SapBERT: Self-Alignment Pretraining for Biomedical Entity Representations

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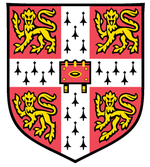

UNIVERSITY OF CAMBRIDGE

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Intro

1 Study Object: Biomedical Entities

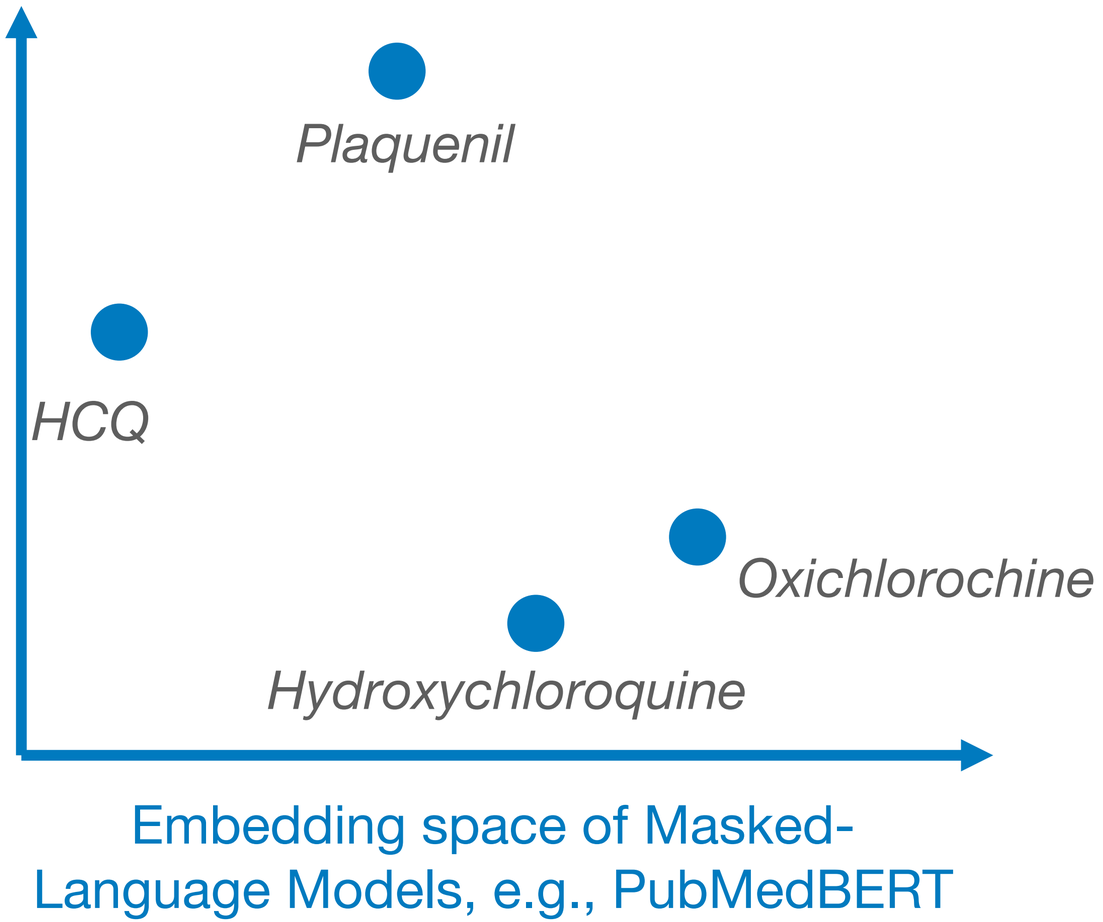
What counts as a biomedical entity?

- A single word (e.g. *fever*)
- A compound (e.g. *SARS-COV-2*)
- A phrase (e.g. *abnormal retinal vascular development*)

2 Challenge: Heterogeneous Naming

Biomedical names referring to the same concept have drastically different surface forms in biomedical text:

- *Hydroxychloroquine*
- *Oxichlorochine* (alternative name)
- *HCQ* (social media)
- *Plaquenil* (drug name)
- ……

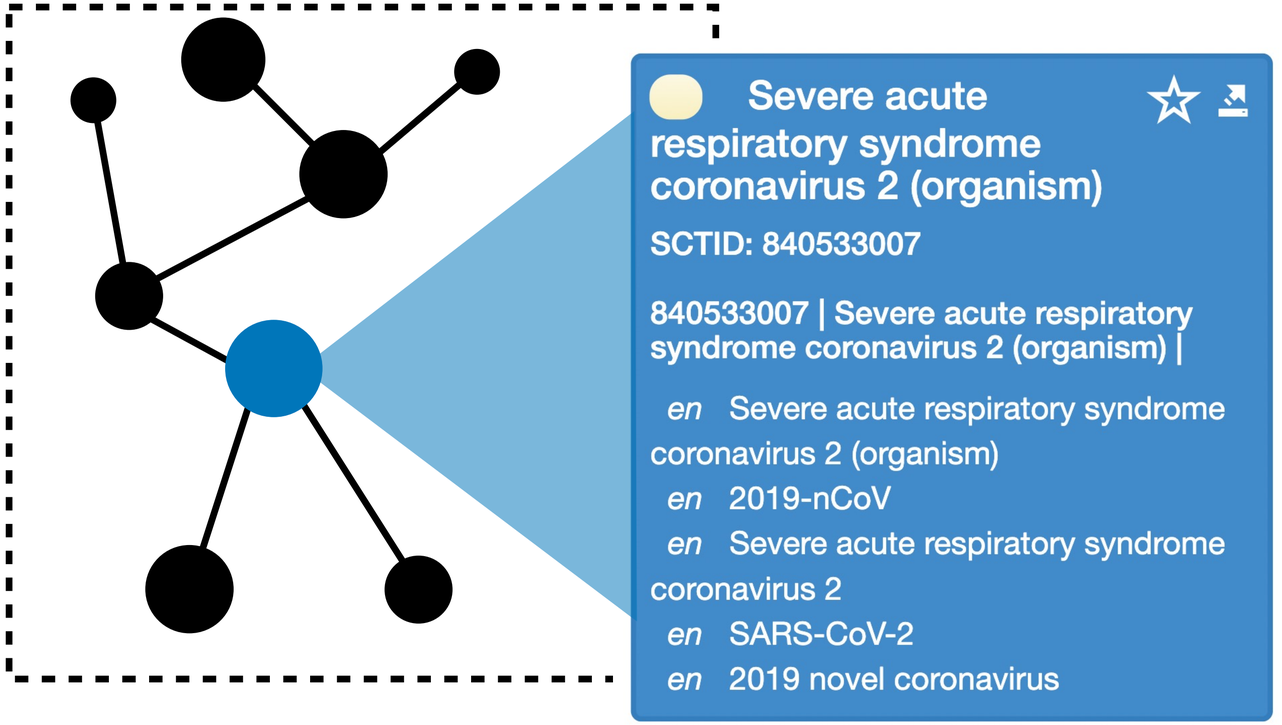


Embedding space of Masked-Language Models, e.g., PubMedBERT

3 Solution: Knowledge Injection from Ontologies

We use UMLS, the largest interlingua of biomedical ontologies:

- 4M+ concepts
- 10M+ synonyms
- 150+ controlled vocabularies (e.g. SNOMED, RxNORM, …)

