Protein-STORY: Semantic Text-Oriented Representation Yields biologically meaningful Protein embeddings

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Abstract

Unsupervised representation learning using masked language modeling on the *'language of life'* has transformed protein research, enabling the analysis of a protein universe that is expanding at an exponential pace. However, most current models rely solely on sequence data, overlooking decades of expert-curated biological knowledge stored in natural language. While recent multimodal and knowledge-graph-based approaches attempt to bridge this gap, they often rely on shallow functional labels that lack the contextual depth of full textual narratives. We present Protein-STORY, a general pipeline that synthesizes protein embeddings from diverse, multi-source text descriptions. At the core of our approach is a novel network architecture designed for the semantic compression of multi document embeddings, which integrates high-fidelity functional and structural insights into a unified representation. Our experiments demonstrate that Protein-STORY produces biologically meaningful embeddings ($r \approx 0.75$) that outperform existing models on diverse downstream tasks ($+2\%$ F1 in function prediction). Furthermore, by projecting the *'story'* of a protein into a natural language semantic space, our model enables effective zero-shot text-prompted protein search. Our codes and data are available at https://github.com/kiharalab/Protein-STORY.

1 Introduction

Proteins are the fundamental building blocks of life, governing a complex network of interconnected functional mechanisms within an organism (Levitt, 2009). As their biological functions and 3D structures are primarily encoded in their amino acid sequences, effectively the *'language of life'*(Heinzinger et al., 2019), a plethora of research has been conducted to develop sequence-based protein representation learners (Ibtehaz and Kihara, 2023). This trend has been further inspired by the success of Natural Language Processing , employing unsupervised masked language modeling (Devlin et al., 2019), which has managed to learn robust protein representations suitable for several applications (Meier et al., 2021; Lin et al., 2023). While the exponential growth of unannotated protein databases makes unsupervised learning a necessity (Bateman et al., 2023), this paradigm often overlooks decades of expert-curated biological knowledge stored in textual formats.

While unsupervised representation learning is the standard in NLP due to the scarcity of large-scale annotations, protein research benefits from decades of expert-curated biological knowledge. Current protein language models largely overlook these insights, treating even well-studied proteins as unannotated and fails to leverage established textual information. We argue that integrating such structured knowledge into representation learning captures higher-order biological insights that sequence-only models cannot fully comprehend.

Recent efforts have leveraged knowledge graphs (KGs) to incorporate functional semantics. For example, OntoProtein (Zhang et al., 2022) and its successors, KeAP (Zhou et al., 2023) and Kara (Zhang et al., 2025), utilize Gene Ontology (GO) terms to align sequence embeddings with textual descriptions. However, these models rely exclusively on restricted functional annotations and consequently focus on narrow downstream tasks. While broader KG-based learners, such as, OtterKnowledge (Lam et al., 2023) incorporate pathways and protein families, they often utilize only category names, lacking the contextual depth necessary for nuanced biological reasoning. Consequently, a significant gap remains in developing general-purpose representations that move beyond simple label-matching to integrate high-fidelity text-based biological knowledge.

To address these limitations, we propose Protein-STORY, a pipeline for generating unified protein

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representations from variable, heterogeneous textual data. Our primary contributions include:

- A semantic compression network specifically designed to distill multi-view document embeddings into a cohesive semantic signature.
- The integration of high-fidelity biological narratives, capturing structural, functional and evolutionary contexts that enhance performance on downstream tasks.
- A text-aligned embedding space that facilitates zero-shot protein search, bridging the gap between natural language and proteins.

2 Methodology

2.1 Problem Formulation

We consider a protein as a set of text annotations describing it, e.g., structure, function, evolution, interaction etc. Formally, a protein $\mathcal{P}$ is defined as $\mathcal{P} = \{t_1, t_2, \ldots, t_n\}$

Our goal is to generate a unified embedding $\mathcal{E} \in \mathbf{R}^d$ that aggregates all aforementioned text information, i.e., $\mathcal{E} = \textsc{Protein-Story}(\mathcal{P})$

In a way, we aim to perform semantic compression of a set of embeddings, maintaining a balance between local and global context.

