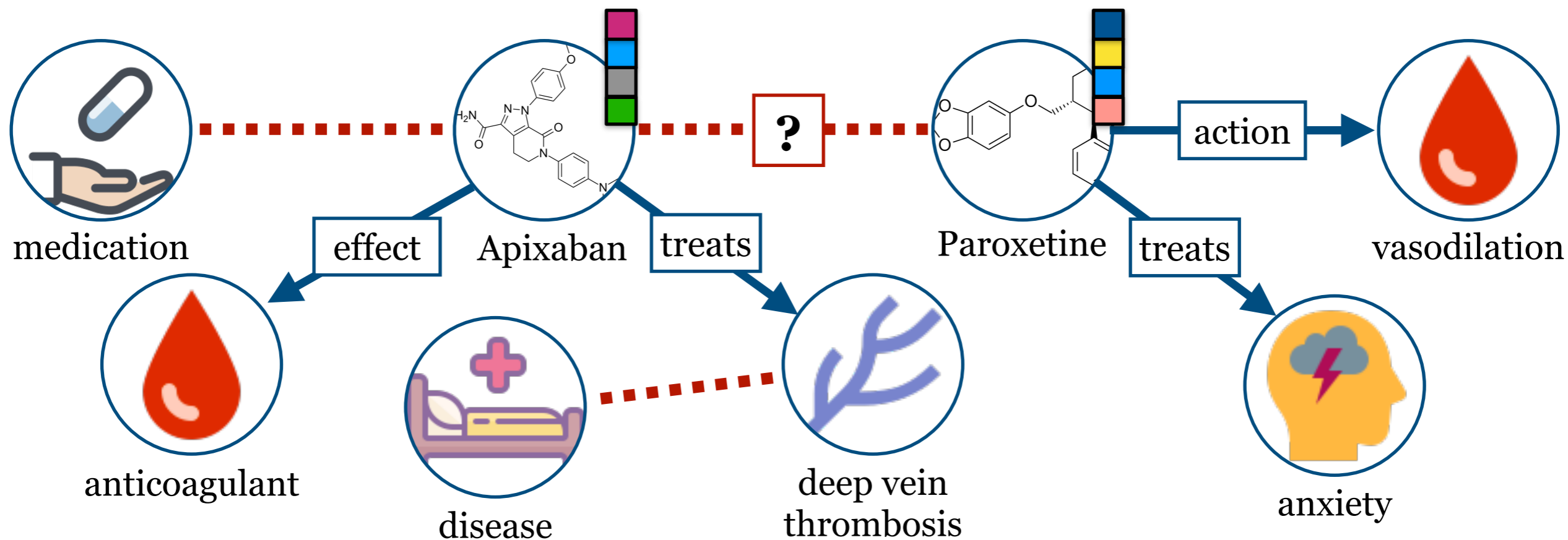


# Neural Link Prediction



$$P(\text{Apixaban} \xrightarrow{\text{interacts}} \text{Paroxetine}) \propto$$

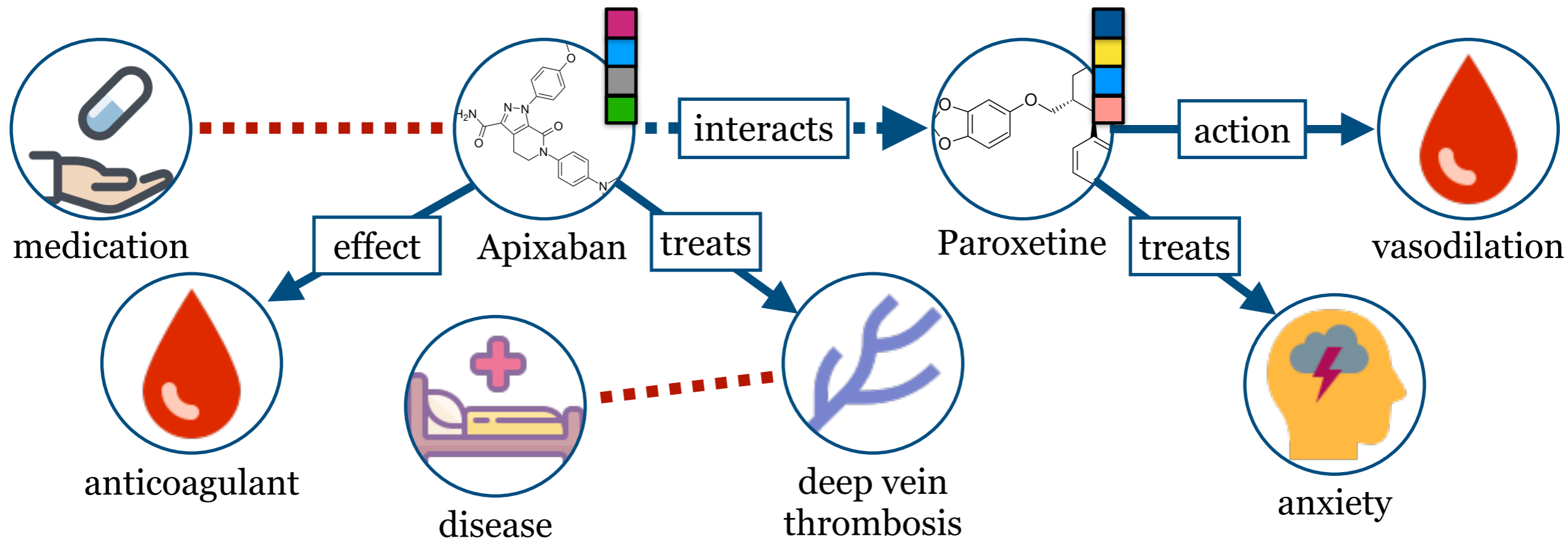
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$$P(\text{Apixaban} \xrightarrow{\text{interacts}} \text{Paroxetine}) \propto \phi_{\text{interacts}} \left( \begin{matrix} \text{Apixaban} \\ \text{Paroxetine} \end{matrix} \right)$$



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# Complex Queries on Incomplete Graphs

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BetaE — Ren et al. [ICLR 2020]

Q2B — Ren et al. [NeurIPS 2020]

GQE — Hamilton et al. [NeurIPS 2018]