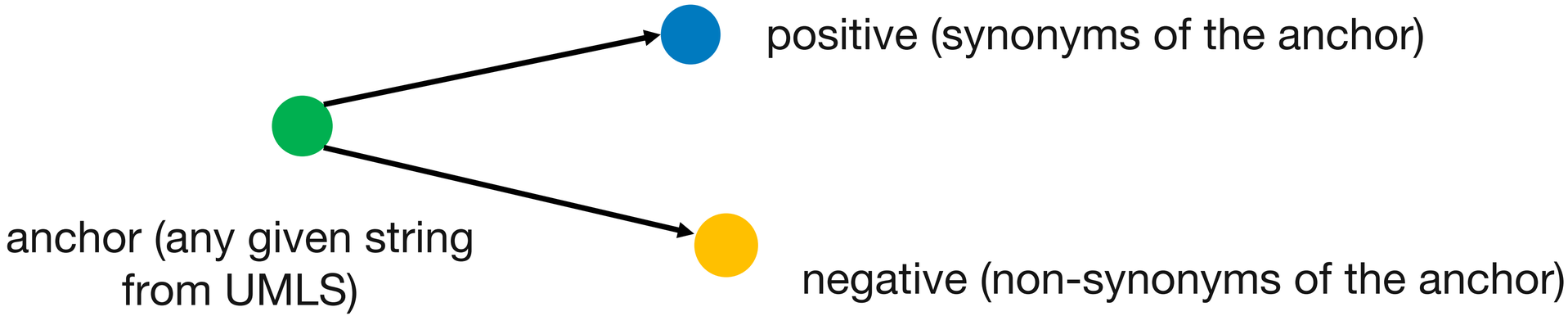


Synonym relations extracted from UMLS can inform language models' representations

Method

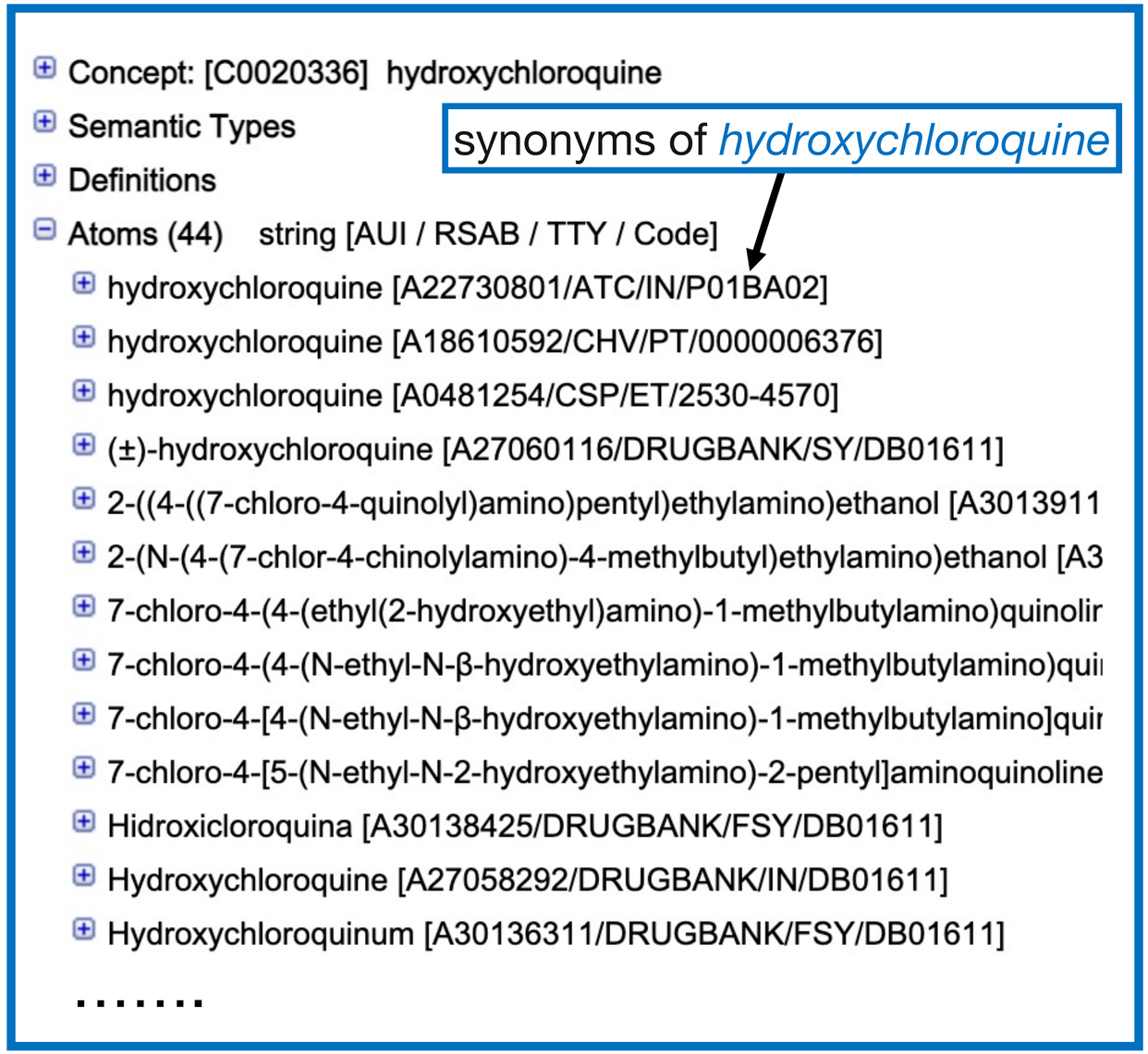
4 Method: Self-Alignment Pretraining

Constructing positives and negatives



4 Method: Self-Alignment Pretraining

Technical challenge: UMLS is gigantic, but not always informative



Most of *hydroxychloroquine*'s variants are easy:

- *Hydroxychlorochin*
- *Hydroxychloroquine (substance)*
- Hidroxicloroquina
- ……

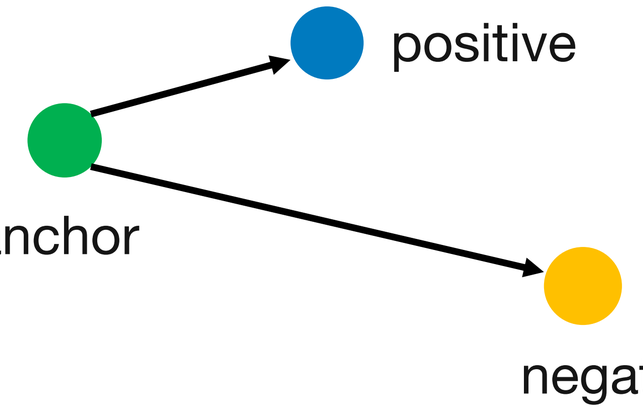
But a few can be very hard:

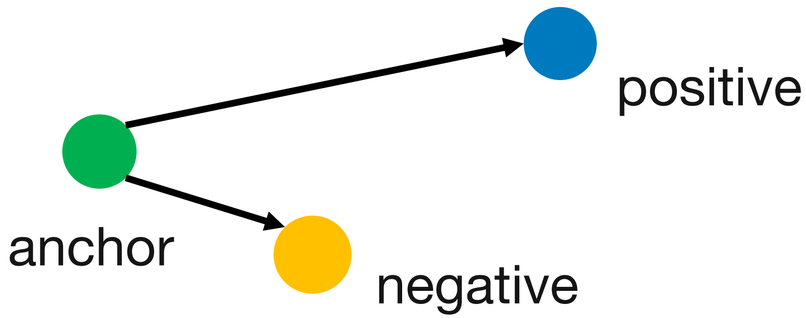
- *HCQ*
- *Plaquenil*
- ……

Can we focus on/learn more from the hard/informative examples?

