

# A transformer-based method for zero and few-shot biomedical named entity recognition

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## ABSTRACT

Supervised named entity recognition (NER) in the biomedical domain is dependent on large sets of annotated texts with the given named entities, whose creation can be time-consuming and expensive. Furthermore, the extraction of new entities often requires conducting additional annotation tasks and retraining the model. To address these challenges, this paper proposes a transformer-based method for zero- and few-shot NER in the biomedical domain. The method is based on transforming the task of multi-class token classification into binary token classification (token contains the searched entity or does not contain the searched entity) and pre-training on a larger amount of datasets and biomedical entities, from where the method can learn semantic relations between the given and potential classes. We have achieved average F1 scores of 35.44% for zero-shot NER, 50.10% for one-shot NER, 69.94% for 10-shot NER, and 79.51% for 100-shot NER on 9 diverse evaluated biomedical entities with PubMedBERT fine-tuned model. The results demonstrate the effectiveness of the proposed method for recognizing new entities with limited examples, with comparable or better results from the state-of-the-art zero- and few-shot NER methods.

## 1. Introduction

Supervised machine learning algorithms depend on large amounts of annotated or labeled data that is often hard or expensive to obtain (Van Engelen and Hoos, 2020). This is particularly true for textual data in the biomedical domain. For disease understanding and drug discovery, it is important to recognize many entities in text, often novel ones (with no previously annotated data), and explore relationships between them (Milošević and Thielemann, 2023). Recognized named entities, such as names of mentioned genes, drugs, chemicals, diseases, biomarkers, cells, cell lines, tissues, organs, DNA or RNA sequences, can be useful for information retrieval (Lu, Kim and Wilbur, 2009), de-identification of medical records (Milosevic, Kalappa, Dadafarin, Azimae and Nenadic, 2020; Dehghan, Kovacevic, Karystianis, Keane and Nenadic, 2015), relationship extraction, knowledge graph creation (Luo, Lai, Wei, Arighi and Lu, 2022a), question answering (Toral, Noguera, Llopis and Munoz, 2005), automatic summarization (Aramaki, Miura, Tonoike, Ohkuma, Masuichi and Ohe, 2009) and many other tasks. In the biomedical domain, text annotation costs are especially high, because the annotation has to be done by professionals (medical doctors, biologists, chemists, etc.). Carrell, Cronkite, Malin, Aberdeen and Hirschman (2016) estimated that the price for a single annotated instance can be between 0.71\$ and 377\$, depending on the complexity and number of annotators. In our previous work, we paid 2.6 euros per annotated sentence (Milošević and Thielemann, 2023). Given that training a good machine learning model for named entity recognition requires several hundred, sometimes several thousand annotated examples for each entity type, these costs can scale fast.

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Zero and few-shot machine learning algorithms can help address issues with a lack of annotated data. Zero-shot learning allows recognizing named entities in text based on no given examples during the training (Xian, Lampert, Schiele and Akata, 2018; Nguyen, Gelli and Poria, 2021), while few-shot learning allows training a more efficient model for named entity recognition based on a few annotated example sentences (Hofer, Kormilitzin, Goldberg and Nevado-Holgado, 2018; Fritzler, Logacheva and Kretov, 2019; Moscato, Napolano, Postiglione and Sperli, 2023). Several zero-shot and few-shot algorithms have been proposed in the last several years for medical terms (Ziletti, Akbik, Berns, Herold, Legler and Viell, 2022), general NER (Aly, Vlachos and McDonald, 2021), and mix of domains, such as general, AI, literature, music, politics, and natural science Nguyen et al. (2021). The biomedical domain has specific language vocabulary (usage of Latin and Greek words or phrases, heavy usage of acronyms and abbreviations). Biomedical entities are more diverse and complex than general entities and therefore require specifically crafted approaches and language models.

In this paper, we present an approach for biomedical named entity recognition based on **specific input representation of labels and input text, and a domain-specific transformer-based models** (BioBERT (Lee, Yoon, Kim, Kim, Kim, So and Kang, 2020) and PubMedBERT (Gu, Tinn, Cheng, Lucas, Usuyama, Liu, Naumann, Gao and Poon, 2021)).

## 2. Background

Named entity recognition (NER) is an information extraction task that consists of recognizing mentions of certain information units or *named entities* in text. While there is no definite agreement as to the scope of the term *named*

*entity* (Marrero, Urbano, Sánchez-Cuadrado, Morato and Gómez-Berbís, 2013), it usually refers to generic units such as personal names, locations, organizations, etc., or domain-specific units such as names of genes, proteins or enzymes (Li, Sun, Han and Li, 2020). The first published research papers on NER date from the early nineties and mostly focus on the recognition of personal, location, or organization names in news reports, scientific or religious texts, and later in emails (Nadeau and Sekine, 2007). Early NER systems relied on handwritten rules in the form of regular expressions (Appelt, Hobbs, Bear, Israel and Tyson, 1993) or syntactic-lexical patterns (Morgan, Garigliano, Callaghan, Poria, Smith, Urbanowicz, Collingham, Costantino, Cooper, Group et al., 1995; Grishman, 1995), often augmented with gazetteers (Iwanska, Croll, Yoon and Adams, 1995). Even though these systems can lead to high precision, they depend on the quality and breadth of the rules and named entity lists and require a lot of time and skill to build. Therefore, later efforts started relying on machine learning algorithms to deduce rules either from a fully hand-annotated text (supervised methods) (Zhou and Su, 2002; Curran and Clark, 2003; McCallum and Li, 2003; Li, Bontcheva and Cunningham, 2005), a small set of named entities and NE contexts (semi-supervised methods) (Carreras, Marquez and Padró, 2002; Agerri and Rigau, 2016), or context alone with the help of different lexical resources (unsupervised methods) (Etzioni, Cafarella, Downey, Popescu, Shaked, Soderland, Weld and Yates, 2005; Munro and Manning, 2012). Nowadays, state-of-the-art results in NER are achieved using deep learning (Yadav and Bethard, 2019; Li et al., 2020).