**Process**

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## Process

1. Generate *millions* of complex query-answer pairs
2. Train a deep neural model to answer complex queries

# Complex Queries on Incomplete Graphs

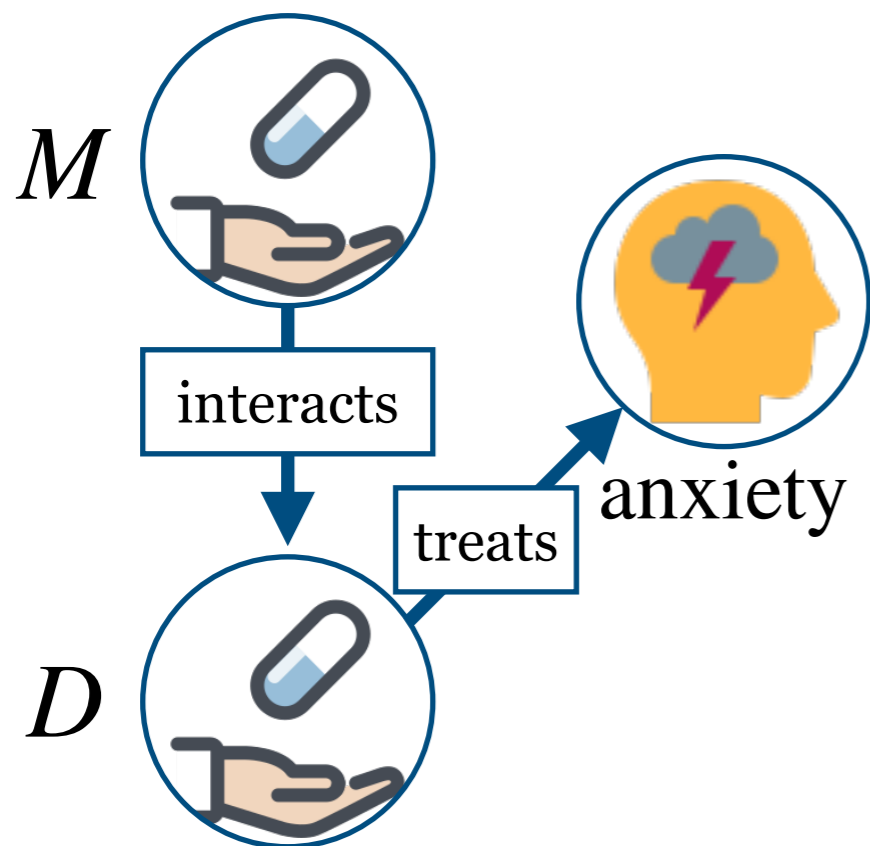
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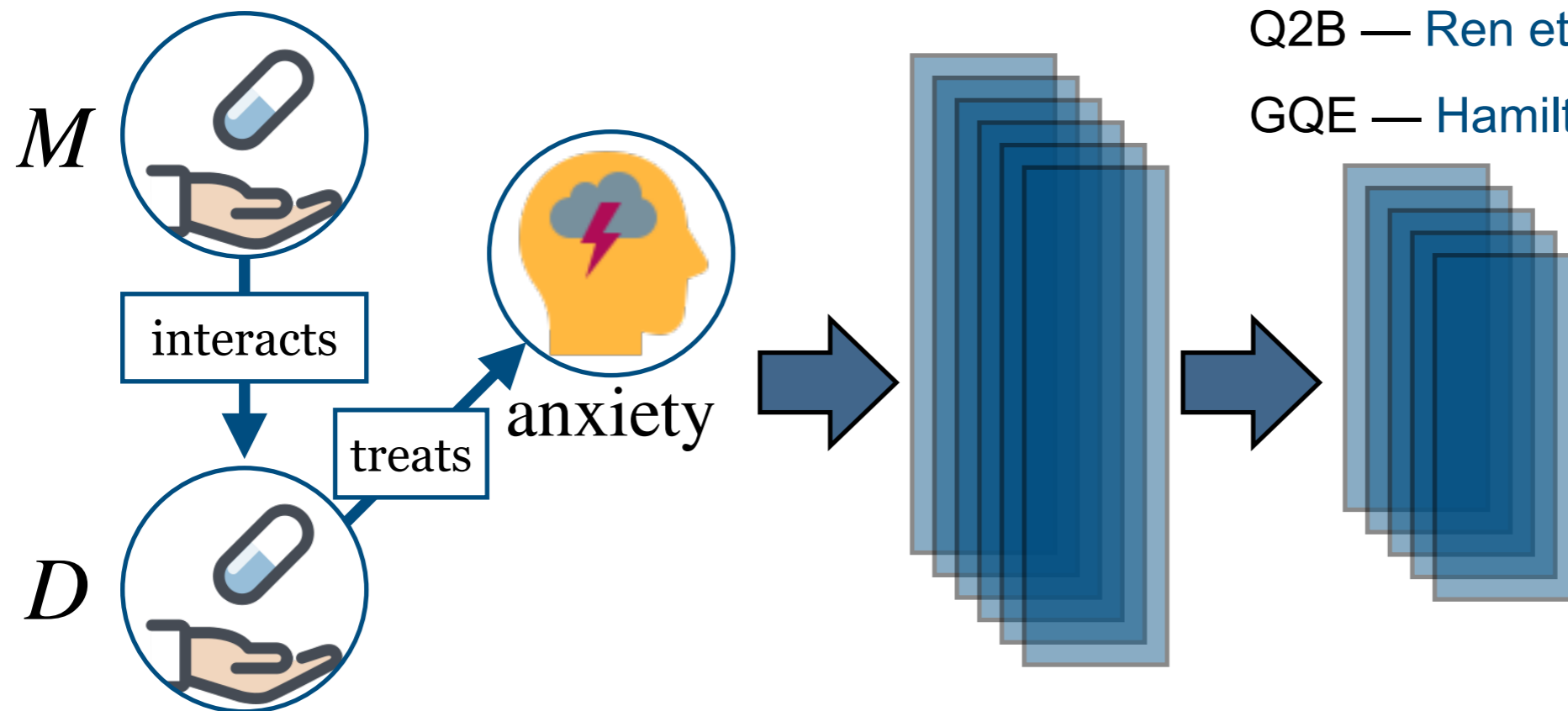
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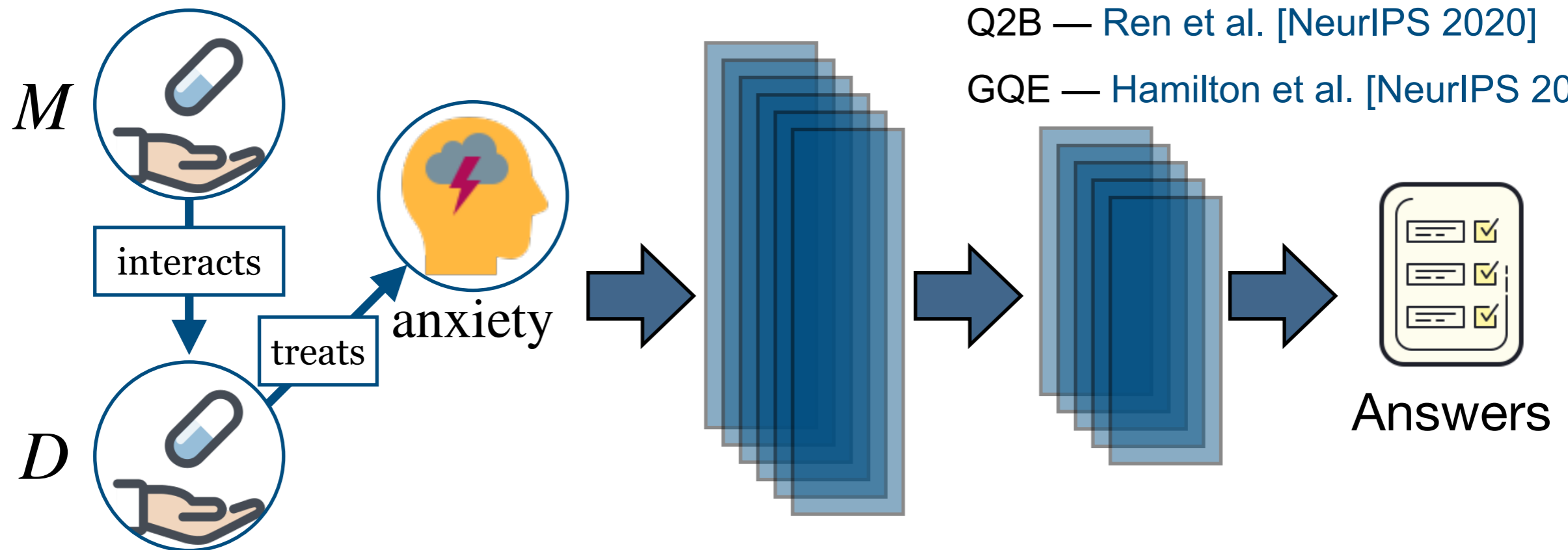
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## Problems

