Answering Complex Queries on Very Large and Incomplete Knowledge Graphs

Pasquale Minervini
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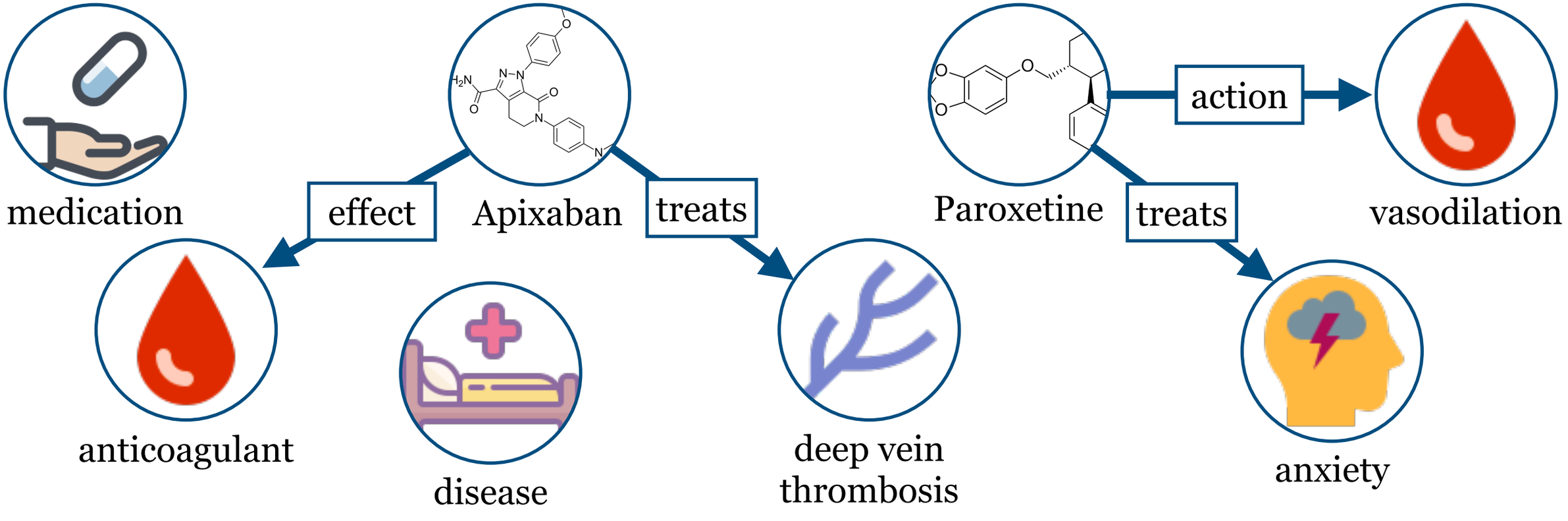
Complex Query Answering with Neural Link Predictors

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

Outstanding Paper Award 🏆 @ ICLR 2021

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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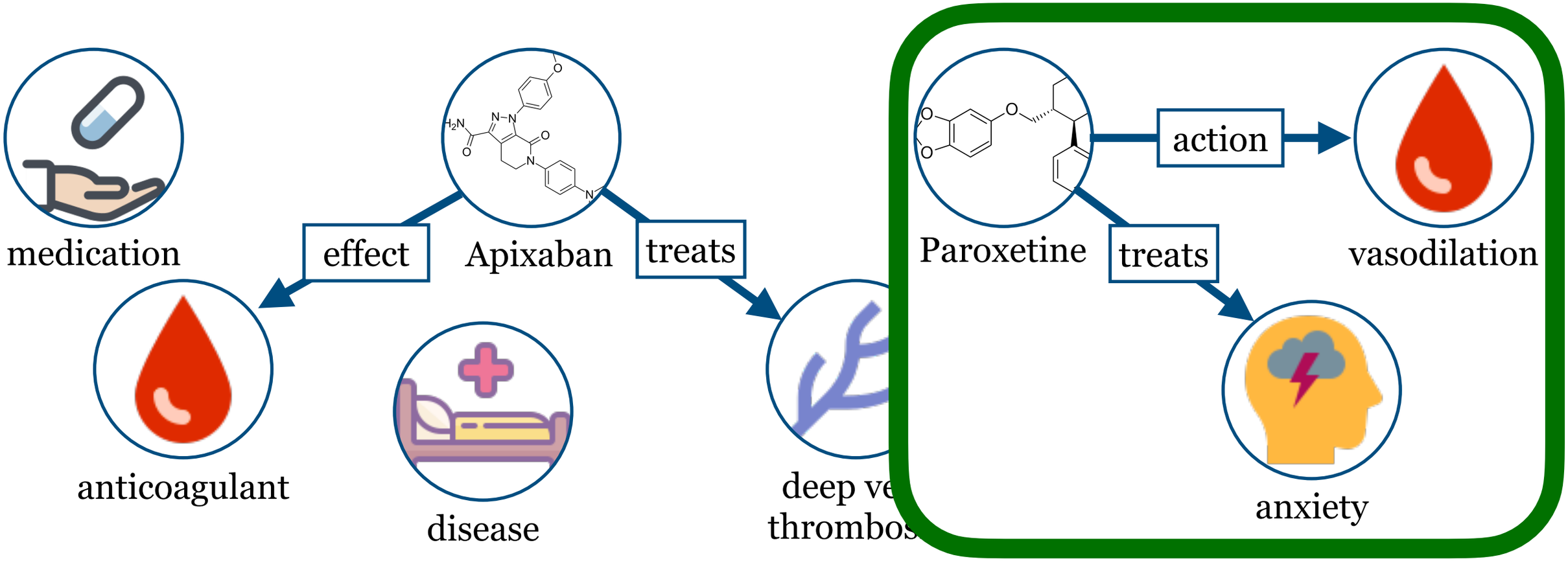

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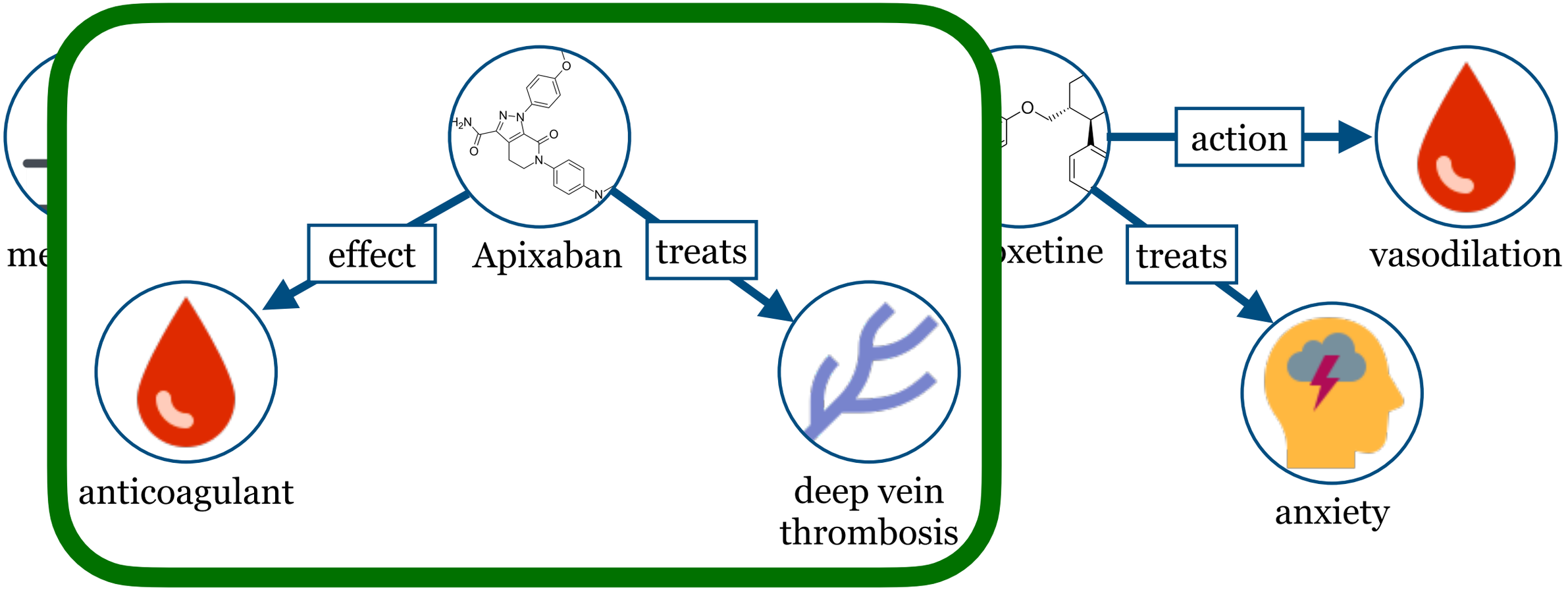