The early 2000s marked the appearance of the first publicly available biomedical corpora (Kim, Ohta, Tateisi and Tsujii, 2003; Hirschman, Yeh, Blaschke and Valencia, 2005). The availability of data further spurred research in the domain of recognizing mentions of proteins, genes, drugs/chemicals, and similar named entities in different kinds of biomedical texts (bioNER), largely through shared tasks such as BioCreative (Hirschman et al., 2005) or JNLPBA (Collier and Kim, 2004). Early bioNER systems range from entirely rule-based ones (Gaizauskas, Demetriou, Artymiuk and Willett, 2003), those based on machine learning methods such as Naive Bayes (Nobata, Collier and Tsujii, 1999), Support Vector Machine (Mitsumori, Fation, Murata, Doi and Doi, 2005), Hidden Markov Model (Zhou, Shen, Zhang, Su and Tan, 2005), Maximum Entropy (Dingare, Nissim, Finkel, Manning and Grover, 2005) and Conditional Random Fields (Settles, 2004). While each of those types of systems has its advantages, what they have in common is that building them is time-consuming and requires constant manual adaptation (of rules or features) when data changes. Deep learning systems such as (Habibi, Weber, Neves, Wiegandt and Leser, 2017) alleviate this issue by automatically generating the features, but they require large amounts of annotated data to train.

Introduction of the transformer neural architecture (Vaswani, Shazeer, Parmar, Uszkoreit, Jones, Gomez, Kaiser and Polosukhin, 2017) revolutionized the field of natural language

processing and artificial intelligence in general. Key components of transformer architecture are its encoder and decoder. The encoder of the transformer model takes short text as input and outputs a sequence of embeddings that correspond to the tokens of the input text. The encoder can be separately trained utilizing both unsupervised and supervised transfer learning (Devlin, Chang, Lee and Toutanova, 2018). An encoder of the transformer model can be trained on unannotated structured text corpora, and the model weights created in the training process can then be transferred to a specific downstream task, which as a result requires a smaller amount of annotated data. Base encoder transformer models are usually pre-trained on general-domain data and do not yield satisfactory results when applied to domain-specific areas (Lee et al., 2020). Therefore, researchers started training the models on biomedical data before fine-tuning them for the bioNER task. Two representative examples are BioBERT (Lee et al., 2020), a BERT-based model, and SciFive (Phan, Anibal, Tran, Chanana, Bahadroglu, Peltekian and Altan-Bonnet, 2021), a T5-based model. Both were initialized using weights of the original models and additionally trained on PubMed abstracts and PubMed Central (PMC) full-text articles. They were further fine-tuned for bioNER and other NLP tasks. Gu et al. (2021) argued that training models on biomedical data from scratch makes a difference in model performance on downstream tasks. In addition to proposing a model trained in such a way, PubMedBERT, they also proposed BLURB, a Biomedical Language Understanding and Reasoning Benchmark, that tracks state-of-the-art model performance for different biomedical tasks, including bioNER. BioGPT, a domain-specific generative transformer language model pre-trained on large-scale biomedical literature is proposed as an alternative to BioBERT and PubMedBERT, which, due to the lack of generative ability, limits their scope of application (Luo, Sun, Xia, Qin, Zhang, Poon and Liu, 2022b), but is not evaluated on NER task. We therefore further exploit possibility of using encoder only transformer in order to achieve zero-shot NER task.

The need to recognize entities in a growing number of scarcely annotated or unannotated texts has led researchers in the direction of zero- and few-shot learning for NER. Few-shot learning for general-domain NER is fairly explored (Huang, Li, Subudhi, Jose, Balakrishnan, Chen, Peng, Gao and Han, 2020), and while there is some work done on zero-shot learning for general-domain NER (Aly et al., 2021; Nguyen et al., 2021; Van Hoang, Mulvad, Rong and Yue, 2021), there is little work done on few- and zero-shot learning specifically for bioNER. This is where bioNER can benefit from such approaches in different text classification tasks. An approach proposed by Halder, Akbik, Krapac and Vollgraf (2020) transforms different tasks of sentence classification (question type classification, sentiment, and topic classification) into a generic binary classification problem. Feeding the information to the model in the form of a "sentence, label" tuple for each of the tasks and continually fine-tuning the same model for each of the tasks allows the model to make zero-shot predictions, as long as there is enough

similarity between tasks. However, TARS faces scalability issues when dealing with a large number of classes - an issue Ziletti et al. (2022) tackle by proposing xTARS. xTARS combines BERT-based multi-class classification ensembles to deal with scalability problems and improve prediction stability and the TARS zero/few-shot learning approach, while making specific choices about the examples shown to the model. Recently, GPT models and ChatGPT gained popularity for many NLP tasks. Hu, Ameer, Zuo, Peng, Zhou, Li, Li, Jiang and Xu (2023) used ChatGPT with a specific prompt design for a clinical zero-shot approach for clinical NER. **QaNER system formulated a NER problem as a QA task and tried to approach it with prompt engineering (Liu, Xiao, Zhu, Zhang, Li and Arnold, 2022).**

### 3. Methodology

We hypothesize that semantic information contained in the named entity label will enable the model to correctly classify the words corresponding to that label even though the model has not seen explicit examples during zero-shot fine-tuning process. Training the model on a large number of named entity classes will enable the model to deduce semantic relationships between these classes. Based on this, the model may be able to infer the semantic relationship of unseen named entity class with the previously seen ones, and label sequences in input text accordingly.