4 Method: Self-Alignment Pretraining

Techniques: (1) smart online sampling

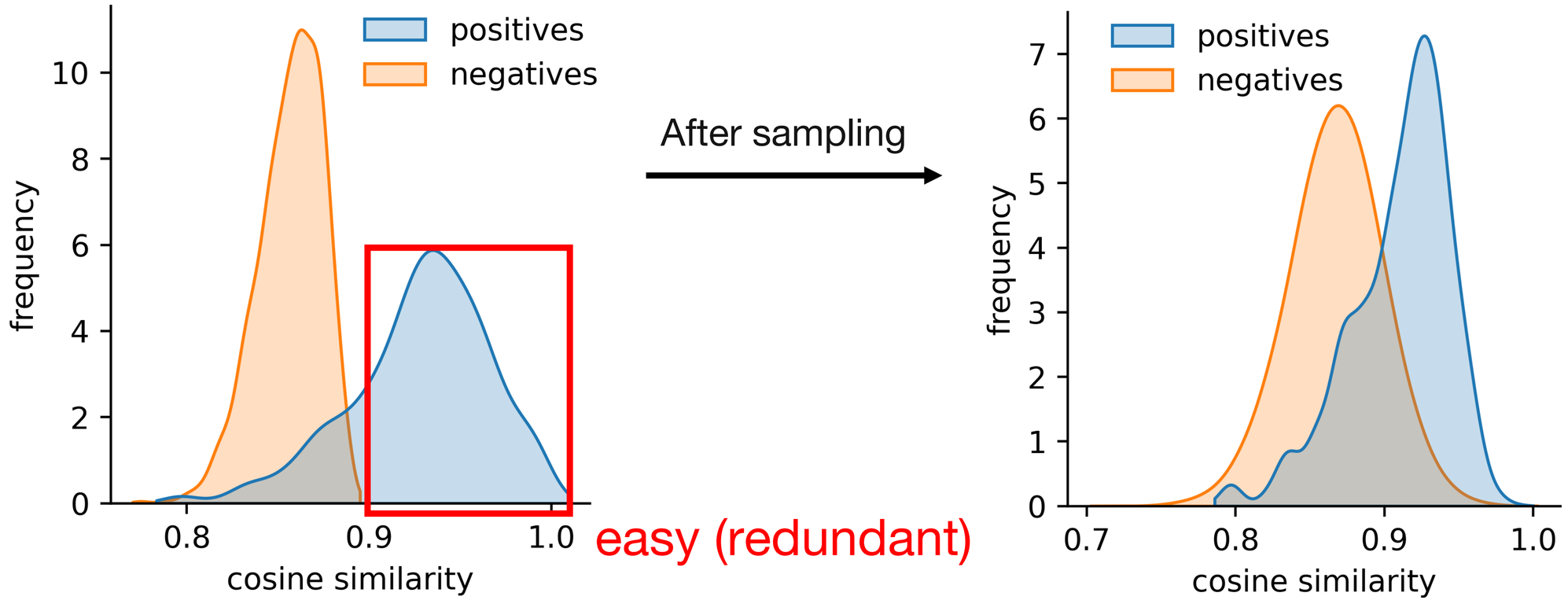




$$\|f(x_a) - f(x_p)\|_2 > \|f(x_a) - f(x_n)\|_2 + \lambda$$

4 Method: Self-Alignment Pretraining

Techniques: (1) smart online sampling



4 Method: Self-Alignment Pretraining

Techniques: (2) multi-similarity loss

push away negatives

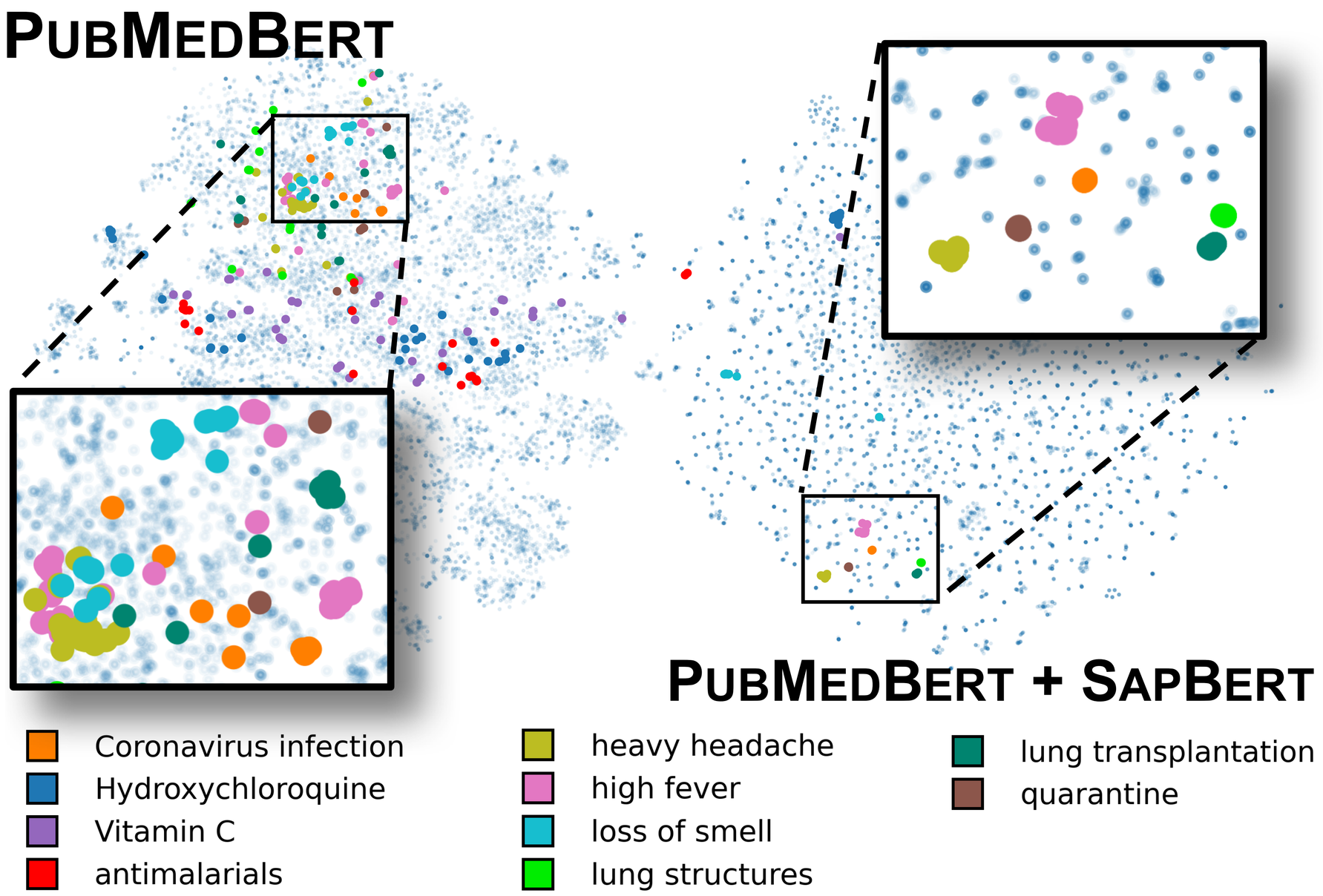
$$\mathcal{L} = \frac{1}{|\mathcal{X}_b|} \sum_{i=1}^{|\mathcal{X}_b|} \left(\frac{1}{\alpha} \log \left(1 + \sum_{n \in \mathcal{N}_i} e^{\alpha(\mathbf{S}_{in} - \epsilon)} \right) + \frac{1}{\beta} \log \left(1 + \sum_{p \in \mathcal{P}_i} e^{-\beta(\mathbf{S}_{ip} - \epsilon)} \right) \right),$$