2.2 Data Source

Proteins, being well-studied, are analyzed in millions of literature and hundreds of curated databases. For this work, we limit our text description data to the following features:

i) Family: Proteins sharing origin and function.

ii) Domain: Independent functional or structural unit of a protein.

iii) Homologous Superfamily: Proteins possibly evolutionarily related, having low sequence similarity but sharing a structural fold.

Domains and families offer local vs global context, while homologous superfamilies imply distant evolution and remote homology that is challenging to detect. For each protein, we collect the text descriptions of the associated domains, families and superfamilies from InterPro (Blum et al., 2021), which is a compilation of 13 large databases of these features and also provides expert curated, literature supported rich text descriptions for them.

We collected 11.29 M proteins from InterPro database, having 312,517 different combinations of aforementioned text features. Proteins from SwissProt database (Poux et al., 2017), which are expert curated, are used in different evaluations and thus proteins having similar features are removed from the training dataset, reducing the dataset size to 6.59 M proteins and 309,930 feature combinations.

2.3 Proposed Architecture

We propose a multi-stage architecture to decompose protein-related textual descriptions into a unified embedding. The model is engineered to handle heterogeneous data from diverse sources and in varying quantities; it is specifically designed to project the textual narrative of a protein into the semantic representation space of natural language. The primary components are as follows (Fig. 1):

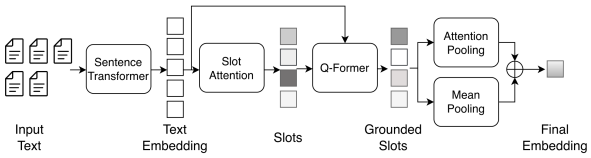


Figure 1: Overview of Protein-STORY.

i) Embedder: Individual texts are encoded using a Sentence Transformer model to generate consistent and comparable embeddings. Specifically, we employ the `pubmedbert-base-embeddings` model (Mezzetti; Gu et al., 2022) due to its proficiency in processing biomedical literature.

$$e_i = \textit{Sentence-Transformer}(t_i), \forall t_i \in \mathcal{P}$$

ii) Disentangler: Protein descriptions often contain redundancy and varying levels of focus. To address this, we employ slot attention (Locatello et al., 2020) and disentangle the descriptions. This module samples $k(= 8)$ slots, S from a normal distribution, which then compete to understand the input features through an iterative competitive attention mechanism. This process partitions the input into a set of specialized concepts, suppressing redundancy while preserving distinctive features.

$$S = \textit{Slot-Attention}(\{e_1, e_2, \ldots, e_n\})$$

iii) Contextual Grounder: To ensure that the abstracted slots remain contextually faithful to the original input, we utilize a novel Slot-Conditioned Q-Former (Li et al., 2023). Rather than using globally learned query vectors, we utilize the slots themselves as queries to attend over the sequence of embeddings (e). This grounding mechanism allows the model to refine disentangled representations by re-incorporating fine-grained details from the raw input context. Furthermore, by conditioning on dynamic slots rather than static learnable queries,

the model can accommodate open-ended protein descriptions without the template-based biases inherent in learnable but shared query sets.

$$x = \textit{QueryFormer}(q = S, kv = e)$$

iv) Aggregator: Finally, we aggregate the grounded slots using an attention-based pooling mechanism, driven by a single layer of multi-head self-attention. To preserve global information, we incorporate a residual connection by adding the mean of the grounded slots to the attention output. This fusion of learned attention and mean pooling generates our final protein representation, $\mathcal{E}$.

$$\mathcal{E} = \textit{Attn-Pool}(x) + \textit{Mean-Pool}(x)$$

By aligning the embedding $\mathcal{E}$ with the sentence transformer's representation space, we effectively capture the protein's *'story'* within a single vector.