Our approach was inspired by the approach proposed by Halder et al. (2020), where input is created by combining a label of entity, together with the sentence. For underlying models that we have fine-tuned, we selected encoder-based domain-specific pre-trained language models, such as BioBERT (Lee et al., 2020) and PubMedBERT (Gu et al., 2021). Our dataset was constructed by a suitable transformation of six standard biomedical datasets consisting of common biomedical entities (such as genes, drugs, diseases, adverse events, chemicals, etc.) into a single common format. We expand more on our methodology in the following sections.

#### 3.1. Dataset integration

We integrated six publicly available corpora which were predominantly manually annotated for named entity classes:

- **CDR** (Wei, Peng, Leaman, Davis, Mattingly, Li, Wiegers and Lu, 2016) is a biomedical dataset annotated for chemicals, diseases, and chemical-disease interactions on 1500 PubMed articles. We used exclusively named entity annotations.
- **CHEMDNER** (Krallinger, Rabal, Leitner, Vazquez, Salgado, Lu, Leaman, Lu, Ji, Lowe et al., 2015) consists of 10000 PubMed abstracts annotated with chemical entity mentions.
- **BioRED** (Luo et al., 2022a) is a biomedical relation extraction dataset with multiple entity types and relation pairs annotated at the document level, on a set

of 600 PubMed abstracts. We have used exclusively named entity annotations from this dataset.

- **NCBI Disease** (Doğan, Leaman and Lu, 2014) is a biomedical dataset annotated with disease mentions, using concept identifiers from either MeSH or OMIM and containing 793 PubMed abstracts.
- **JNLPBA** (Collier and Kim, 2004) is a biomedical dataset that comes from the GENIA version 3.02 corpus created with a controlled search on MEDLINE, consisting of 2404 PubMed abstracts with term annotation.
- **N2C2** (Henry, Buchan, Filannino, Stubbs and Uzuner, 2020) consists of drug administration-relevant annotations extracted from a total of 1243 de-identified discharge summaries.

The selected datasets focus on scientific literature in the biomedical domain, but they also contain other types of documents (e.g. hospital discharge summaries). While entities across datasets overlap to some degree, they still cover a diverse set of biomedical named entities.

#### 3.2. Input modeling: Preparing data for zero and few-shot NER task

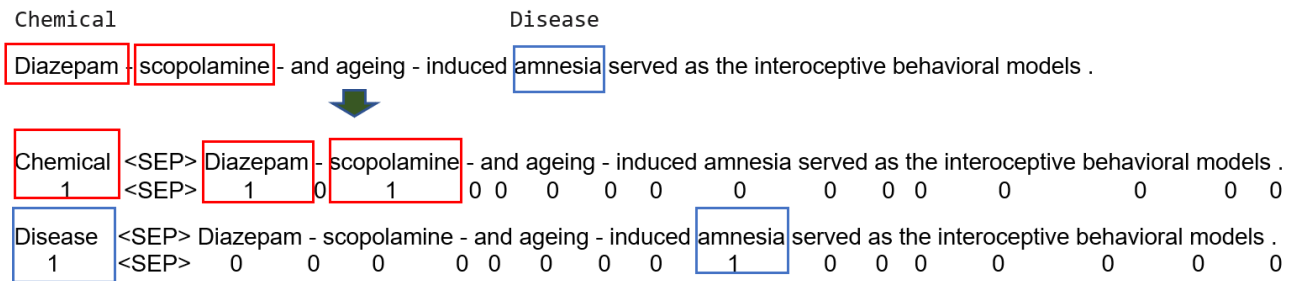
In the given datasets, all the named entities were annotated on a document level. The datasets were in different annotation and file formats. Therefore, we first performed processing that would unify all the datasets into a single format.

**Firstly, documents were split into sentences. We split the sentences that contain multiple classes of entities into separate sentences. Each sentence contained a single annotated named entity class.** The intuition was to create a method and dataset in which each sentence has a specification of entity type that should be annotated. Therefore, data was formatted as:

*< Label Name >< Separator >< Sentence >*

Where the label name is a class that is being annotated, and the sentence is a sentence example. In order to create a training set, for each sentence we have created an output vector by aligning annotations with sentence tokens, and labeling tokens annotated with defined label name with 1, while labeling unannotated tokens with 0. For the label name, we have created two variants. In one variant, the label name was also annotated with 1, with the intuition that model may learn relationships between label names and named entities that are being annotated. In the other variant, the label name was annotated with 0. We wanted to compare these two approaches and evaluate whether the annotation of label name influences the results. This technique allowed us to transform token classification from a multi-class into a binary classification problem. The example of building input and expected output sequences in the new dataset can be seen in Figure 1

### Input example transformed from multiclass into binary representation



**Figure 1:** Example of transforming one annotated sentence to the new format of input and expected output. The sentence comes from the CDR dataset, with 2 annotation classes (Chemical and Disease), and therefore is transformed to two training sequences.

Considering the fact that our focus was on recognizing biomedical named entities, we wanted to include a broad range of different biomedical subdomains (drugs, diseases, chemical compounds, etc.). We also included some subclasses of previously gathered classes (for example, specific disease for disease, protein type for protein), which will be used to explore the model’s transfer learning behavior from more generic to specific classes and vice versa.