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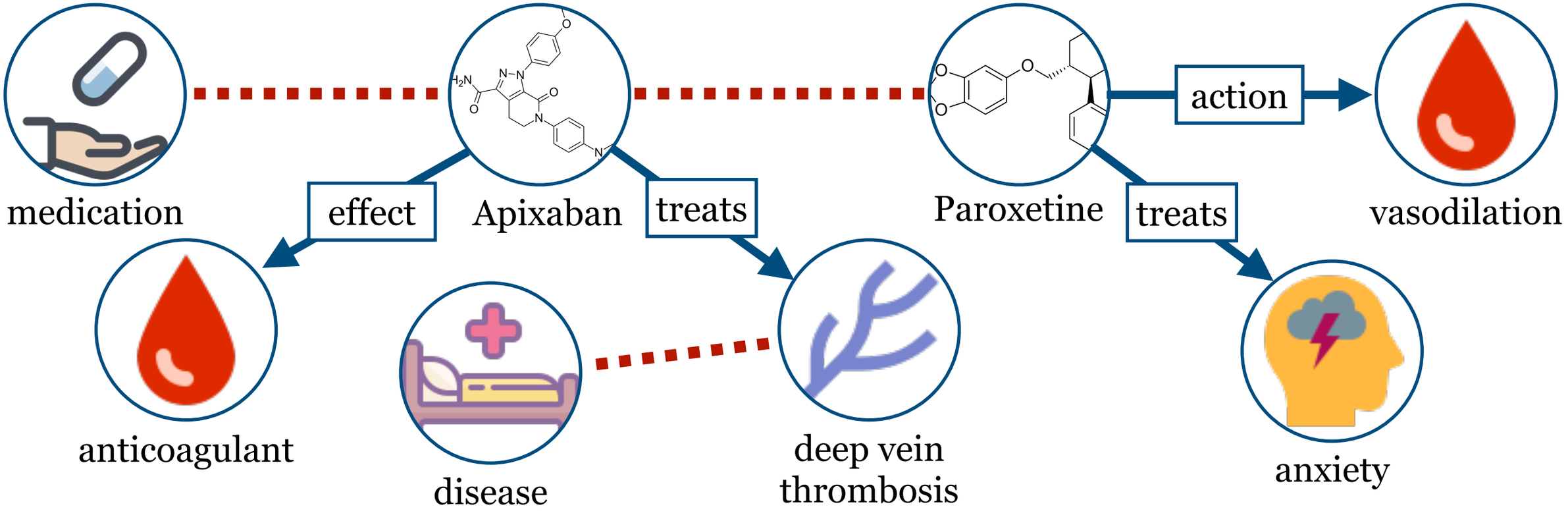
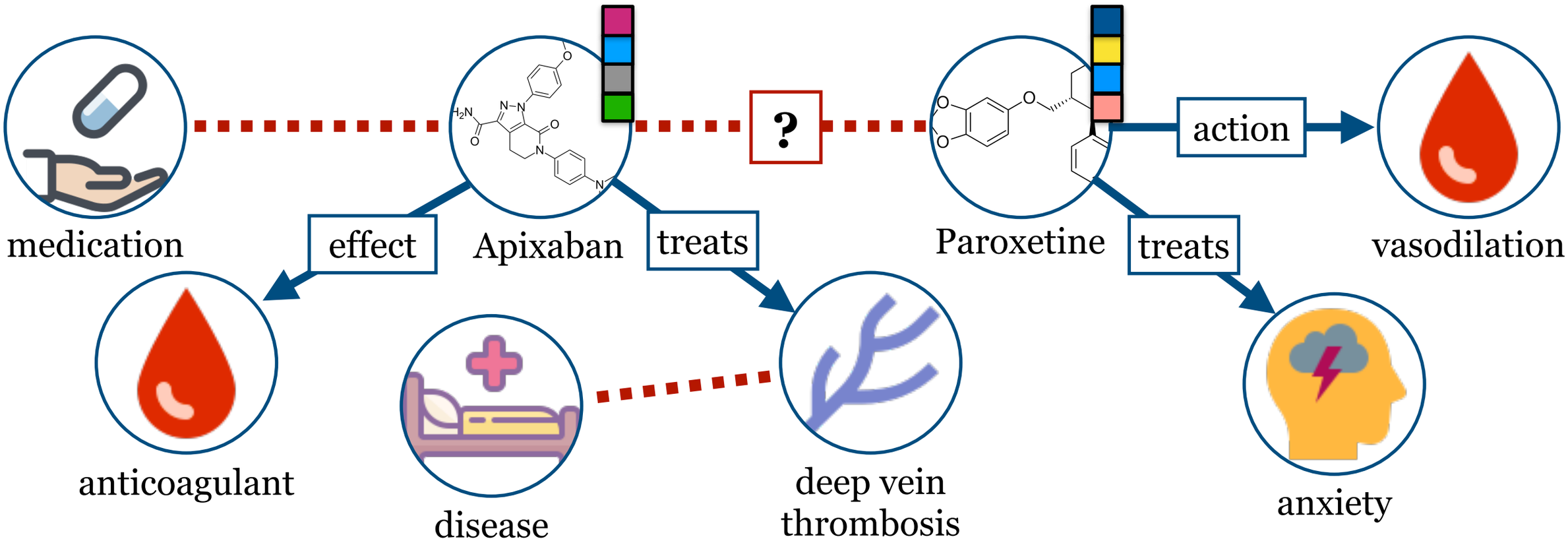


Neural Link Prediction



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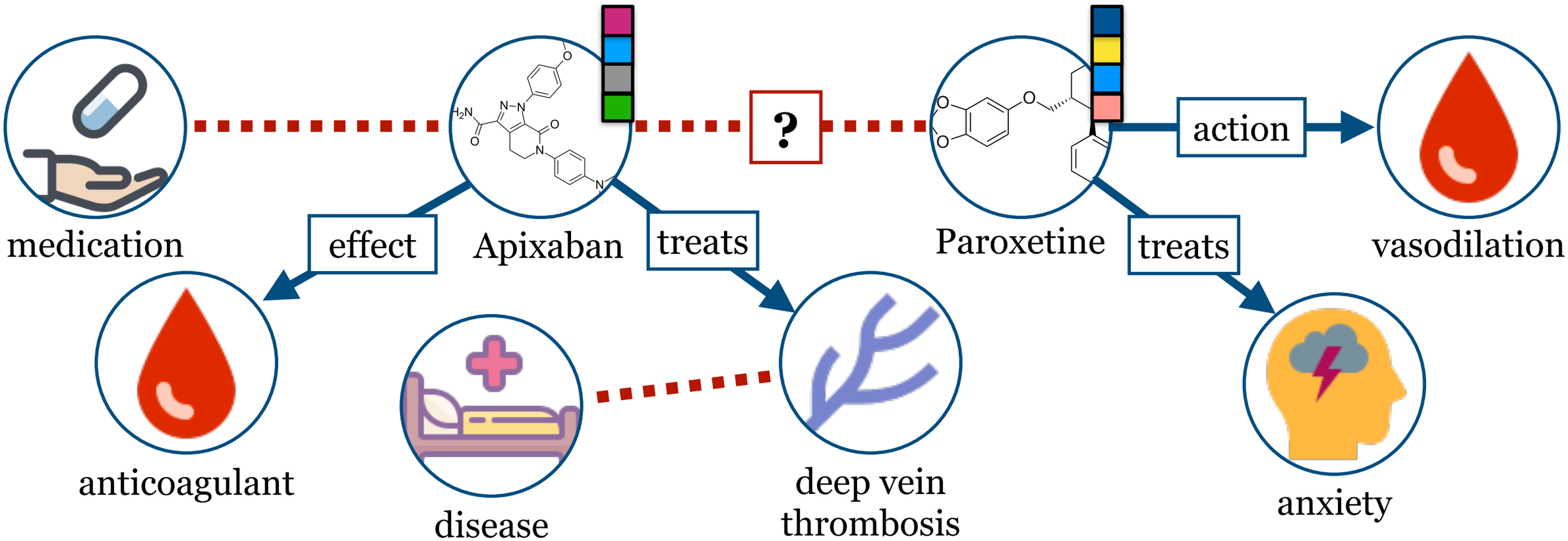