2.4 Training

We train the model primarily with the retrieval loss based on SupCon (Khosla et al., 2020). Moreover, we propose some coverage, activity and diversity loss for regulating our slots (see Appendix). The model was trained for 30 epochs with the AdamW optimizer (Loshchilov and Hutter, 2019). 20% of the training data was used as the validation split.

3 Experiments and Results

3.1 Multi-Document Retrieval Performance

We evaluate our ability to generate compressed yet informative representations through a retrieval task: the aggregated embedding serves as a query to retrieve its constituent input embeddings from a shared vector space. To ensure robustness, we select proteins from SwissProt with at least 10 associated text features, resulting in 3,801 proteins.

We compare our approach against several baselines: mean and attention pooling, multi-head self-attention (via a [CLS] token), and the Set Transformer (Lee et al., 2019). As shown in Table 1, we report Mean Average Precision (mAP), Normalized Discounted Cumulative Gain (nDCG), Recall@|R| (total relevant items), and Median Positive Rank. Our method consistently outperforms all baselines across all metrics. This demonstrate our model's capacity to aggregate disparate information into a unified representation while preserving the fine-grained signals of individual views, effectively balancing global context with local detail.

3.2 Biologically Meaningful Embedding Space

Protein-STORY embeddings provide a compressed representation of rich biological information. While protein language models (PLMs) are the de-facto standard (Weissenow and Rost, 2025), sequence-based patterns alone often fail to capture the depth of curated experimental and expert knowledge. We evaluate Protein-STORY's representational quality against ESM2-3B (Lin et al., 2023), a state-of-the-art PLM.

First, we measure the correlation between embedding similarity and biological similarity (funSim (Schlicker et al., 2006) for function, TM-score (Zhang and Skolnick, 2004) for structure). Protein-STORY embeddings show strong correlations (76.03 and 74.50), surpassing the weak alignment of ESM2-3B (32.65 and 1.42; Fig. 2). Additionally, linear probing for Enzyme Commission (EC) and CATH class prediction (Sillitoe et al., 2021) (Table 3) confirms that our representations substantially outperform ESM2-3B in macro F1 scores.

These results demonstrate that while unsupervised pLMs are versatile, Protein-STORY more effectively condenses heterogeneous biological knowledge into a unified embedding that can accurately reflect essential protein attributes.

We further compare our representation with ProtTrek (Su et al., 2025), a recent state-of-the-art multimodal protein language model that utilizes large-scale contrastive learning to align sequence and structural information with natural language. While ProtTrek exhibits much stronger correlations than ESM (67.70 and 49.16), reflecting its explicit training on textual descriptions, it still lags behind Protein-STORY by margins of 8.33 and 25.34, respectively. Furthermore, despite its improved alignment, ProtTrek underperforms in linear probing tasks, even relative to ESM models, which is consistent with its reported results.

These findings reinforce our core claims: while the multimodal nature of proteins suggests that integrated embeddings are advantageous, properly grounding representation learning in decades of scientific text offers noteworthy potential and should be considered as a major research direction.

3.3 Downstream Task Performance

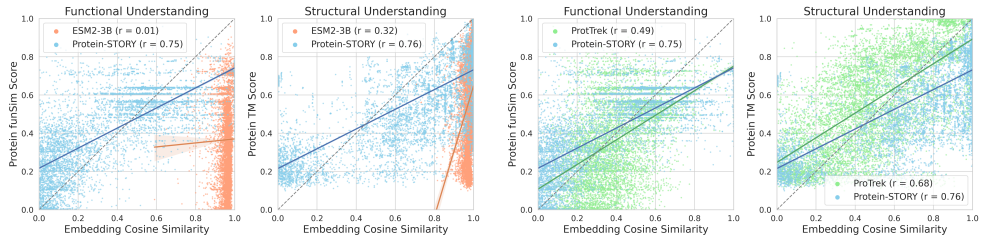
To evaluate the downstream utility of our embeddings, we utilize the PROBE benchmark (Unsal et al., 2022) across three tasks: semantic similarity,

Table 1: Retrieval performance of multi-view embeddings compared to baselines.