We merged all six datasets into one. In doing so, we also matched same classes in previously different datasets (e.g. 'Cell Line' was present in both BioRED and JNLPBA corpus).

The dataset was split into training (85%), validation (5%) and test (10%) sets in a way that each named entity class has the same percentage representation in all dataset parts.

### 3.3. Dataset statistics

The final dataset consists of around 750,000 samples (sentences), containing 26 biomedical entities.

Comparison between the number of labeled and unlabeled tokens in our dataset is given in Figure 2, while the share of each class is given in Figure 3. There are about 3% of labeled tokens and the biggest class overall is *Chemical*, followed by *Protein*.

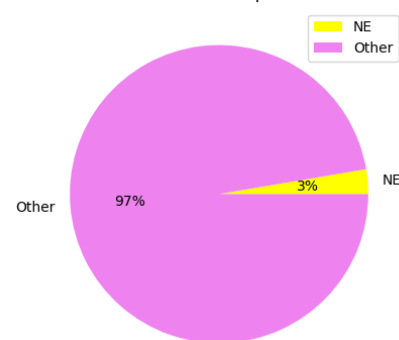
The distribution of classes per dataset is given in Table 1.

### 3.4. Model architecture and training method

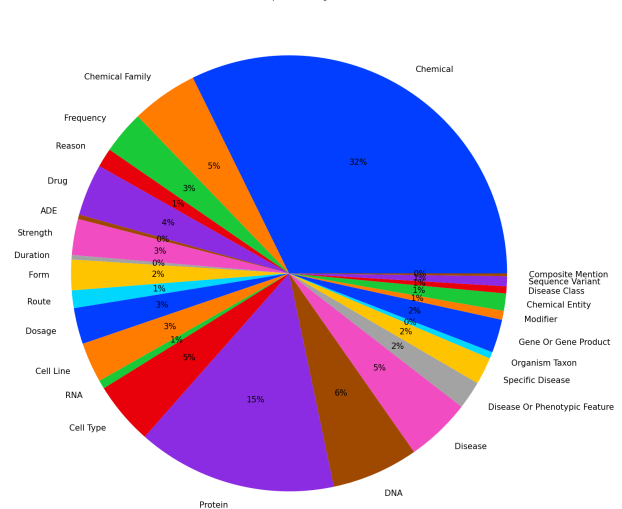
Training samples are first tokenized using either PubMedBERT or BioBERT tokenizers. It is important to note that tokenizers for BioBERT and PubMedBERT differ significantly as explained in detail in [Gu et al. \(2021\)](#).

The model is based on BERT architecture adapted for NER based on BioBERT (biobert-v1.1) and PubMedBERT models (PubMedBERT-base-uncased). One linear and one softmax layer for token classification are added on top of the base model. The model classifies each token as containing or not containing the searched named entity (see Figure 4).

BERT architecture is pre-trained on the next sentence prediction task alongside with masked language modelling Lee et al. (2020). Next sentence prediction task is conducted



**Figure 2:** Amount of labeled tokens (NE), compared to unlabeled tokens (Other) in the created dataset.



**Figure 3:** Distribution of entity classes in the dataset.

by splitting input text into two segments. Self attention layers are then able to learn dependencies and relations of the tokens from the first segment (label) to all the tokens from the second segment (sentence to be labelled). We place the text label in the first segment and the text we want to label



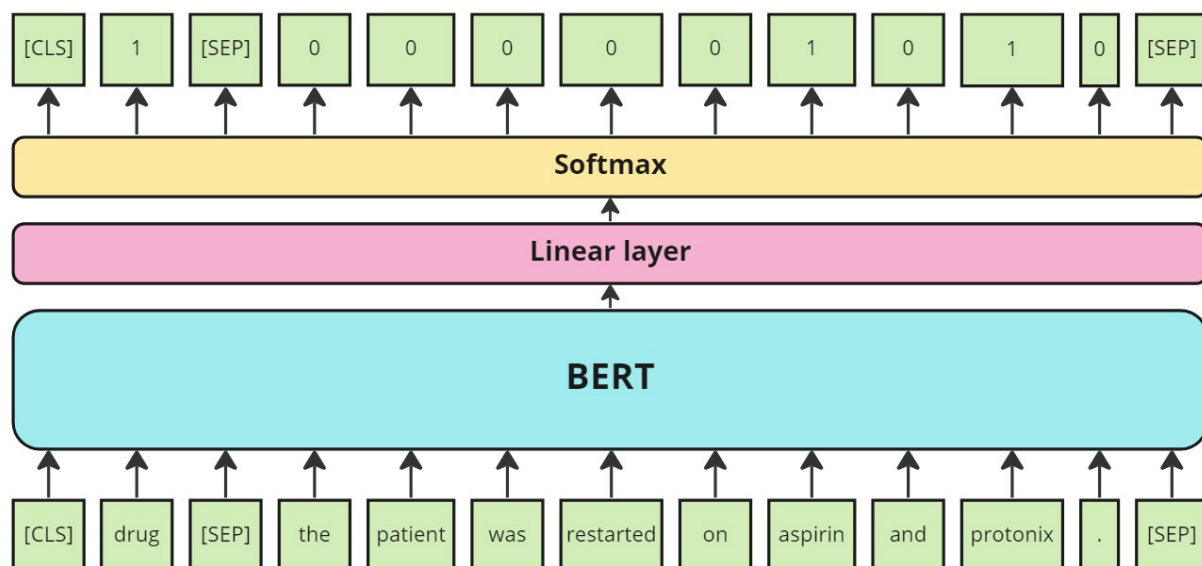


Figure 4: Model architecture.