cluster positives

5 Evaluations

5 Evaluations

(1) T-SNE visualisations



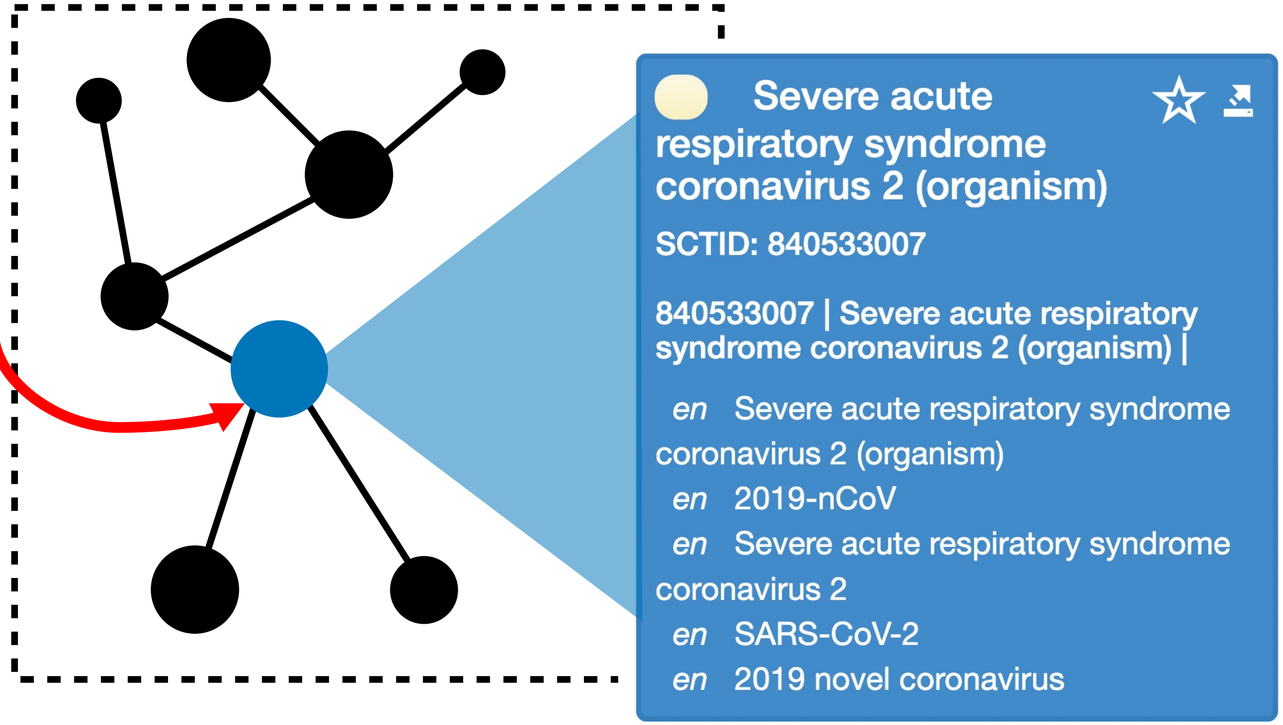
5 Evaluations

(2) Task evaluations: Medical Entity Linking

a medical **entity mention** in *free text*

OMG have u heard that John got the Covid virus ?!

entity linking



a unique concept (**node**) in a biomedical Knowledge Graph

5 Evaluations

The datasets used:

- NCBI-disease
- BC5CDR-disease
- BC5CDR-chemical
- MedMentions

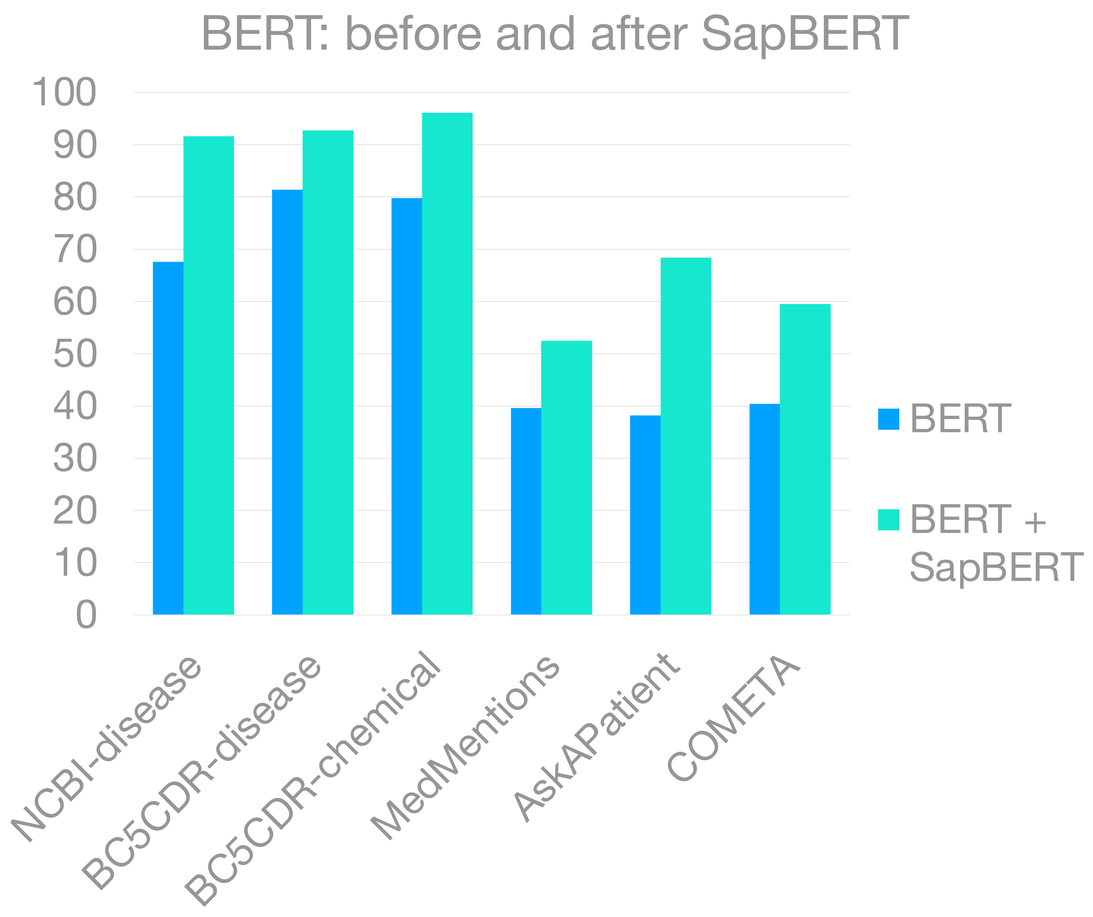
} Scientific

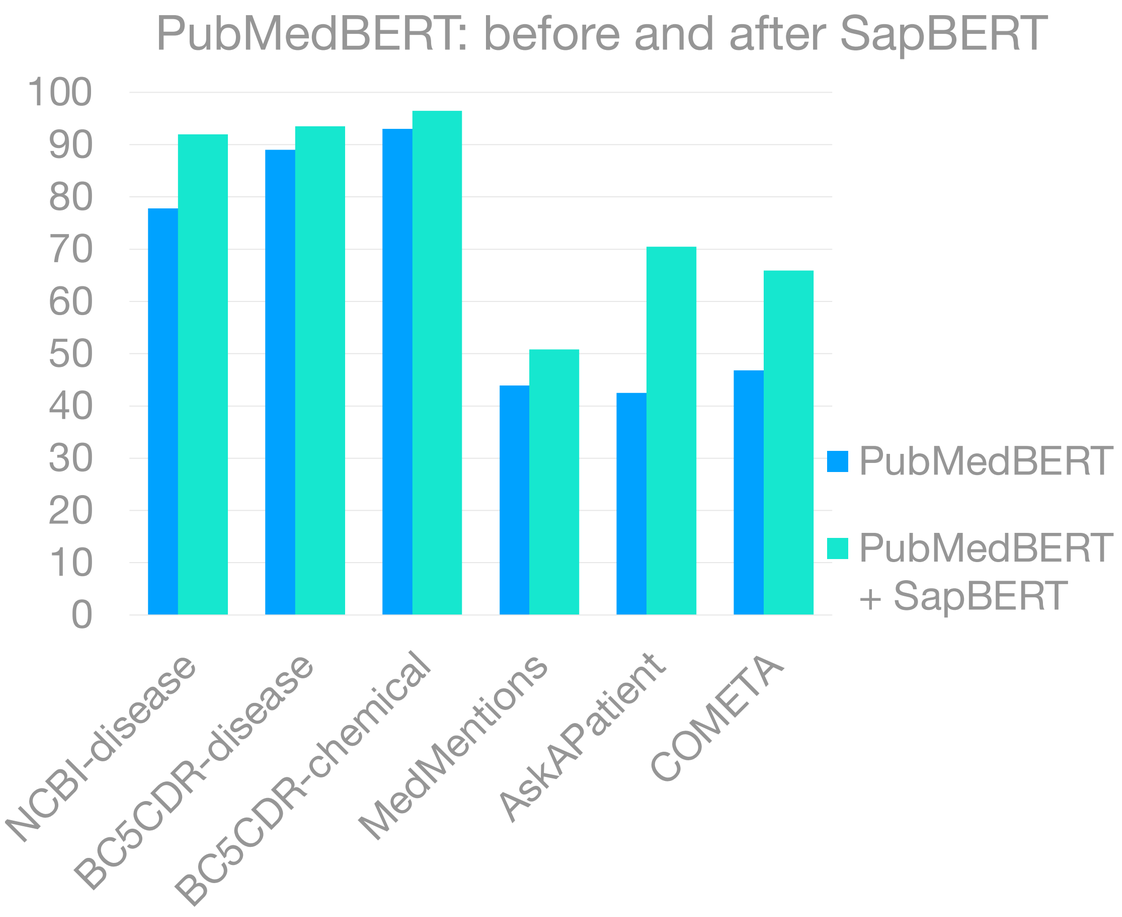
- AskAPatient
- COMETA

} Social media

5 Evaluations

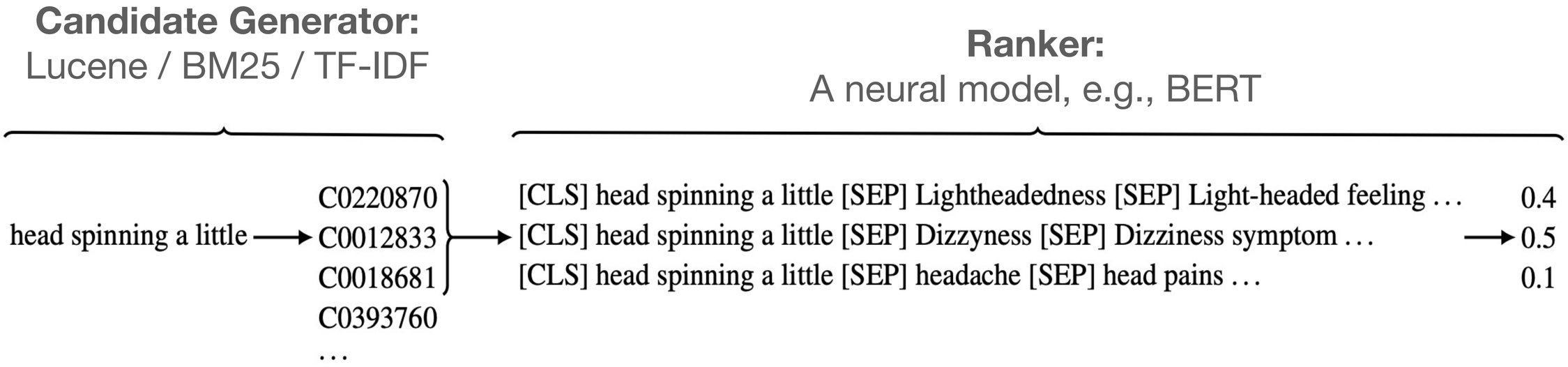
Compare with off-the-shelf pretrained Masked Language Models





5 Evaluations

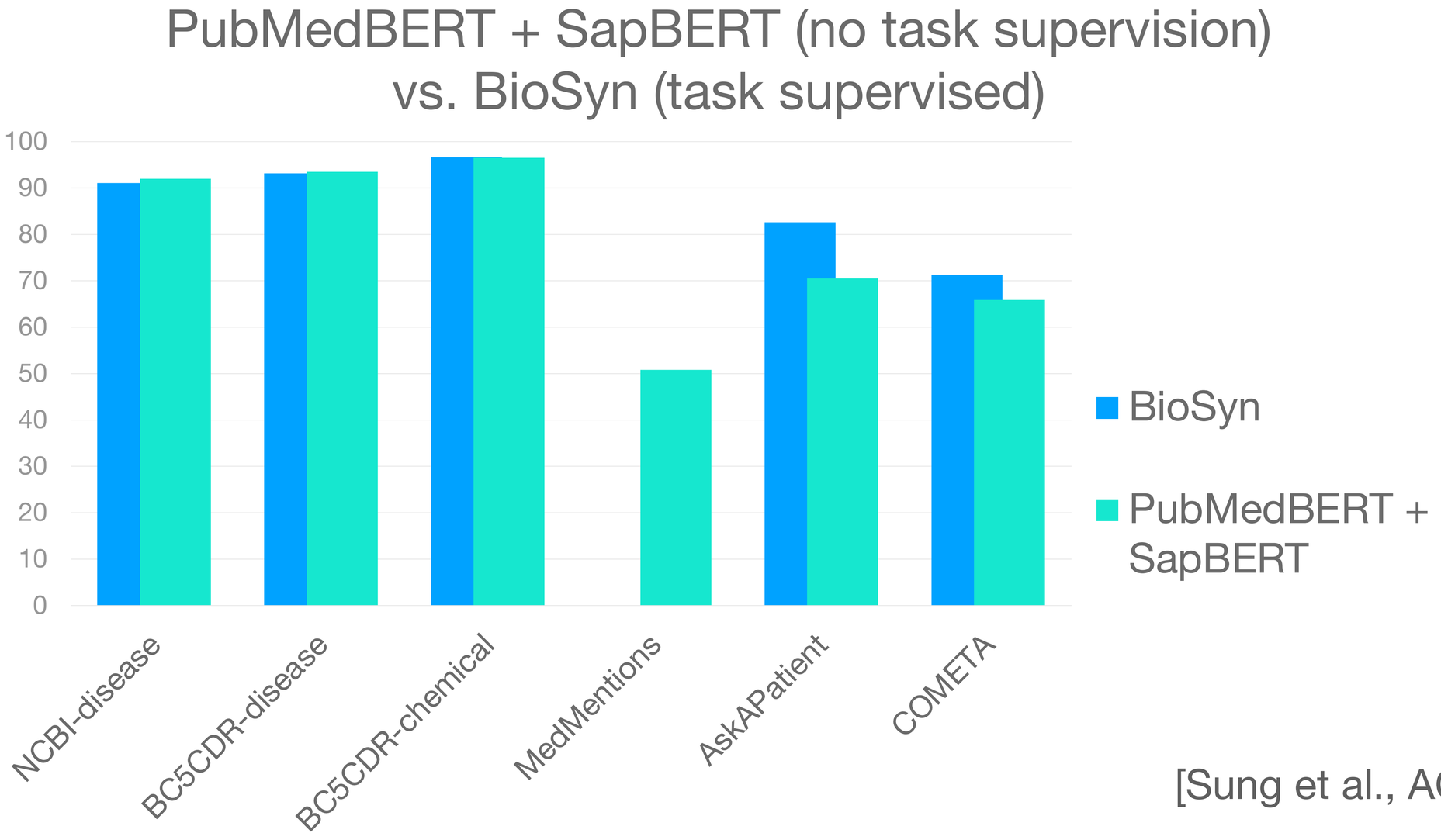
Compare with state-of-the-art biomedical entity linking systems



[Xu et al., ACL 2020] & [Sung et al., ACL 2020]