- Need to train the model on *millions* of generated queries — not clear what happens when evaluating on queries outside of training distribution

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## Problems

- Need to train the model on *millions* of generated queries — not clear what happens when evaluating on queries outside of training distribution
- No explanation on the reasons *why* a given answer was produced by the model

# Query Answering as Optimisation

**Proposed solution:** train a neural model  $\phi$  for answering atomic (simple) queries (e.g. “which drugs treat Anxiety?”), and cast the query answering task as an *optimisation problem*

$$?M : \exists D . \text{interacts}(M, D) \wedge \text{treats}(D, \text{anxiety})$$

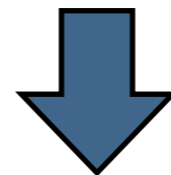


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Optimisation problem



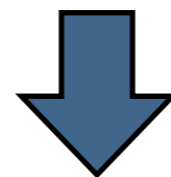
$$\arg \max_{M, D \in \mathcal{E}}$$

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Optimisation problem



$$\arg \max_{M, D \in \mathcal{E}}$$

$$\phi_{\text{interacts}}(\mathbf{e}_M, \mathbf{e}_D)$$

$$\phi_{\text{treats}}(\mathbf{e}_D, \mathbf{e}_{\text{anxiety}})$$

Likelihood that M interacts with D

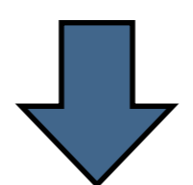
Likelihood that D treats anxiety

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Optimisation problem



Continuous relaxation of the logical AND (t-norm)

$$\arg \max_{M, D \in \mathcal{E}} \left[ \phi_{\text{interacts}}(\mathbf{e}_M, \mathbf{e}_D) \top \phi_{\text{treats}}(\mathbf{e}_D, \mathbf{e}_{\text{anxiety}}) \right]$$

Likelihood that M interacts with D

Likelihood that D treats anxiety

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## Greedy Search

# Query Answering as Optimisation

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## Greedy Search

- Identify the  $k$  most likely values for  $D$

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- Compute the query score for all  $(M, D)$  combinations

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- For each value of  $D$ :
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- Compute the query score for all  $(M, D)$  combinations
- Return the most likely value for  $(M, D)$

# Query Answering as Optimisation

$$\arg \max_{\mathbf{e}_M, \mathbf{e}_D \in \mathbb{R}^k} \left[ \phi_{\text{interacts}}(\mathbf{e}_M, \mathbf{e}_D) \top \phi_{\text{treats}}(\mathbf{e}_D, \mathbf{e}_{\text{anxiety}}) \right]$$

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## Gradient-Based Search

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- Initialise  $\mathbf{e}_M$  and  $\mathbf{e}_D$  randomly

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## Gradient-Based Search

- Initialise  $\mathbf{e}_M$  and  $\mathbf{e}_D$  randomly
- Optimise  $\mathbf{e}_M$  and  $\mathbf{e}_D$  via Gradient Ascent to maximise the score of the query