Table 1

Class and token distribution in individual data sets. Column A: Number of sentences containing the class, Column B: Number of tokens per class, Column C: Percentage of labeled tokens.

	Class	A	B	C
NCBI	Specific Disease	7029	8846	5,39
	Composite Mention	1119	922	3,37
	Modifier	5343	2923	2,26
	Disease Class	4158	2304	2,23
	Sequence Variant	3246	3247	6,16
BIORED	Gene Or Gene Product	6194	10813	6,08
	Disease Or Phenotypic Feature	7599	9132	5,15
	Chemical Entity	5337	5611	4,42
	Cell Line	601	312	1,58
	Organism Taxon	6923	2163	1,35
CDR	Disease	17015	21057	5,89
	Chemical	17015	20366	5,38
CHEMDNER	Chemical	95221	121189	4,11
	Chemical Family	95221	21614	0,81
JNLPBA	Protein	22402	64958	10,98
	DNA	22402	28152	4,53
	Cell Type	22402	20378	3,57
	Cell Line	22402	12706	2,05
	RNA	22402	2786	0,46
n2c2	Drug	36078	16864	2,40
	Frequency	36136	14026	2,01
	Strength	36077	11696	1,52
	Dosage	36077	11749	1,50
	Form	36077	9918	1,40
	Reason	36082	6165	0,88
	Route	36077	5725	0,85
	ADE	36078	1459	0,19
	Duration	36077	1480	0,16

in the second segment. We hypothesise that our model will learn the desired graph connections between different segments through the zero-shot fine-tuning process. We setup this supervision by providing positive class label on tokens in the second segment which correspond to occurrence of the named entity defined in the first segment for seen classes. All

other tokens are labeled as negative class. This is illustrated in Figure 4.

Our architecture is one of the contributions of this paper. Similar ideas have been used in two groups of models in the literature. The first group of models stems from the cross-encoders for sentence similarity where two input segments are filled as input in order to assess similarity measure between them (Humeau, Shuster, Lachaux and Weston, 2020). The second group of models uses two input segments for the classification of the second segment by the class name contained in the second segment (Halder et al., 2020).

In this setup, the name of the named entity class is not strictly defined. Users may place any named entity class in the first segment and the model will identify tokens in the second segment corresponding to the named entity class name from the first segment. This allows for zero-shot named entity recognition where the model will recognize the entity it has not been trained on.

This setup also allows training from any checkpoint and adding new examples with new labels without restrictions. We can add a set of examples to the existing checkpoint. This allows for fine-tuning of few-shot learning methodology and improving the method fast given a few training examples. For few-shot learning, we have used 10 epochs to fine-tune the model on the given set of training samples.

To summarize the procedure, we fine-tune the model in two stages:

- **Zero-shot fine-tuning** - This model is trained on the dataset, excluding one of the classes. It can be used to annotate entities of pre-trained named entity classes as well as unseen classes.

- **Few-shot fine-tuning** - Model is fine-tuned on a few shots (1, 10, or 100 examples) of unseen classes for 10 epochs.

Training of the models was performed with batch sizes 32 on a single A100 GPU. The method used ADAM optimizer (Kingma and Ba, 2014) with recommended values of optimizer parameters. Learning rate value of 5e-5 was used and slight decay of learning rate (0.01) was applied. The implementation was done using Pytorch and Huggingface transformer library.

### 3.5. Model selection and testing

There is no strong consensus in the literature for the criteria of model selection in zero-shot setups. The main challenge is that the input data (e.g. possible classes) during the deployment is unknown.

Throughout our experiments, we considered several validation strategies to select model optimized for zero-shot performance. In order to select model we have used the following approach:

We split dataset into training (85%), validation (5%) and test (10%) sets in a way that each named entity class has the same percentage representation in all dataset parts. One class is selected as unseen for the purpose of zero-shot fine-tuning by removing the examples with that class from train dataset. The examples of the unseen class are selected from test datasets for the purpose of performance testing of our model. Validation set was kept the same as initial validation split containing all classes. We elaborate our decision in discussion section. Few-shot fine-tuning was then conducted with the examples previously removed from train dataset for zero-shot fine-tuning process. The model performance were evaluated with the selected unseen class examples from the test set. We then conducted this procedure for several different classes taking into account semantic relations between different classes.

## 4. Experiments and results

Table 2 and Table 3 show the results of testing 9 classes. The results in the first table are for the model trained with data that had zero in the first segment, and the second table presents the test results if the model was trained with data that had one on the first segment. Both tables include the best epoch for each of the classes.

In both tables, the first group gives the test results when the BioBert model was used as the initial fine-tuning model and the second group when PubMedBert model was fine-tuned.

The column with zero represents the testing of a specific class on the model by training without any examples of that class (zero-shot), and the following columns present results of testing the fine-tuned zero-shot model with 1, 10, and 100 examples of a previously unseen class (1-shot, 10-shot and 100-shot).