5 Evaluations

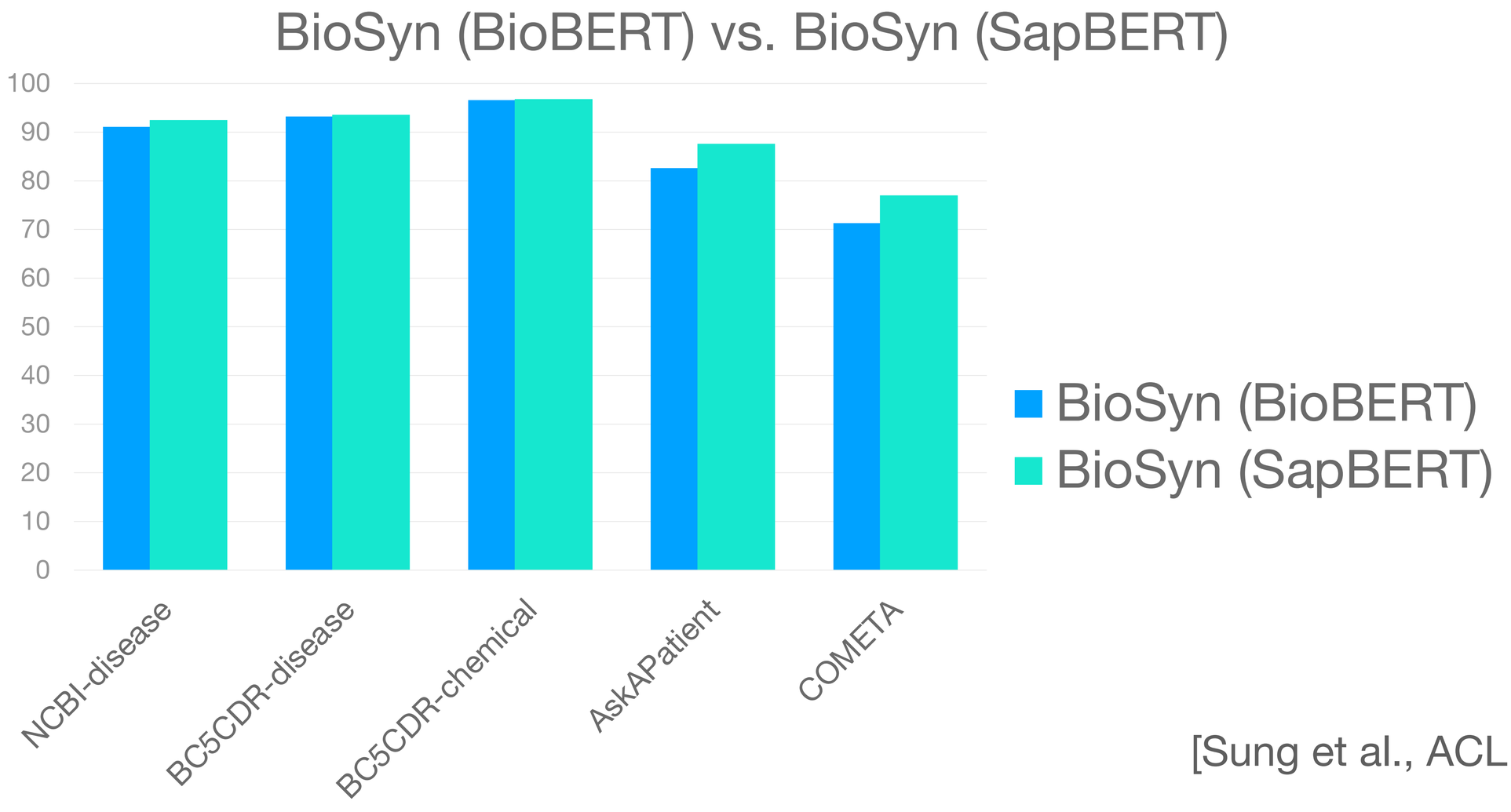
Compare with state-of-the-art biomedical entity linking systems



[Sung et al., ACL 2020]

5 Evaluations

Compare with state-of-the-art biomedical entity linking systems



[Sung et al., ACL 2020]

(2) Task evaluations: Medical Entity Linking (case studies)

[Example]* *I had **cortisone shots** when I was first diagnosed and those helped until the plaquenil built up enough to take away most of the pain.*

[Challenge] Colloquialism: *shot* -> *injection*

- Baseline model* prediction:

*- Cortisone (substance)***

- SapBERT predictions:

- Injection of cortisone (✓)
- Cortisone injection given
- Cortilymph

* All examples and baseline models are taken from the COMETA paper (EMNLP 2020). It's a string matching + BioBERT model.
** The baseline model is a hybrid of neural network and string matching, can thus only produce one prediction instead of a ranking list.

(2) Task evaluations: Medical Entity Linking (case studies)

[Example] *Get Plan B or the **Copper IUD**, if concerned about pregnancy.*

[Challenge] Abbreviation: *IUD* -> *intrauterine device*

- Baseline model prediction:

- *Cuprous oxide*

- SapBERT predictions:

- *Copper-containing intrauterine device (✓)*
- *Copper-containing intrauterine device (product) (✓)*
- *Uses copper intrauterine device contraception (finding)*

(2) Task evaluations: Medical Entity Linking (case studies)

[Example] *Can **A1c tests** be trusted to diagnose diabetes?*

[Challenge] Terminology resolution: *A1c tests* -> *glycerated hemoglobin*

- Baseline model prediction:

- Anticomplement immunofluorescence test (procedure)

- SapBERT predictions:

- Haemoglobin A1c measurement (✓)
- Hemoglobin A1c measurement (✓)
- Hemoglobin A1c measurement (procedure) (✓)

(2) Task evaluations: Medical Entity Linking (case studies)

[Example] *If you can usually sleep off migraine,* ***Benadryl*** *may help but talk to your doctor first obviously.*

[Challenge] Drug brand name

- Baseline model prediction:

- Bengal

- SapBERT predictions:

- Diphenhydramine-containing product (✓)
- Diphenhydramine (✓)
- Product containing diphenhydramine (medicinal product) (✓)

(2) Task evaluations: Medical Entity Linking (case studies)

[Example] *While there are no guarantees with **CAR**-T, and cytokine release syndrome is a real scary dangerous side effect, in your shoes I' d make it your goal to do what it takes to survive till you can get into one.*

[Challenge] Abbreviation

- Baseline model prediction:

  - Car

- SapBERT predictions:

  - Car
  - Has a car
  - CRAT

Correct answer: ***Chimeric antigen receptor***
(Future work: Context modelling)

(2) Task evaluations: Medical Entity Linking (case studies)

[Example] *I do mainly bacon and eggs now, because NO **CARBS**, delicious, and you stay full longer.*

[Challenge] Shortened form/colloquium

- Baseline model prediction:

  - Crabs

- SapBERT predictions:

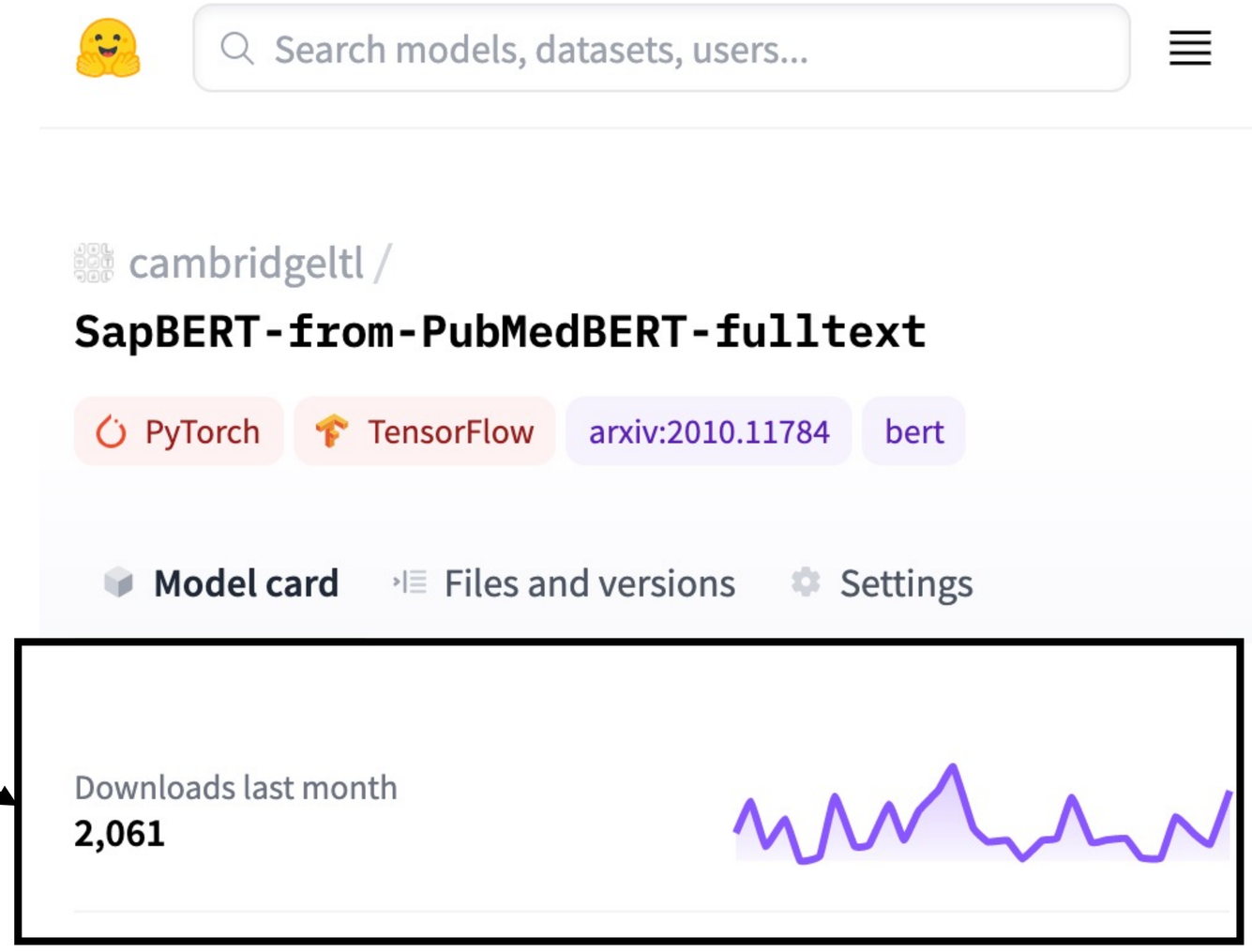
  - Carba mix
  - Carbine, device (physical object)
  - Carbine, device