$$P(\text{Apixaban} \xrightarrow{\text{interacts}} \text{Paroxetine}) \propto$$

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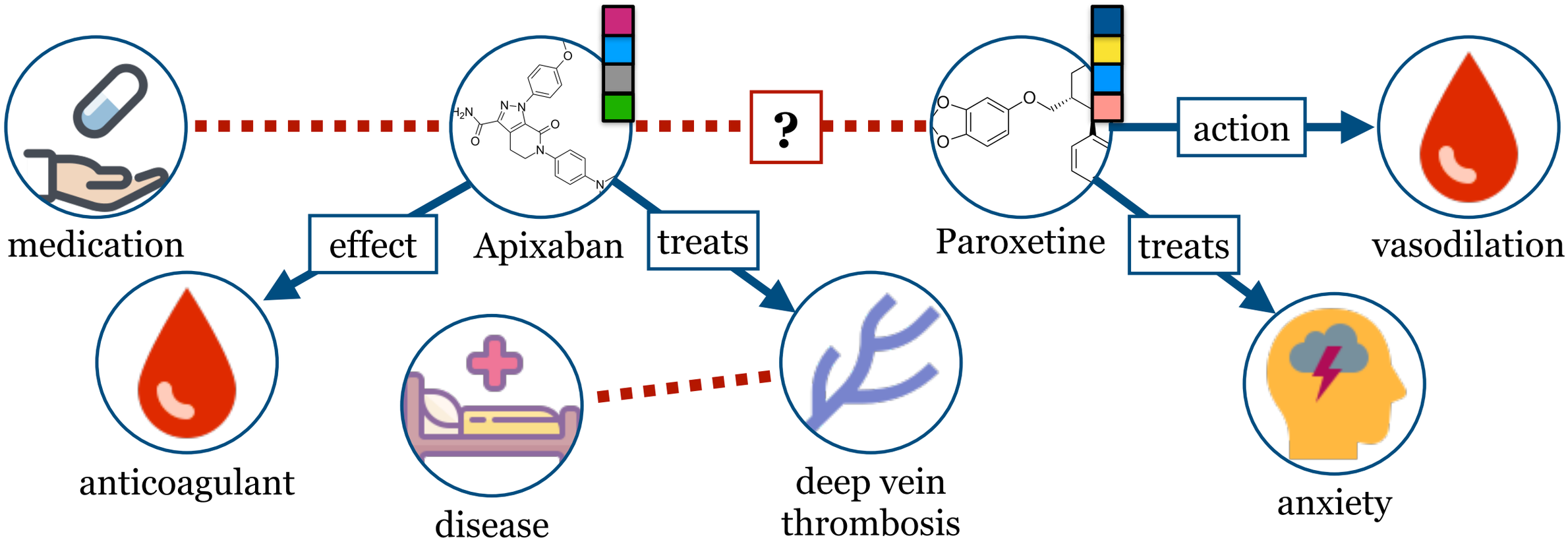
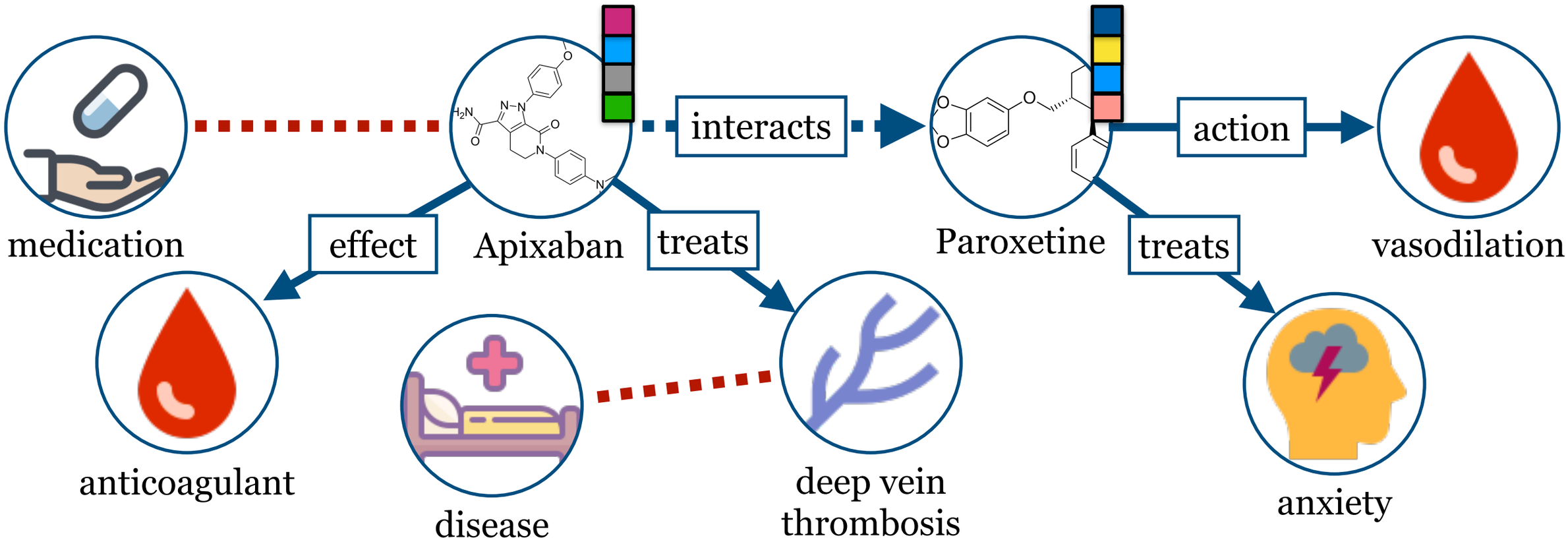


$$P(\text{Apixaban} \xrightarrow{\text{interacts}} \text{Paroxetine}) \propto \phi_{\text{interacts}}\left(\text{Apixaban}, \text{Paroxetine} \right)$$

Neural Link Prediction



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Complex Queries on Incomplete Graphs

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

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$$?M$$

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

Complex Queries on Incomplete Graphs

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

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

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BetaE — Ren et al. [ICLR 2020]

Q2B — Ren et al. [NeurIPS 2020]

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Process

Complex Queries on Incomplete Graphs

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1. Generate *millions* of complex query-answer pairs

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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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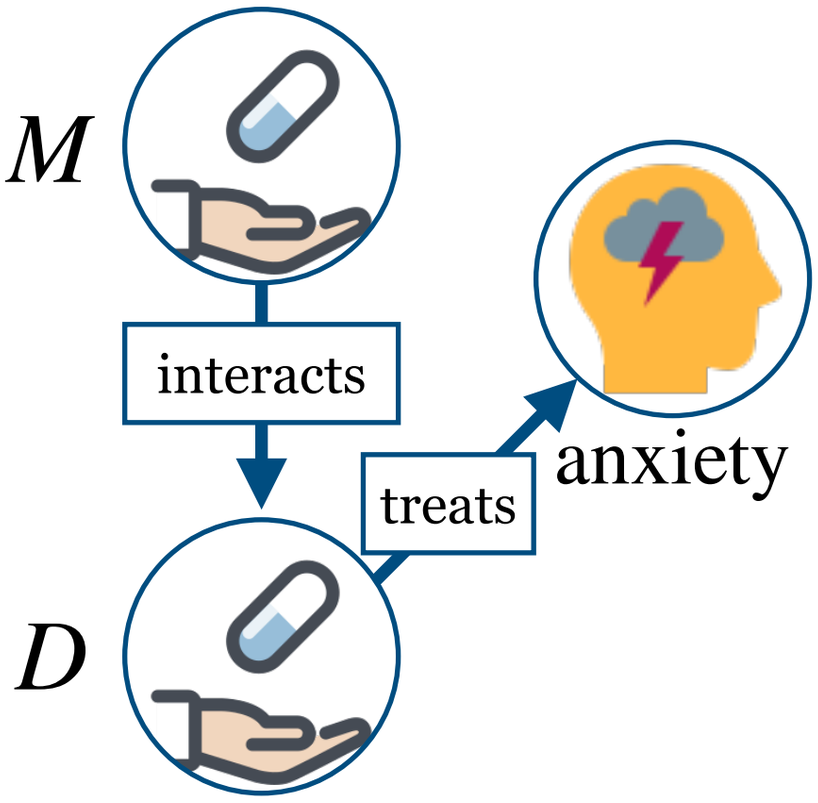