It can be seen from the table that we have the best results in the zero-shot regime for the Disease class in all the cases,

regardless of the base model or whether 1 or 0 are in the first segment. Disease gives the best results also for the case when we train the models with one or ten examples of that class. Disease and Specific Disease are both syntactically and semantically similar classes. Both of them presented promising results when they were excluded, showing that transfer learning using semantically and syntactically similar classes is happening. Class Drug is semantically similar to the class Chemical, but they are syntactically different. It can be seen that Drug shows good results, probably based on the transfer from Chemical, but the other way around the results are much worse. This may be due to the fact that all drugs are chemicals, but not all chemicals are drugs. The Dosage class shows interesting behavior: the zero-shot model is unable to detect it, but learns very well with a few supporting examples, at times exceeding the results for classes that are semantically similar to the classes in the training set. This is because the class Dosage is semantically independent from other classes (both in form and name). However, Dosage has a specific structure (usually measures such as mg, g, ml, etc.), and therefore the method is learning it well based on a few examples. Most of the classes saturate between 75-87% F1 score after 100 shots, depending on the entity, which is not far from the reported state-of-the-art NER results trained on the whole dataset (for example, Kühnel and Fluck (2022) reported F1 score of 87.27% for NCBI corpus and 83.07% for CDR corpus using BioBERT, BioRED reported F1-score of 89.3% (Luo et al., 2022a)).

## 5. Discussion

We have presented a promising approach for zero- and few-shot NER for biomedical named entities. The macro-average for zero-shot NER for PubMedBERT model is 39.66%. Our results are better than many approaches presented in the general domain. For example, Van Hoang et al. (2021) and Aly et al. (2021) reported macro-average F1-score of 23%, and Nguyen et al. (2021) reported macro-average F1-score of up to 30% for zero-shot. Our method significantly outperforms most of these approaches, and in 100 shots it is relatively close to the performance of the method trained on the full dataset. Even, much larger and more complex proprietary chatGPT models (GPT-4 based model) have been, to the best of our knowledge, reporting similar performance - F1 score of 41.8% for exact NER matching in clinical NER (Hu et al., 2023). At present, hosting this proprietary model on consumer electronics is not feasible due to its extensive size, resulting in slow performance and significant costs associated with hosting.

We could note three types of behaviors depending on the entities:

- The first pattern can be seen in entities, such as Dosage, Cell Line or DNA. They have poor performance in zero-shot, but are steeply learned based on the given examples, and reach 75-85% F1 score in 100 shot. Poor zero-shot performance is due to semantic independence of these classes to the seen classes

**Table 2**

F1 (precision, recall) scores and best epoch for models trained with 0 in the first segment.

	Class	Epoch	Number of supporting examples			
			0	1	10	100
BioBert	Drug	2	49.46 (83.97,35.05)	67.36 (76.71,60.04)	73.16 (66.91,80.69)	81.63 (75.86,88.34)
	Protein	2	45.41 (76.67,32.26)	72.13 (71.36,72.92)	80.07 (81.90,78.33)	85.61 (81.94,89.62)
	Dosage	3	0.00 (0.00,0.00)	0.00 (0.00,0.00)	86.01 (92.70,80.22)	85.44 (79.68,92.09)
	Cell Line	3	2.18 (1.80,2.78)	2.52 (2.06,3.23)	46.64 (31.12,93.02)	53.10 (37.27,92.27)
	Disease	3	<b>83.16</b> (88.27,78.61)	<b>85.73</b> (82.48,89.26)	<b>86.79</b> (83.04,90.89)	<b>86.82</b> (85.04,88.66)
	Chemical	2	4.45 (13.48,2.66)	70.20 (62.47,80.11)	72.18 (72.95,71.43)	81.38 (78.86,84.06)
	Specific Disease	2	61.37 (53.16,72.60)	62.12 (53.28,74.48)	63.48 (49.60,88.18)	73.98 (67.71,81.55)
	RNA	2	0.00 (0.00,0.00)	13.70 (8.07,45.21)	13.27 (7.13,95.55)	75.46 (68.33,84.25)
	DNA	2	0.07 (0.47,0.04)	12.00 (28.19,7.63)	78.02 (68.47,90.67)	78.23 (69.91,88.82)
	Average	2.3	<b>27.35</b> (35.31, 24.89)	<b>42.86</b> (42.74,48.10)	<b>66.63</b> (61.54,85.44)	<b>77.96</b> (71.62,87.74)
PubMedBert	Drug	1	72.36 (79.48,66.41)	80.91 (76.46,85.91)	78.65 (71.77,87.00)	80.22 (73.16,88.78)
	Protein	2	70.16 (84.39,60.04)	73.26 (80.19,67.44)	78.99 (80.93,77.15)	83.43 (76.19,92.18)
	Dosage	3	0.00 (0.00,0.00)	1.93 (3.41,1.35)	0.00 (0.00,0.00)	<b>87.01</b> (82.39,92.17)
	Cell Line	3	2.95 (2.58,3.45)	1.87 (1.69,2.10)	47.65 (32.07,92.65)	61.18 (46.04,91.15)
	Disease	4	<b>80.17</b> (87.11,74.26)	<b>82.57</b> (86.01,79.41)	<b>85.74</b> (84.87,86.63)	86.86 (82.44,91.78)
	Chemical	1	50.08 (65.00,40.74)	61.80 (66.12,58.01)	74.29 (71.16,77.72)	80.92 (74.83,88.10)
	Specific Disease	4	64.59 (55.16,77.90)	63.55 (53.61,78.01)	64.59 (55.16,77.90)	76.83 (73.71,80.22)
	RNA	2	15.14 (9.74,33.90)	27.70 (17.26,70.21)	14.30 (7.73,95.21)	75.73 (69.01,83.90)
	DNA	3	1.46 (18.26,0.76)	10.64 (17.57,7.63)	.78.06 (68.78,90.23)	79.45 (72.30,88.16)
	Average	2.6	<b>39.66</b> (44.64, 39.72)	<b>44.92</b> (44.70,50.01)	<b>58.03</b> (52.50,76.05)	<b>79.07</b> (72.23,88.49)

**Table 3**

F1 (precision, recall) scores and best epoch for models trained with 1 in the first segment.