Correct answer: ***Carbohydrate***
(Some layman language can not be learned from standardized vocabularies.)

6 Open-Source

SapBERT is receiving positive feedbacks and gaining popularity within the Machine Learning and Natural Language Processing communities

The SapBERT model gets 2,000+ downloads per month



7 Work-in-Progress

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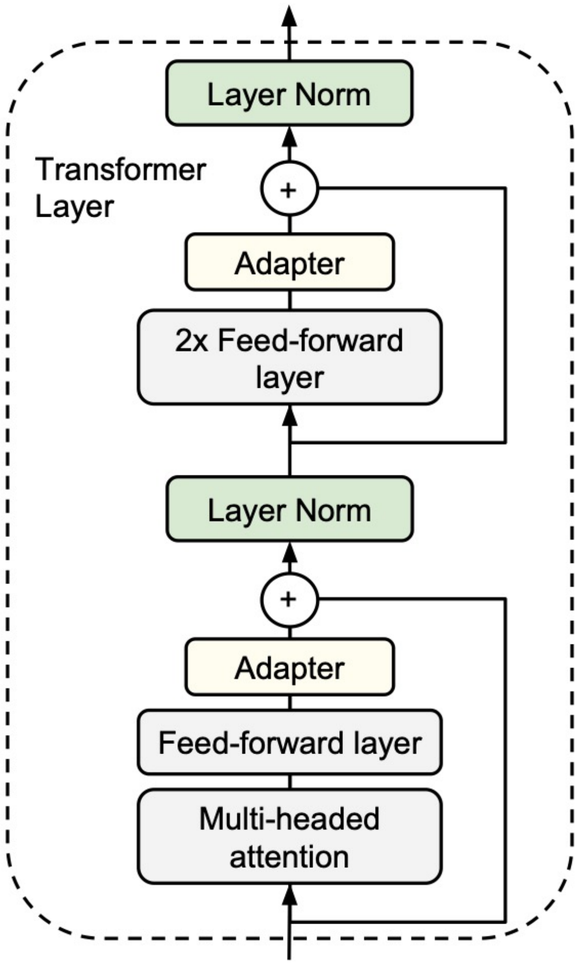
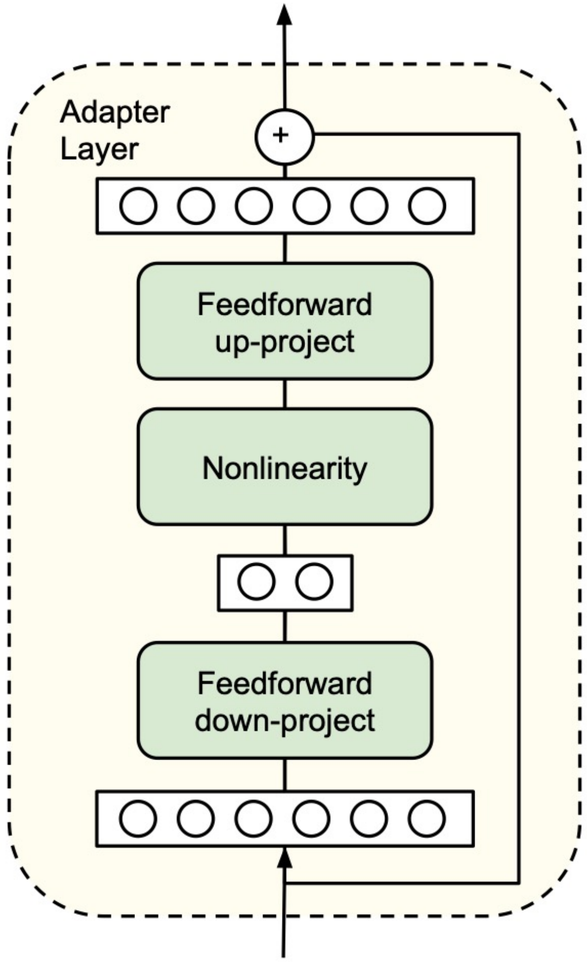
How about sentence-level tasks? (QA, text classification, etc.)

Adapters!