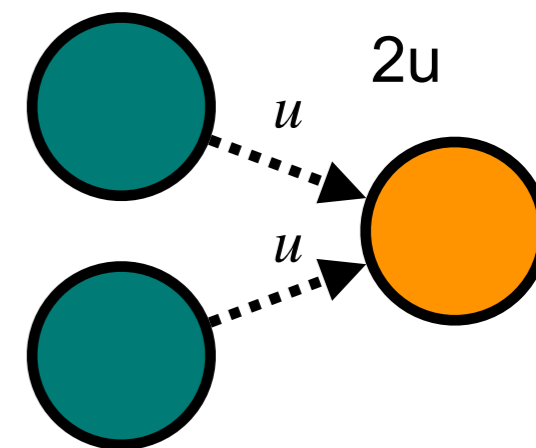
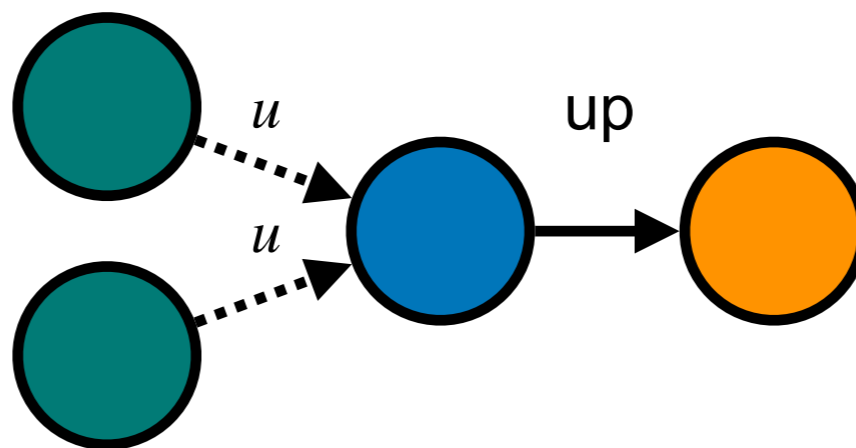
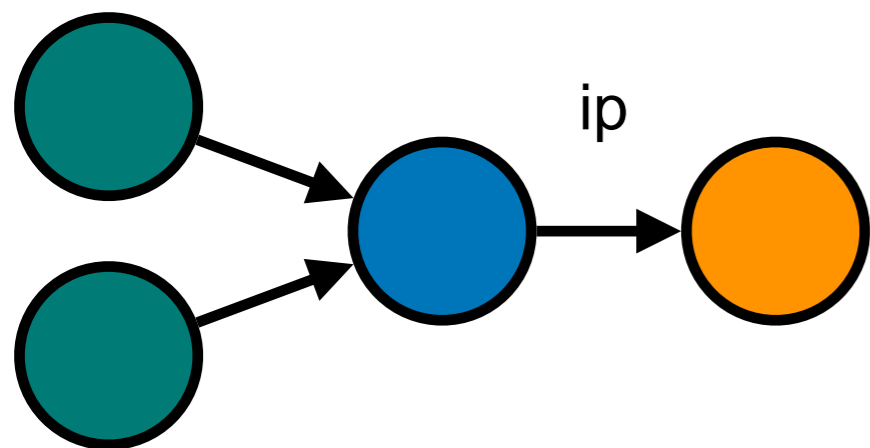
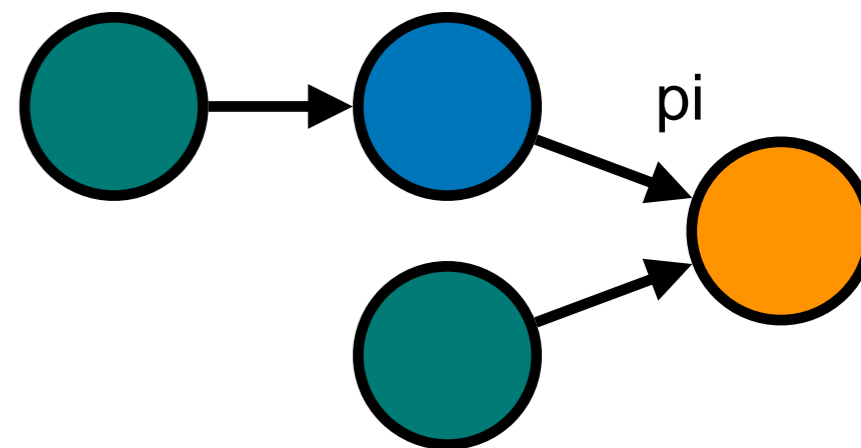
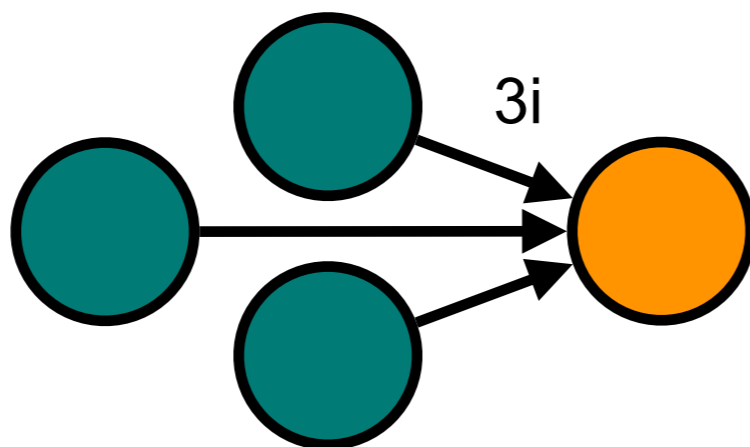
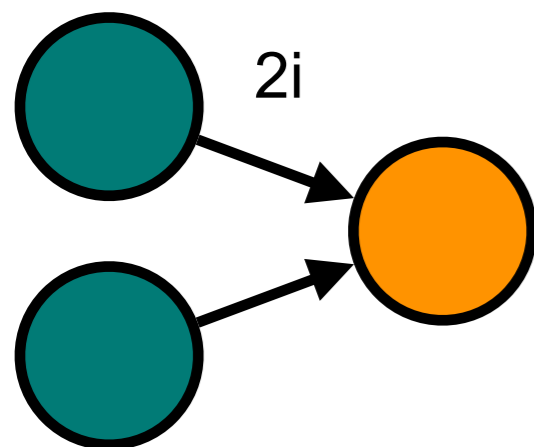
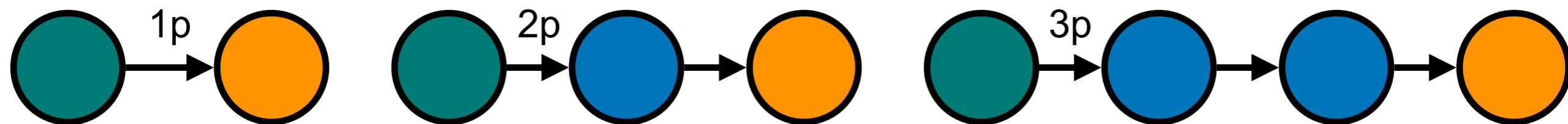
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- Initialise  $\mathbf{e}_M$  and  $\mathbf{e}_D$  randomly
- Optimise  $\mathbf{e}_M$  and  $\mathbf{e}_D$  via Gradient Ascent to maximise the score of the query
- Replace  $\mathbf{e}_M$  with the representations of all entities, and rank them based on the resulting query score