	Class	Epoch	Number of supporting examples			
			0	1	10	100
BioBert	Drug	2	30.57 (79.41,18.93)	79.83 (82.37,77.44)	78.00 (76.41,79.67)	78.74 (71.69,87.32)
	Protein	2	63.84 (76.13,54.96)	71.74 (71.13,72.36)	77.51 (78.13,76.89)	84.96 (79.41,91.35)
	Dosage	2	0.00 (0.00,0.00)	0.15 (0.91,0.08)	78.03 (76.73,79.38)	87.95 (83.88,92.42)
	Cell Line	3	1.90 (1.61,2.33)	3.49 (2.85,4.50)	48.54 (33.25,89.87)	55.63 (40.49,88.82)
	Disease	3	<b>81.36</b> (87.61,75.94)	<b>86.22</b> (84.99,87.48)	<b>86.72</b> (82.68,91.19)	<b>85.87</b> (82.90,89.06)
	Chemical	1	6.61 (19.26,3.99)	73.89 (66.86,82.58)	73.63 (74.47,72.79)	82.51 (80.40,84.74)
	Specific Disease	1	53.06 (48.58,58.45)	60.08 (51.76,71.60)	63.32 (50.94,83.65)	73.71 (64.77,85.52)
	RNA	1	5.53 (3.09,26.03)	14.38 (7.78,94.52)	13.44 (7.24,92.81)	58.50 (45.30,82.53)
	DNA	2	1.63 (7.81,0.91)	18.64 (16.01,22.29)	78.56 (71.25,87.55)	77.25 (67.18,90.89)
	Average	1.9	27.17 (35.94,26.84)	<b>45.38</b> (42.74, 56.98)	66.42 (61.23,83.75)	76.12 (68.45,88.07)
PubMedBert	Drug	2	66.92 (73.20,61.63)	77.73 (72.67,83.56)	80.10 (77.74,82.60)	81.94 (75.57,89.48)
	Protein	3	71.18 (83.13,62.23)	73.85 (73.65,74.05)	80.80 (82.10,79.53)	87.08 (84.29,90.06)
	Dosage	3	0.00 (0.00,0.00)	52.42 (45.11,62.54)	85.67 (95.36,77.78)	<b>86.99</b> (82.91,91.50)
	Cell Line	3	2.47 (2.10,3.00)	3.54 (2.92,4.50)	64.10 (51.91,83.80)	58.94 (43.55,91.15)
	Disease	2	<b>81.50</b> (91.65,73.37)	<b>85.19</b> (85.09,85.30)	<b>87.28</b> (84.38,90.40)	85.52 (80.39,91.34)
	Chemical	1	12.79 (32.08,7.99)	74.96 (68.66,82.54)	75.37 (75.45,75.29)	83.46 (79.35,88.02)
	Specific Disease	2	61.83 (53.66,72.93)	60.94 (52.16,73.26)	65.70 (53.43,85.30)	77.03 (68.59,87.85)
	RNA	2	20.87 (12.18,72.60)	17.39 (9.72,82.53)	14.59 (7.90,95.21)	77.62 (73.25,82.53)
	DNA	2	1.44 (12.65,0.76)	4.86 (4.44,5.37)	75.87 (66.73,87.91)	76.98 (65.42,93.50)
	Average	2.2	35.44 (40.07,39.39)	<b>50.10</b> (46.05,61.52)	<b>69.94</b> (66.11, 84.20)	<b>79.51</b> (72.59,89.49)

during zero-shot fine-tuning. However, these classes appear in the very specific context and algorithm can learn very fast from such specific context in few-shot fine-tuning. For example, class Dosage is often followed by quantity information such as milligram.

- The second pattern can be seen in entities such as Drug and Protein where zero-shot performance is fairly good and few shot performance increases also in satisfactory manner and approaches limits of many shot learning. This pattern is attributed to the semantic similarity of unseen class to the classes seen during zero-shot fine-tuning. Classes Drug and Protein are semantically subordinate to the seen class Chemical (hyponymy).
- The third pattern can be seen in class Disease where excellent zero-shot success is obtained. This is due to the fact that class disease is both semantically and syntactically related to specific disease in super-ordinate relation (hypernymy).

It is important to note that the base model using the mentioned datasets can be trained on 26 biomedical entities, and can be used for recognizing any of these entities. For these entities, it would perform close to state-of-the-art. However, in addition, the model would be able to recognize new entities, that the model has never seen. The model would attempt to find similarity between the new class and some of the previously trained classes. In addition to this, the model can be fine-tuned with additional few examples of the new class. We have shown that the model can significantly improve the results for the new class based on just a few given examples.

During our experiments, we noticed challenges in selecting the right validation method for selecting the best-performing zero-shot base model and the instability of zero-shot results during different runs.

**Table 4**

Comparison of validation on BioBert with 1 on the first segment with and without seen class in the validation set. Results are given as F1 score (precision, recall).