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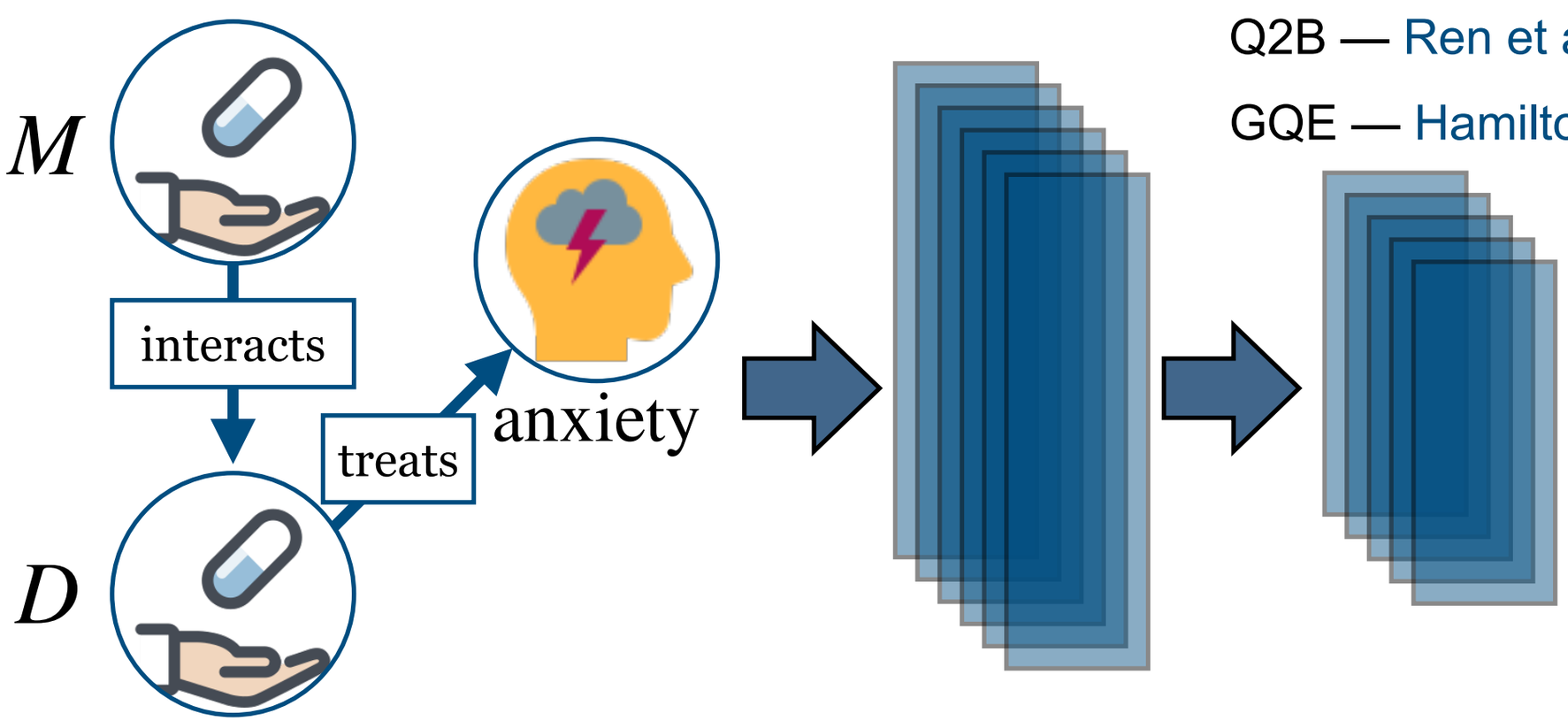

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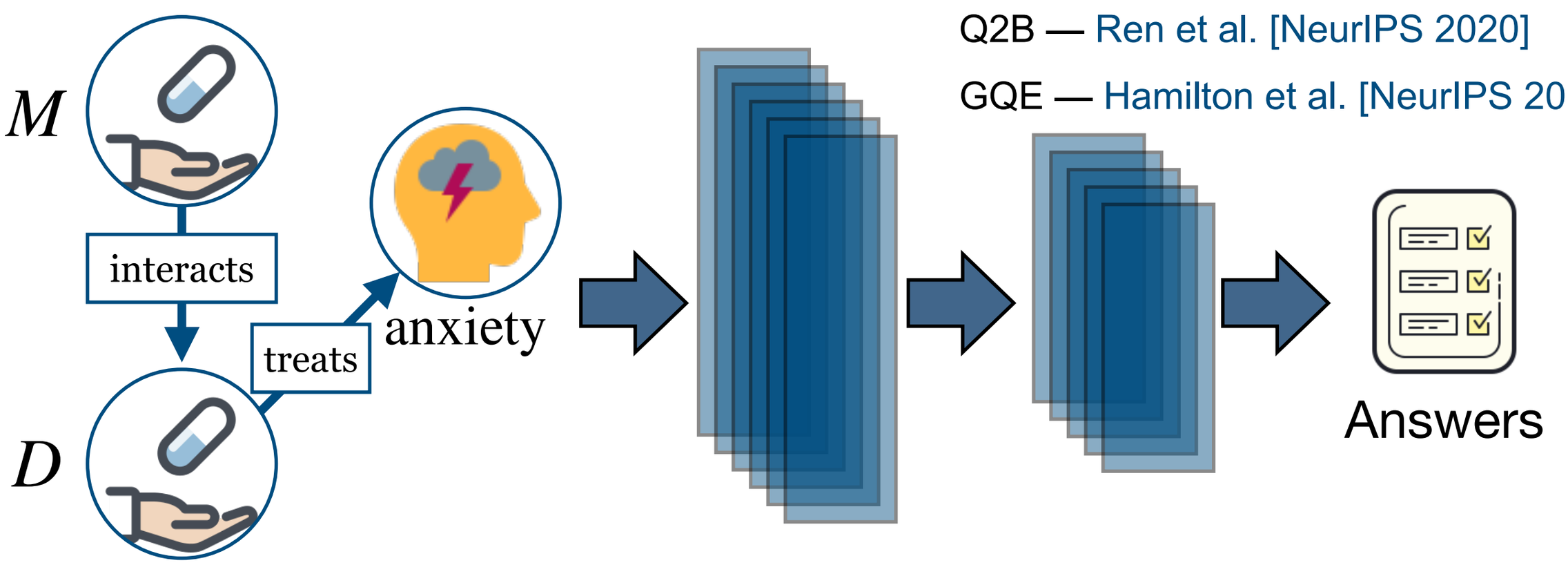

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Problems

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Problems

- Need to train the model on *millions* of generated queries
- No explanation on the reasons *why* a given answer was produced by the model

Query Answering as Optimisation

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

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Optimisation problem

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

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Optimisation problem

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

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**)

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

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Greedy Search

Query Answering as Optimisation

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

Greedy Search

- Identify the k most likely values for D

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- For each value of D:

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

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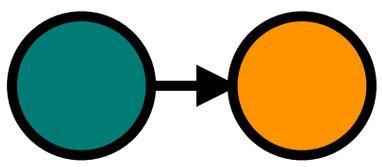
Greedy Search

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

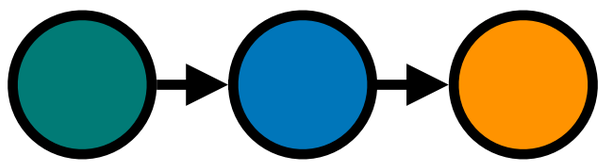
Complex Query Types 1/2

1p (atomic)



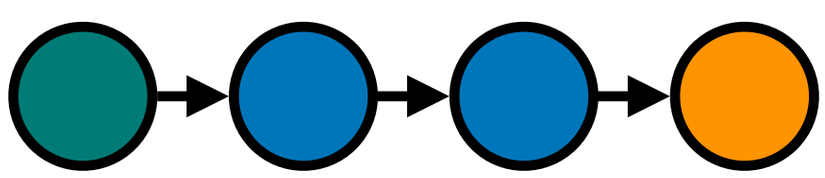
$$?T : p(a, T)$$

2p



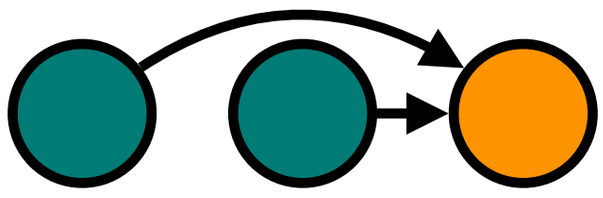
$$?T : \exists V_1 \,.\, p_1(a, V_1) \wedge p_2(V_1, T)$$

3p



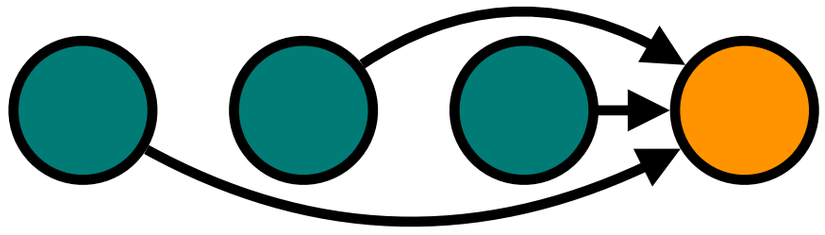
$$?T : \exists V_1, V_2 \,.\, p_1(a, V_1) \wedge p_2(V_1, V_2) \wedge p_3(V_2, T)$$

2i

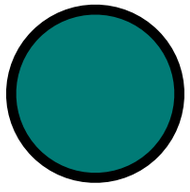


$$?T : p_1(a_1, T) \wedge p_2(a_2, T)$$

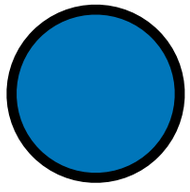
3i



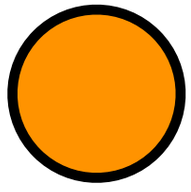
$$?T : p_1(a_1, T) \wedge p_2(a_2, T) \wedge p_3(a_3, T)$$