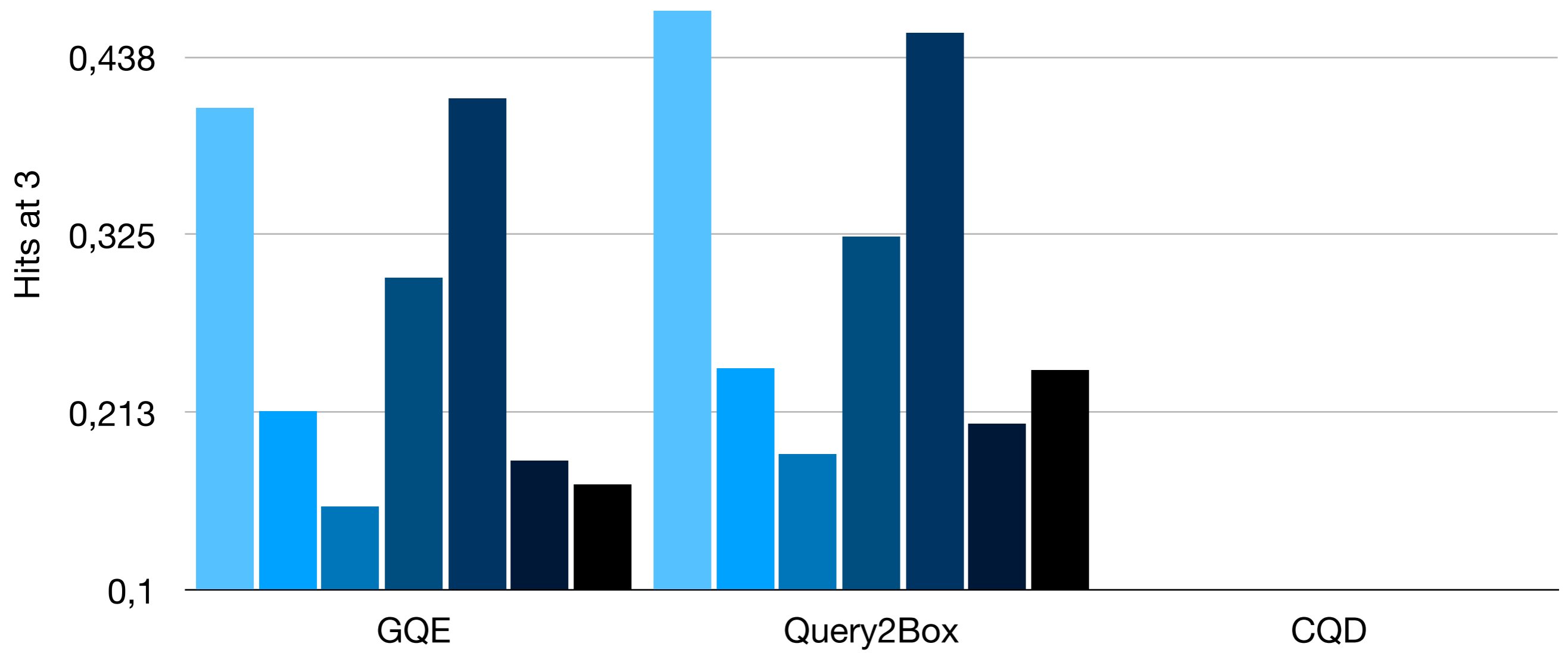
# Types of Complex Queries





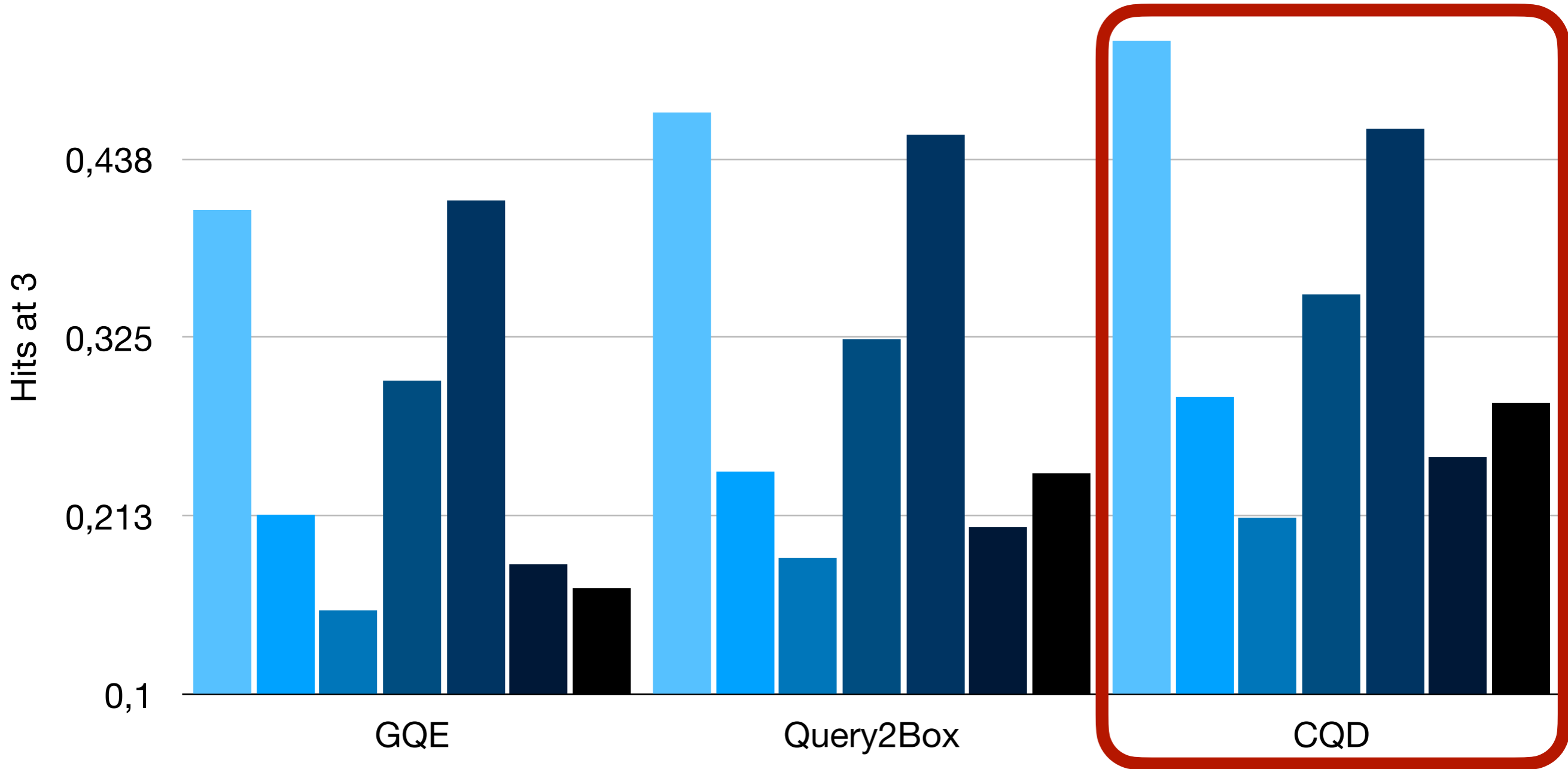
# Experiments

Query types: 0,55 1p 2p 3p 2i 3i