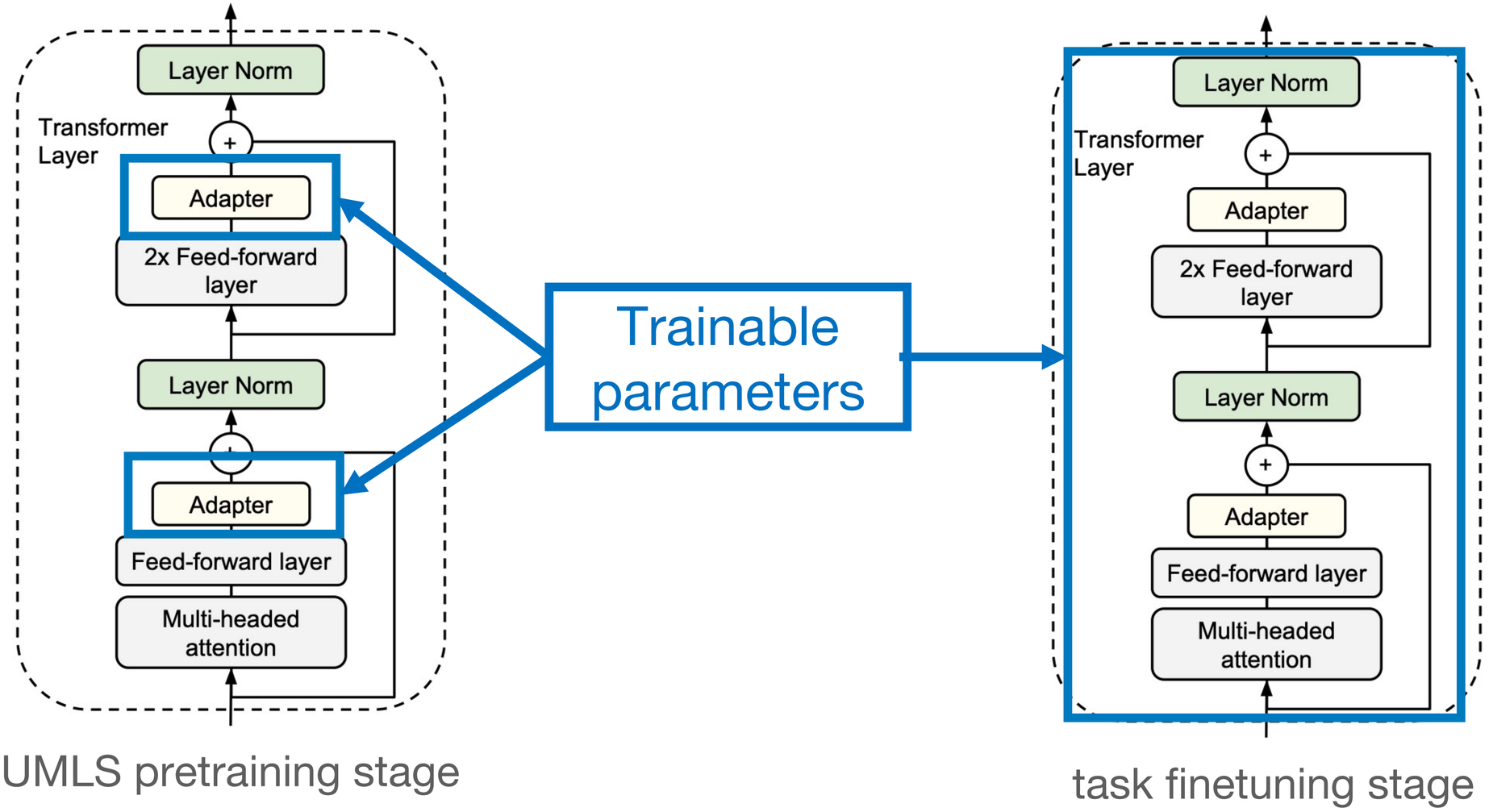




[Houlsby et al., ICML 2019]

7 Work-in-Progress

Adapter UMLS pretraining and task finetuning



UMLS pretraining stage

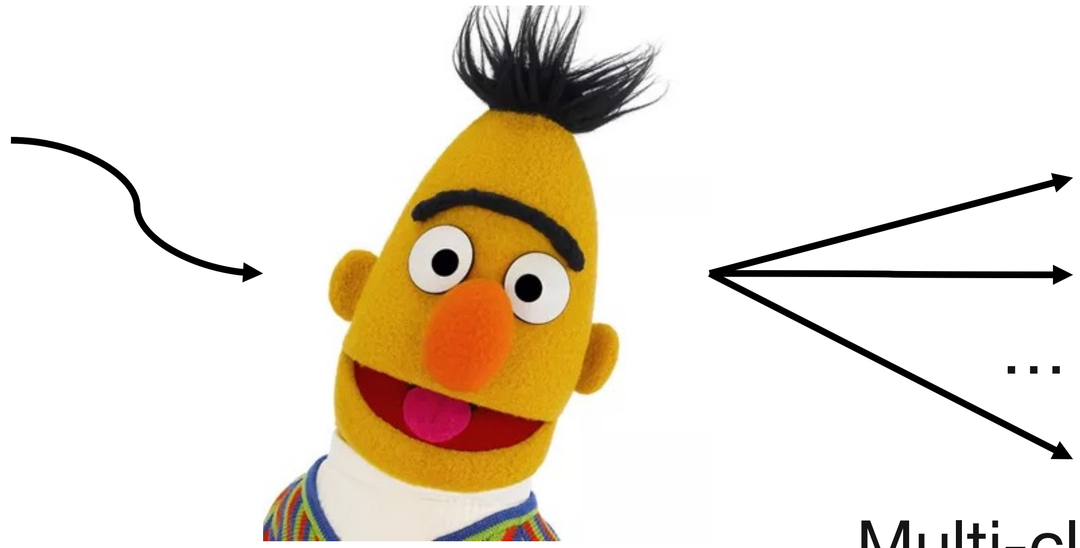
task finetuning stage

7 Work-in-Progress

We train a knowledge graph completion objective on UMLS triples:

(chemical_A, *interact_with*, ?)

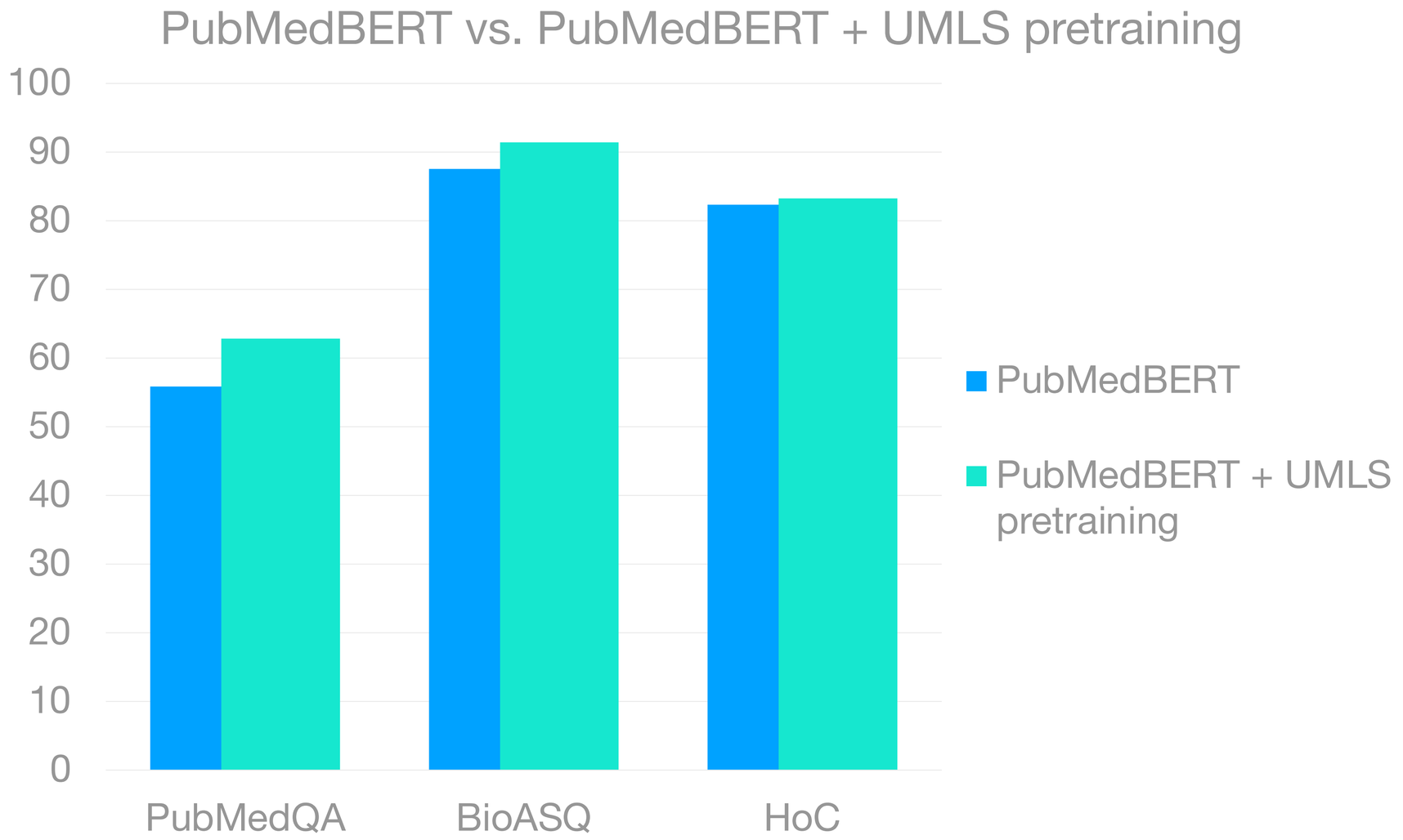
Input: [CLS] chemical_A [SEP] interact [SEP]



Multi-class classification

7 Work-in-Progress

Sentence-level tasks results



Thank you!

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