Anchor



Variable



Target

Complex Query Types 2/2

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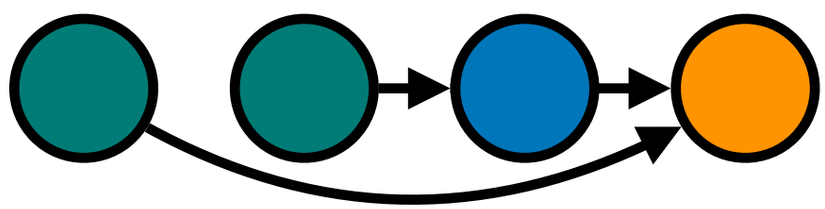
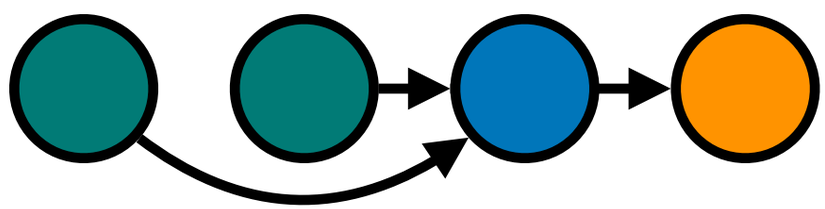


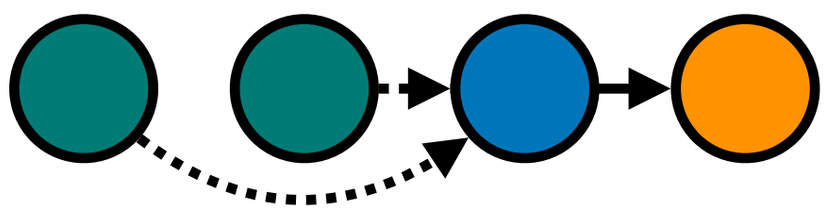
$$?T : \exists V \,.\, p_1(a_1, V) \wedge p_2(V, T) \wedge p_3(a_2, T)$$

ip



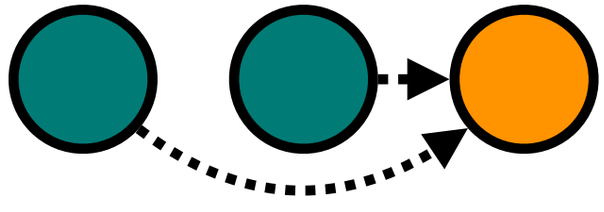
$$?T : \exists V \,.\, p_1(a_1, V) \wedge p_2(a_2, V) \wedge p_3(V, T)$$

up



$$?T : \exists V \,.\, \left[p_1(a_1, V) \vee p_2(a_2, V)\right] \wedge p_3(V, T)$$

2u



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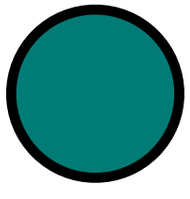

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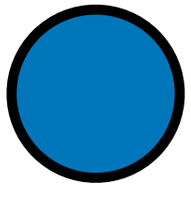
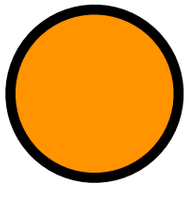


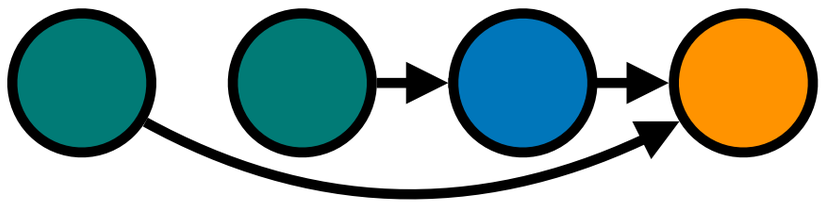
Variable



Target

Complex Queries — Examples

pi



$$?T : \exists V \,.\, p_1(a_1, V) \wedge p_2(V, T) \wedge p_3(a_2, T)$$

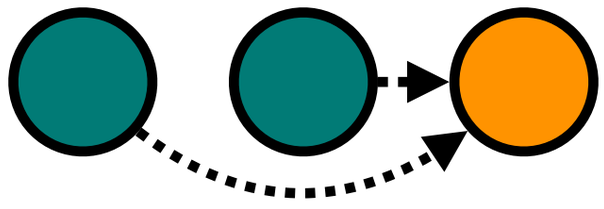
Query: Which medications used for treating fibromyalgia interact with drugs for treating Diabetes?

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

Anchor Variable Target

Complex Queries — Examples

2u

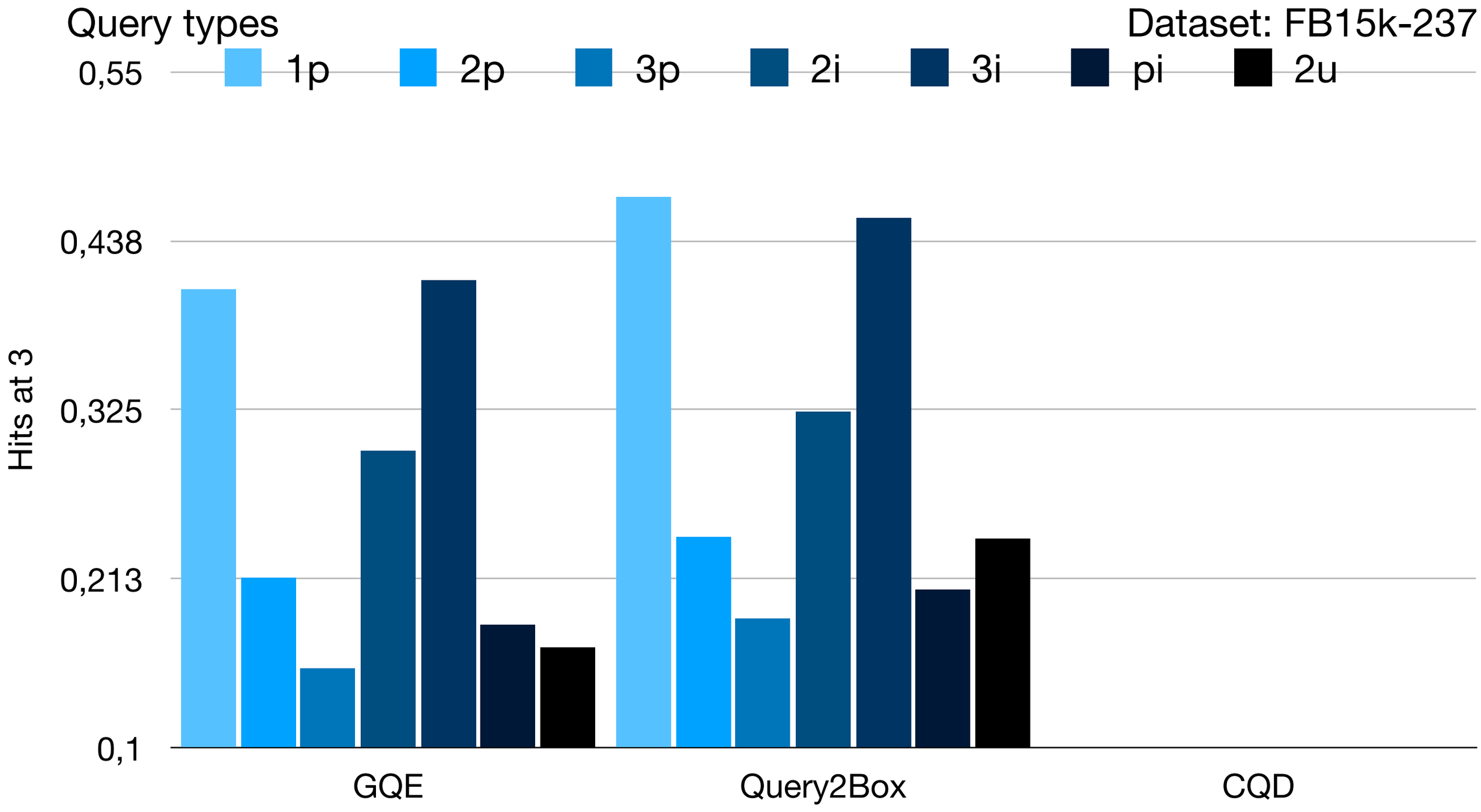


$$?T : p_1(a_1, T) \vee p_2(a_2, T)$$

Query: Which actors played in King's Speech or in Dunkirk?

$$?A : \text{playsIn}\left(A, \text{king's speech}\right) \vee \text{playsIn}\left(A, \text{dunkirk}\right)$$