pi 2u Dataset: FB15k-237

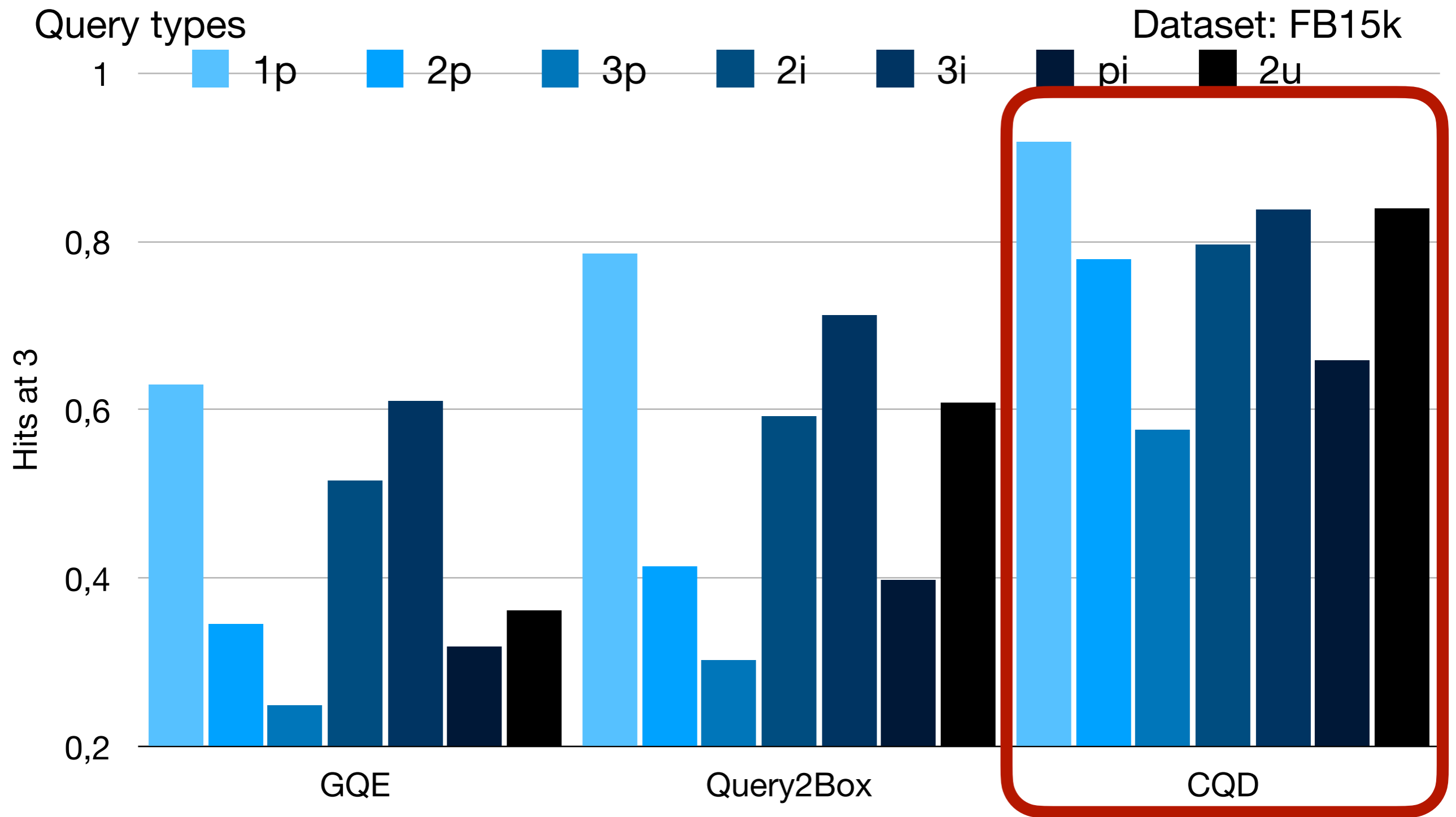


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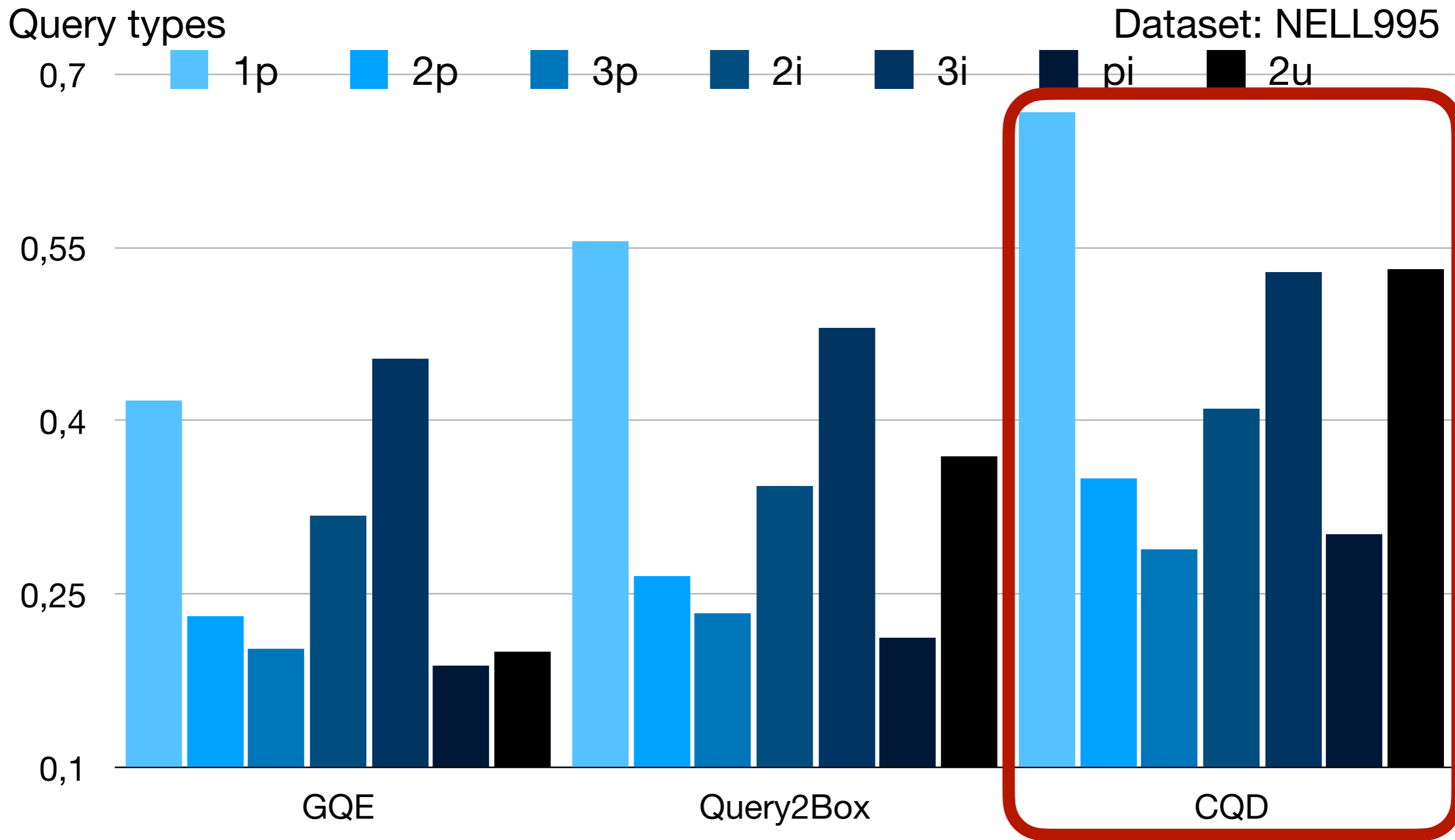