Model	Class	Number of supporting examples			
		0	1	10	100
No unseen	Chemical	2.10 (6.83, 1.24)	25.15 (45.30, 17.41)	72.33 (69.04, 75.95)	78.21 (67.84, 92.33)
	Protein	49.18 (78.46, 35.81)	74.28 (77.42, 71.39)	80.02 (82.77, 77.44)	86.05 (80.92, 91.89)
	Disease	81.36 (87.61, 75.94)	86.22 (84.99, 87.48)	87.16 (83.98, 90.59)	85.24 (80.02, 91.19)
With unseen	Chemical	6.61 (19.26, 3.99)	73.89 (66.86, 82.58)	73.63 (74.47, 72.79)	82.51 (80.40, 84.74)
	Protein	63.84 (76.13, 54.96)	71.74 (71.13, 72.36)	77.51 (78.13, 76.89)	84.96 (79.41, 91.35)
	Disease	81.36 (87.61, 75.94)	86.22 (84.99, 87.48)	86.72 (82.68, 91.19)	85.87 (82.90, 89.06)

### 5.1. Selecting the model during zero-shot fine-tuning

There is no consensus in the literature about how to perform validation for selecting a zero-shot model. We have considered five options:

- Create a validation dataset containing all of the classes, including the unseen class
- Create a validation dataset containing all of the seen classes, excluding the one we want to evaluate for zero-shot performance
- Create a validation dataset containing only single unseen class
- Create a validation dataset containing a few unseen classes
- Manual inspection of various models occurring throughout zero shot fine-tuning process.

For each of these options, there are theoretical and practical benefits and shortcomings. In the case of creating a validation set containing only the unseen class, it may be likely that the model will perform best during the evaluation. We may obtain a similar gain in performance if the validation dataset contains samples from both seen and unseen classes. Although, in this case, we may argue that the validation is still primarily done on seen classes and that the unseen class will generalize to any unseen class. Therefore, it may help the model to have some unseen class in the validation set, but it may be best to test it on different unseen classes. The practical case would be to train and validate the dataset on seen classes only, since we do not know what will be the unseen class during the deployment.

During validation, we have used both seen and unseen class validation. The motivation was based on the fact that we were training for a zero-shot class. However, this, in reality, may not always be practical, even though one unseen class may generalize for others. Also, we later came to the conclusion that validation should probably use only seen classes. The run for creating the base model lasted for over 6h per run, and therefore re-running all the models was not possible. However, we present a comparison of the results of three different classes based on two validation sets (with and without unseen classes) using the BioBERT model. The results can be seen in Table 4.

As mentioned before, for two classes results are slightly better for zero-shot, while for one class they are the same (Disease). The selection of the model can be influenced and improved by adding an unseen class that the model will be evaluated to the validation set.

### 5.2. Instability of zero-shot results

While performing the experiment, we noticed that the results for the zero-shot NER may be unstable. Namely, in different runs, using the same datasets, and same models, we were obtaining different results for zero-shot NER. In a few-shot regime, the results would stabilize and would not differ much, but in zero-shot, the difference could be high. For example, for the class Drug, in four training runs on the same data, we obtained F1 score results ranging from 0.96% to 44.66%. In order to create reproducible results, we have fixed seed (we have used seed = 0) and set PyTorch to use deterministic methods. The previous tables and text reported results with the fixed seed and using deterministic methods.

This possibly happens due to gradient descent to some of the local minimum and remaining there, instead of reaching the global minimum. Given that we work with text, in high dimensional vector space, it is likely that our objective function is non-convex and complex with many local minima and maxima. Gradient descent can get stuck in a local minimum if the gradient is flat or small in that region, preventing the algorithm from exploring other parts of the search space (Noel, 2012). In our future work, we will explore methods to reliably reach a local minimum, such as adjusting the learning rate, adding regularization, adding momentum to the optimization algorithm, and exploring other adaptive learning rate methods.

## 6. Conclusion and future work

In this paper we have presented a method for zero- and few-shot named entity recognition in the biomedical domain. Since the research idea originated from Bayer Pharmaceuticals, we have focused on biomedical entities, however, the same method can be applied to other domains, given the annotated data for a larger number of classes is available. The method is based on encoder-based transformer models and input data modification that factorizes regular multi-class token classification into binary classification, given the class that the user would like to annotate. The method showed state-of-the-art results for zero-shot NER and, to the best of our knowledge, it is the first method specifically shaped for



zero- and few-shot NER in the biomedical domain. We have evaluated nine common biomedical classes, but the method will behave in a similar fashion for other classes.

The performance of the model on the unseen classes can be improved by providing and fine-tuning the model with several examples. This training is fast and brings the performance of the model to the F1 score of 75-87% after 100 examples. This is often close and comparable to the BERT-based models trained on the whole dataset containing thousands of examples.

In this paper, we also compare and discuss various strategies for zero-shot model validation. We have proposed three strategies - (1) using unseen classes only, (2) using seen classes only, (3) using both seen and unseen classes. We note that using an unseen class in validation may lead to the selection of a better model for zero-shot NER. However, since users do not know what the unseen classes will be, this method has questionable practicality.

The base zero-shot model showed instability issues, which is likely caused by the model not being able to reach the global minimum of the optimization function. We are planning to address this issue in the future work.

We are also planning to investigate active learning approaches that may improve the results of the method even further. Our method could also help in labeling datasets while improving itself by confirmed human annotation. For example, our method can be used instead of the self-correcting network in the approach proposed by Ilić and Tadić (2022). Using active learning, the model can also learn to identify difficult examples and flag them for further review.

## Declaration of competing interest

The authors declare no competing interests.

## Model and code availability

The base model trained on all 26 classes based on PubMedBERT is available at <https://huggingface.co/ProdicusII/ZeroShotBioNER>. The code used to train the models can be found at <https://github.com/br-ai-ns-institute/Zero-ShotNER>.

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