Experiments



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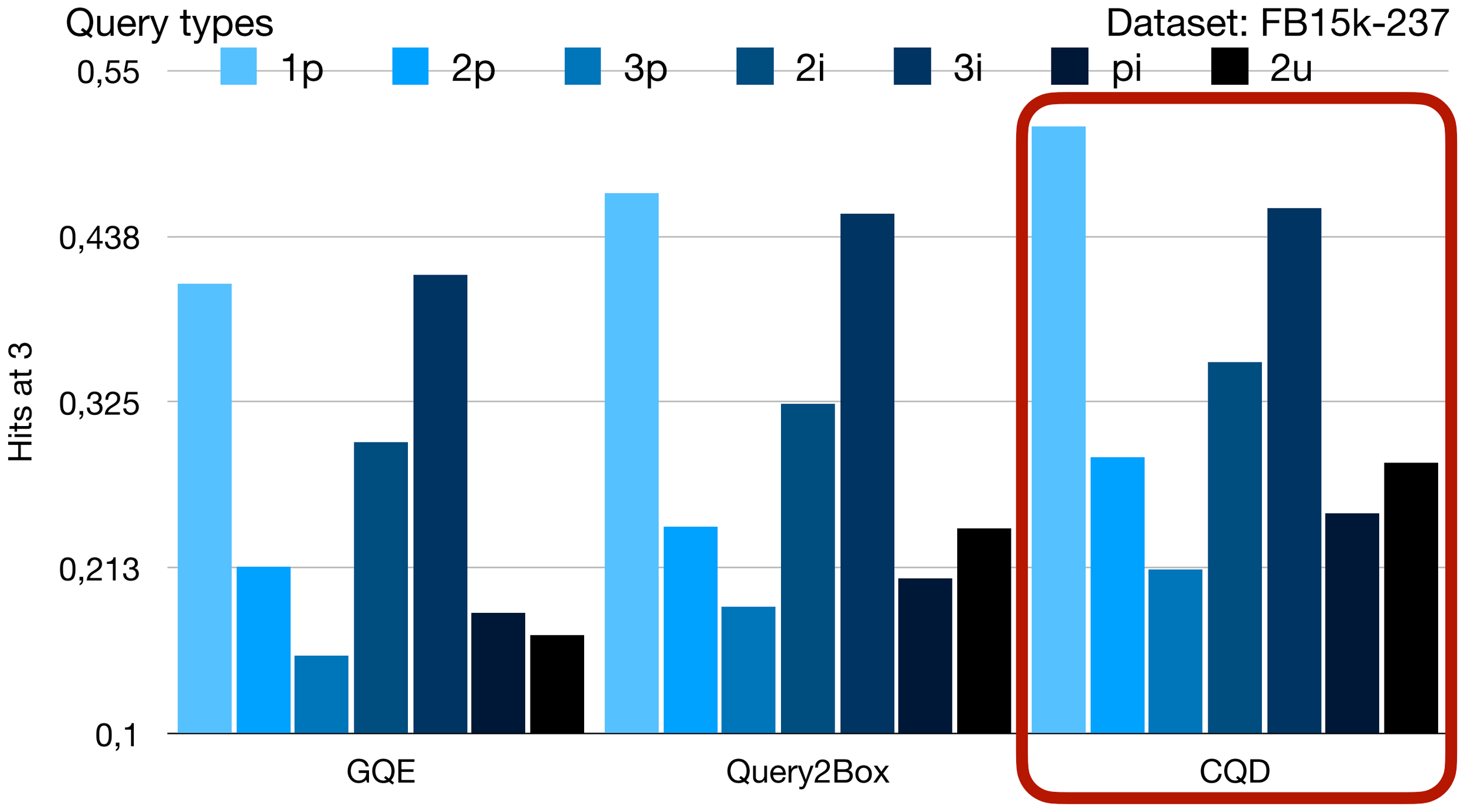

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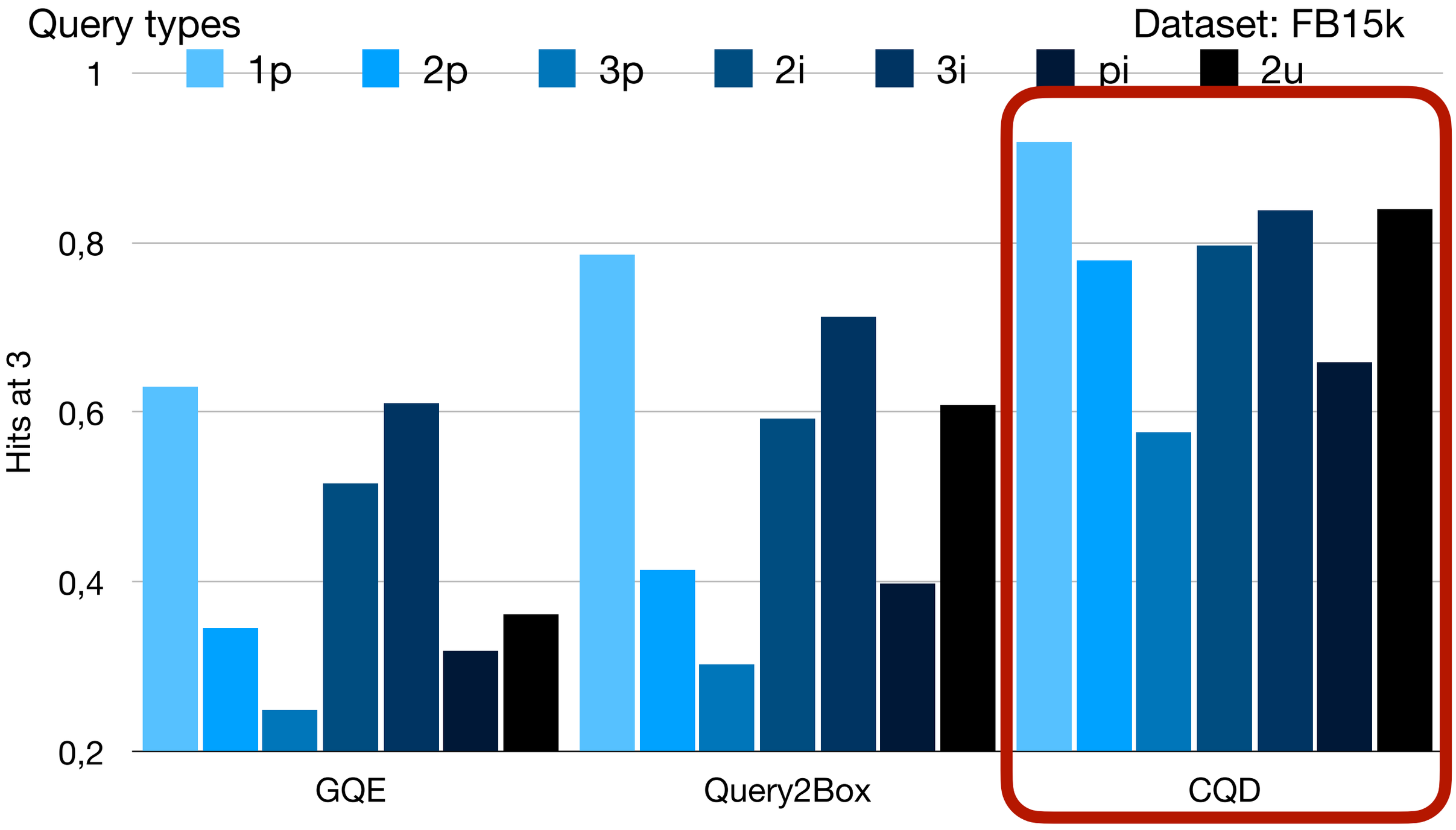