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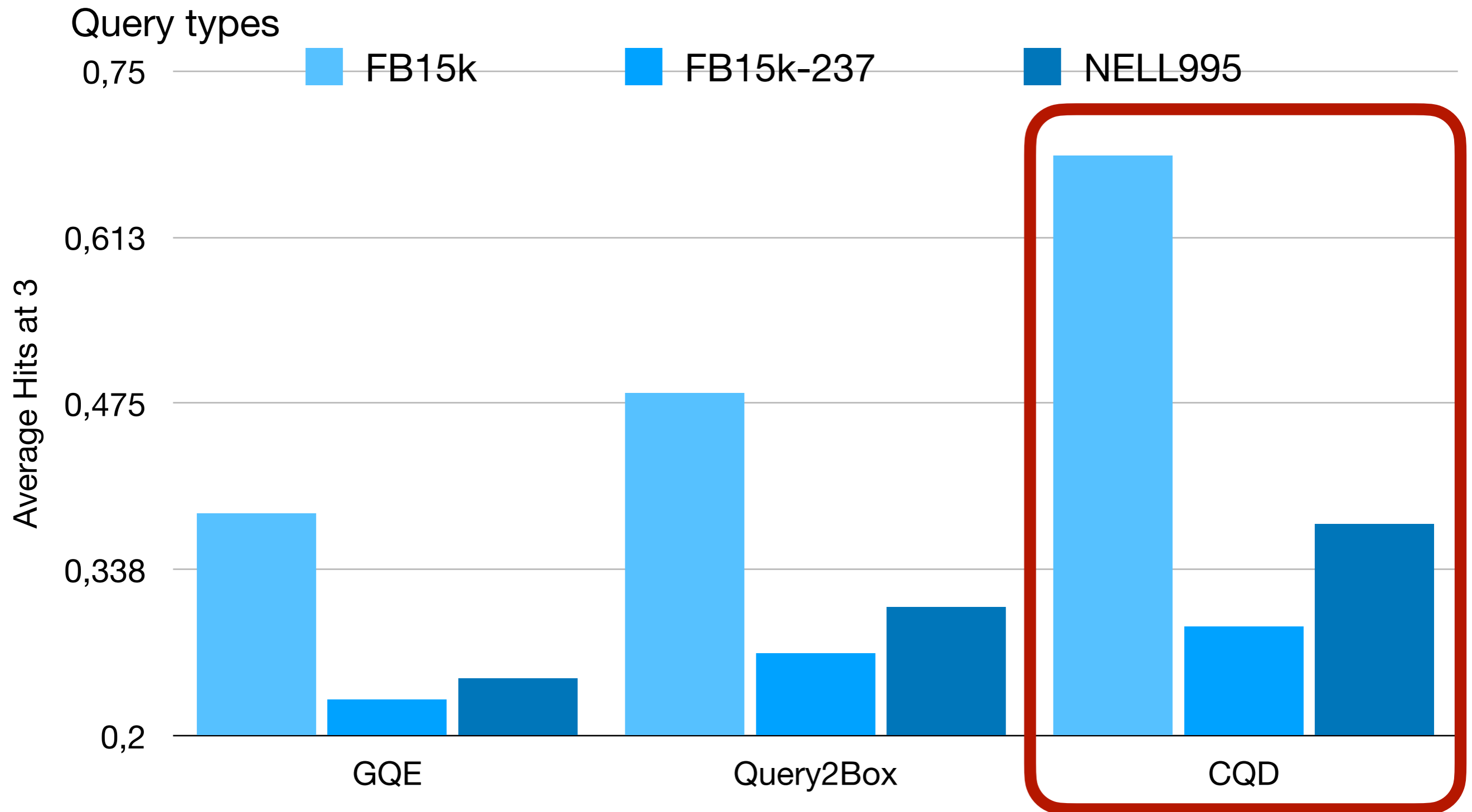
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Query types

0,75



FB15k



FB15k-237



NELL995

Average Hits at 3

0,613

• Data-Efficient

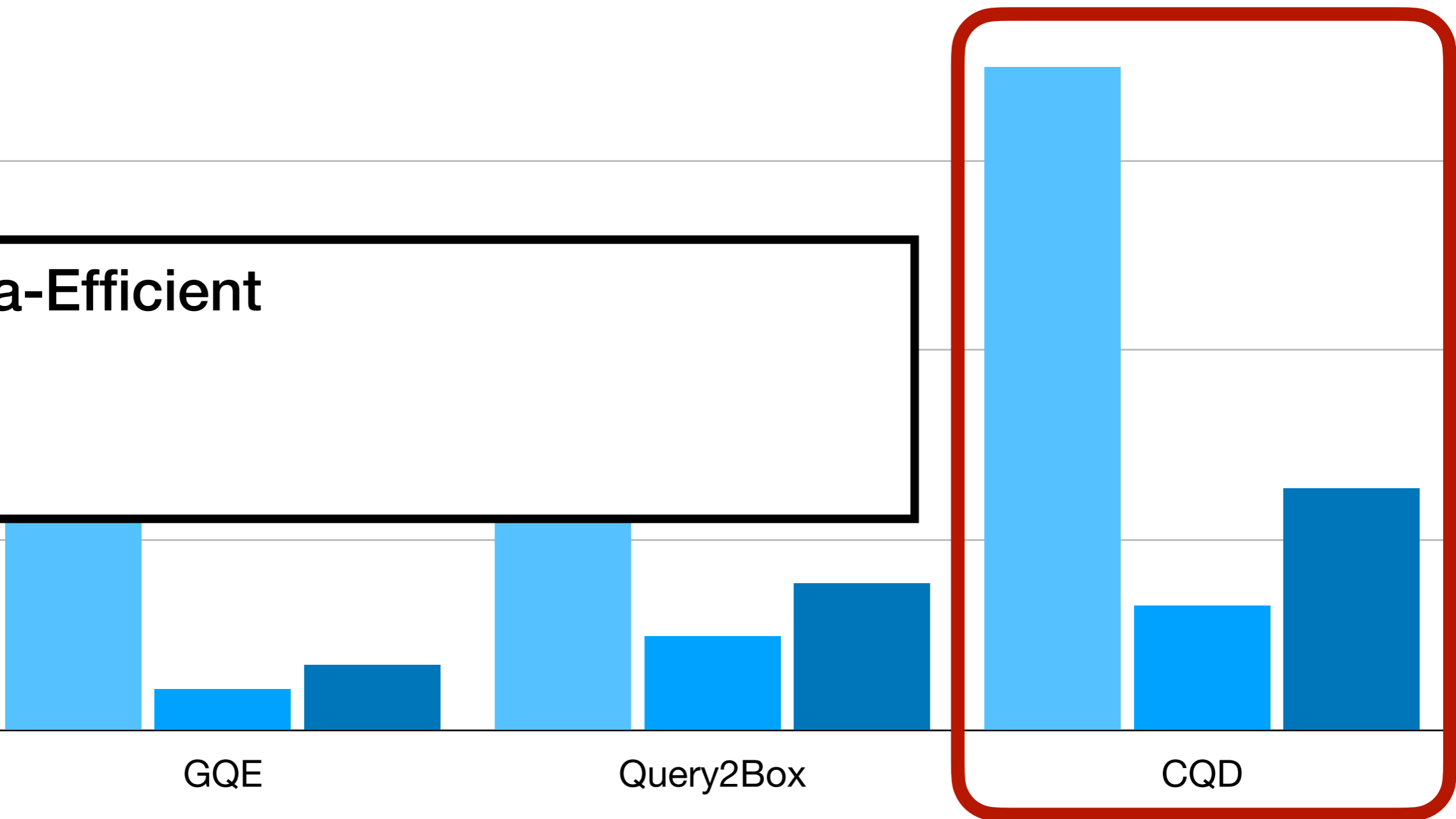
0,338

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GQE

Query2Box

CQD




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Average Hits at 3

- Data-Efficient
- Generalisation to Out-of-Distribution instances

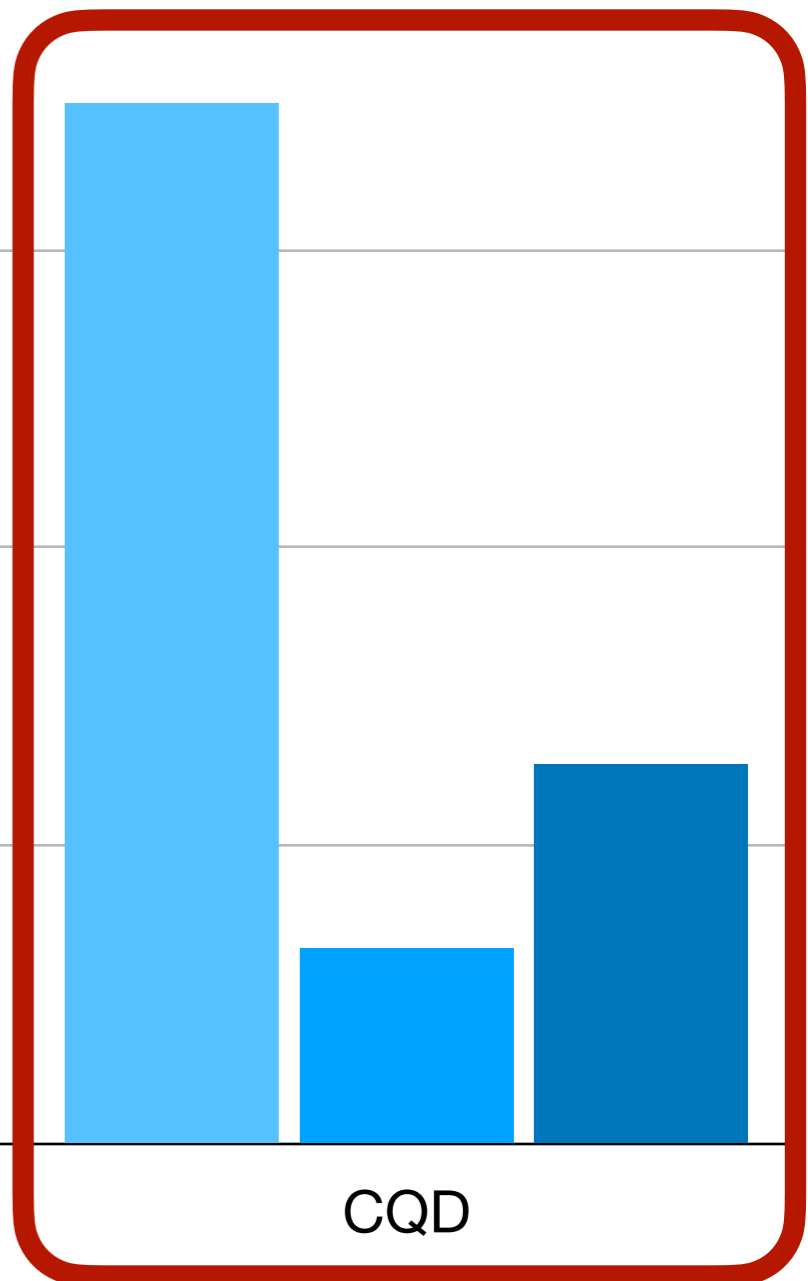
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# Explainability

**Query:** Which medications have side-effects when taken with drugs for treating Anxiety?

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*M*

Apixaban

Amitriptyline

Phenytoin

Duloxetine

Buprenorphine



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<i>M</i>	<i>D</i>	• Explainable
Apixaban	Paroxetine	
Amitriptyline	Paroxetine	
Phenytoin	Paroxetine	
Duloxetine	Pregabalin	
Buprenorphine	Pregabalin	

# Explainability

**Query:** What international organisations contain the country of nationality of Thomas Aquinas?

$?O : \exists C . \text{nationality} (T . \text{Aquinas}, C) \wedge \text{member} (C, O)$

O	C
NATO	United States
OECD	United States
EU	United States
NATO	United Kingdom
OECD	United Kingdom
EU	United Kingdom
OECD	Germany
EU	Germany
WTO	Germany

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Source code: <https://github.com/uclnlp/ctp/>