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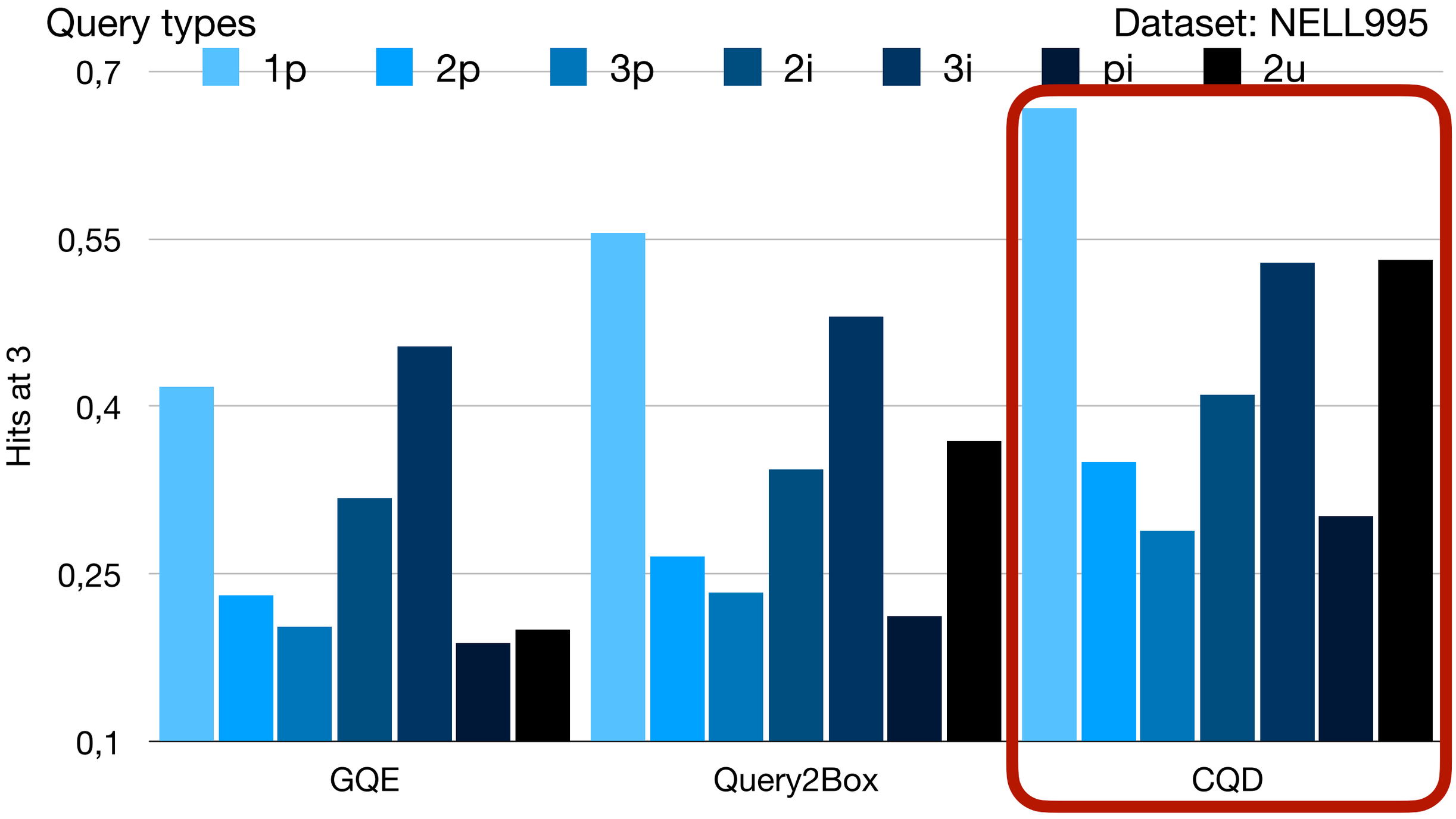

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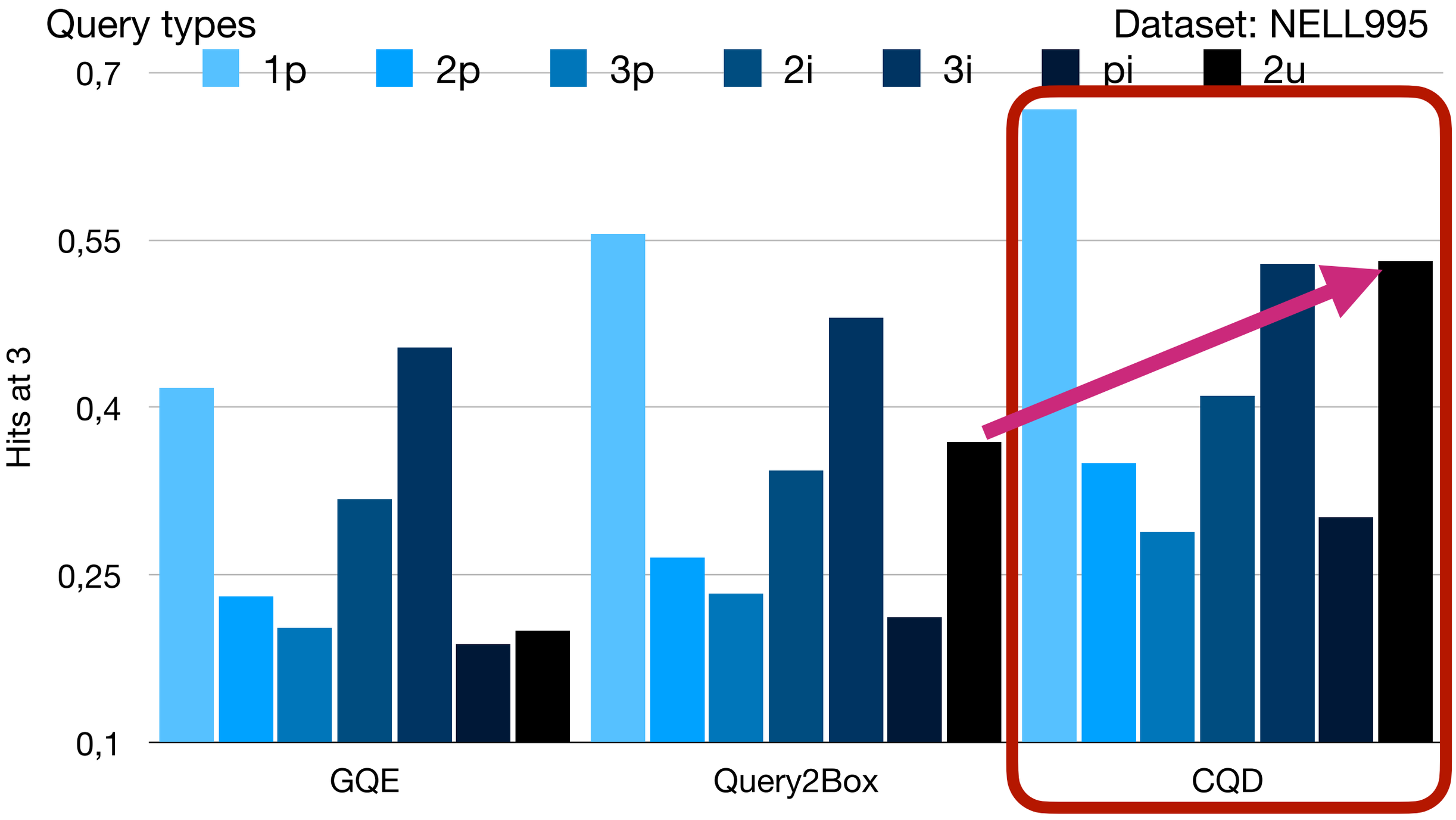
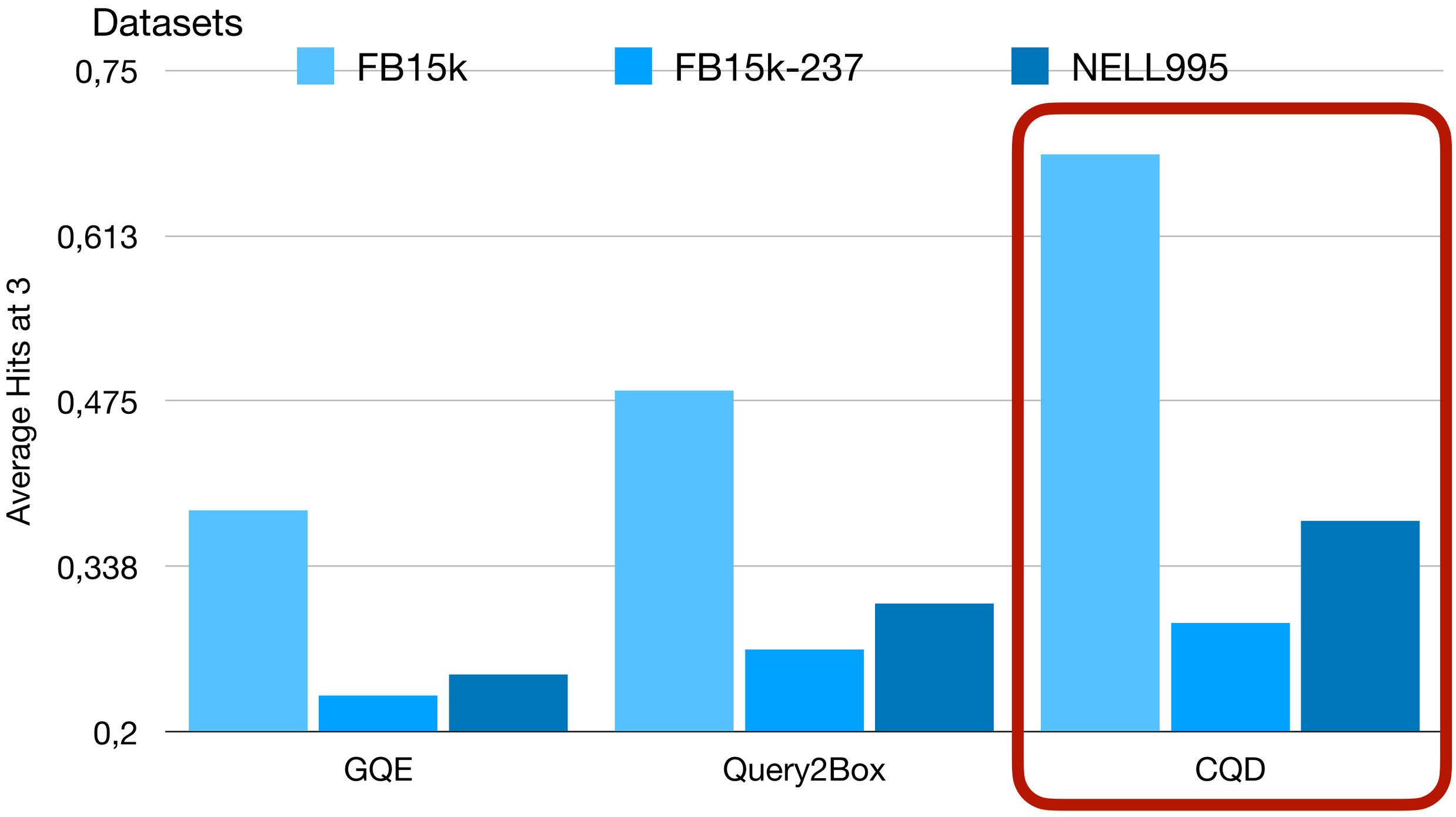
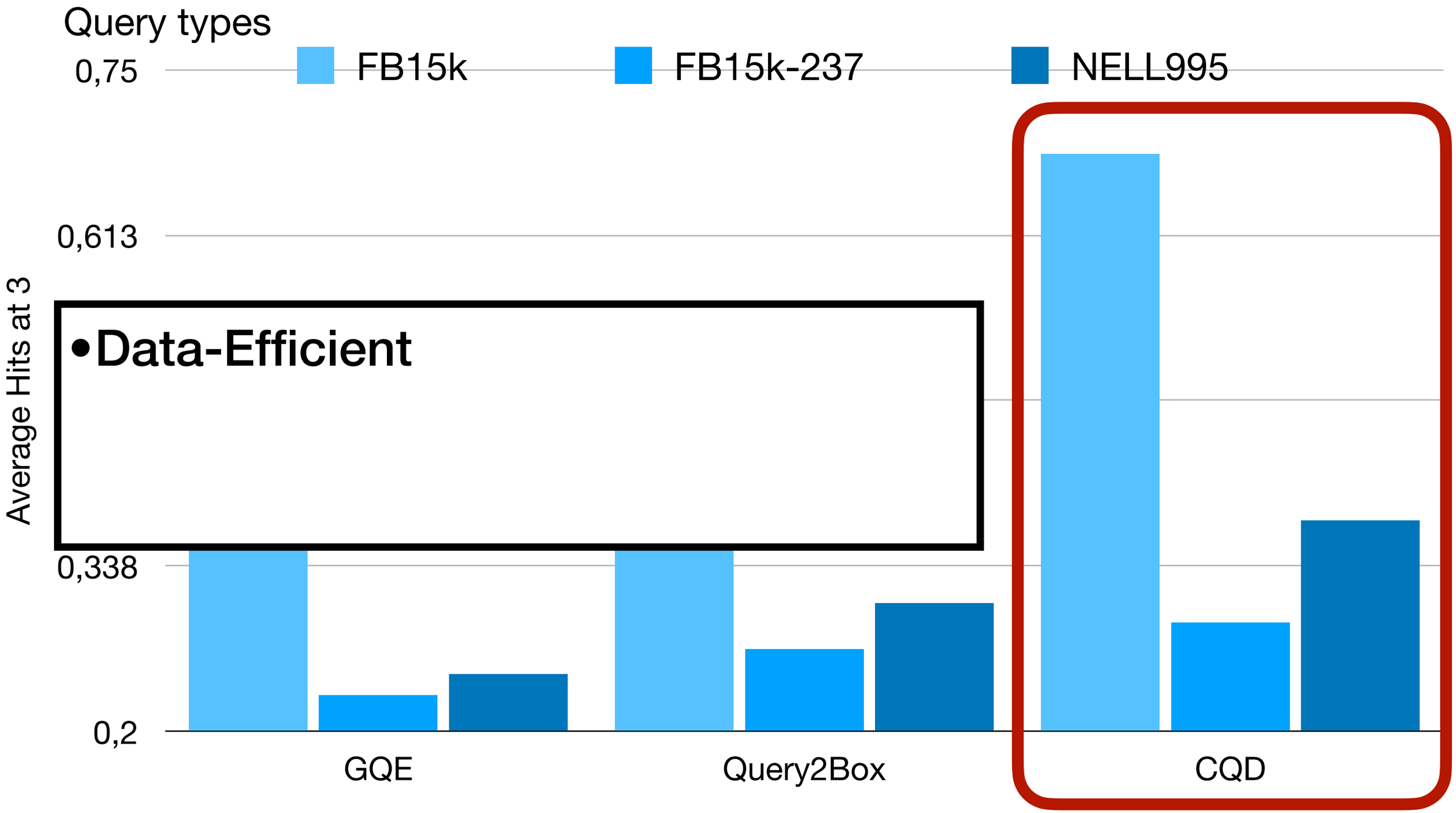


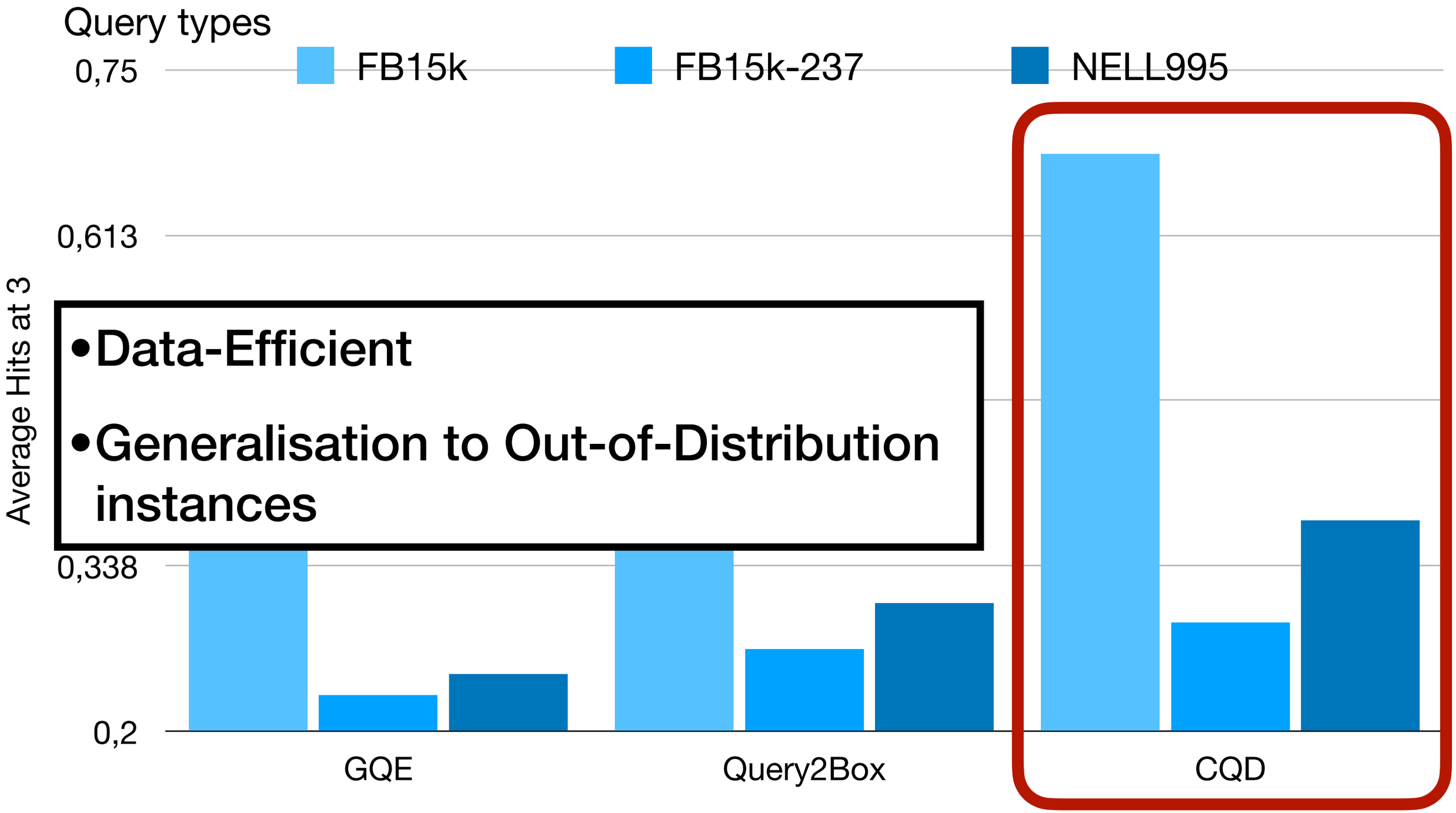
Experiments



Experiments



Experiments



Explainability

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

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

M
Apixaban
Amitriptyline
Phenytoin
Duloxetine
Buprenorphine

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- **Explainable**

M	*D*
Apixaban	Paroxetine
Amitriptyline	Paroxetine
Phenytoin	Paroxetine
Duloxetine	Pregabalin
Buprenorphine	Pregabalin

Summary

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Source code: https://github.com/uclnlp/cqd/