Method	#params	mAP (↑)	nDCG@20 (↑)	Recall@|R| (↑)	Median Positive Rank (↓)
Mean Pooling	0	0.462	0.59	0.456	18
Attention Pooling	0.79 M	0.47	0.597	0.464	17
MHSA	26.78 M	0.494	0.618	0.48	15
Set Transformer	21.06 M	0.486	0.612	0.474	15
Protein-STORY	19.42 M	**0.512**	**0.626**	**0.492**	**14**

Table 2: PROBE benchmark evaluation : we report the best score achieved by any other method as PROBE-best.

	Semantic Similarity (ρ)				Gene Ontology (weighted F1)				Drug Target Protein (MCC)			
	MF	BP	CC	Avg.	MF	BP	CC	Avg.	Random	50%	30%	15%
PROBE-best	0.57	0.58	0.51	0.51	0.92	0.72	0.74	0.79	0.92	0.92	0.92	0.90
Protein-STORY	**0.73**	**0.66**	**0.55**	**0.65**	**0.93**	**0.73**	**0.76**	**0.81**	**0.94**	**0.93**	**0.93**	**0.91**



(a) Protein-STORY vs ESM2-3B

(b) Protein-STORY vs ProTrek

Figure 2: Functional and Structural Meaningfulness of Embeddings.

Table 3: Linear probing macro-F1 Score.

	Protein-STORY	ESM2-3B	ProTrek
EC	**78.24 ± 2.27**	61.1 ± 2.45	58.77 ± 1.86
CATH	**83.45 ± 0.23**	73.29 ± 1.66	66.75 ± 0.93

gene ontology, and drug-target protein family classification. As shown in Table 2, Protein-STORY yields consistent improvements across all metrics.

Notably, our embeddings outperform Domain-PFP (Ibtehaz et al., 2023) by 2%, which is remarkable given that Domain-PFP is specifically developed to leverage the same features through functional alignment. This suggests that our model effectively integrates biologically rich text information for downstream tasks. Furthermore, Protein-STORY achieves higher semantic similarity scores than OntoProtein (Zhang et al., 2022) and KeAp (Zhou et al., 2023). This is particularly striking, as it implies our model implicitly captures functional relationships more effectively than methods that utilize explicit functional information.

3.4 Zero-Shot Protein Search via Natural Language

A key advantage of Protein-STORY is the direct projection of protein representations into the language model's embedding space. This alignment treats proteins as textual narratives, mapping them into a semantic space consistent with natural language and enables text-prompted protein retrieval.

To evaluate this capability, we considered SwissProt protein embeddings as a vector database. Query embeddings were generated by processing natural language prompts through the same sentence transformer model. We performed similarity searches using the FAISS library (Douze et al., 2025), employing an exact search configuration (roughly half a million entries). For each query, we retrieved the top 10 nearest neighbors.

The system was tested using complex functional prompts. For the query: *'Identify extracellular proteins involved in the regulation of blood coagulation that utilize specialized structural modules to bind to membrane phospholipids or other protein mediators.'* all top 10 results belonged to the Fibrinogen C-terminal domain-containing family. These proteins facilitate platelet aggregation via the binding of platelet receptor integrin α(IIb)-β(3) to the fibrinogen C-terminal D domain (Podolnikova et al., 2003). This demonstrates that the systen successfully captures the specific functional and structural requirements specified in the query.

Table 4: Protein-Search Benchmark Retrieval Success Result.

Success Rate	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
C1	7	3.6	4	4.2	4.8	7.4	13.8	12.2	11.6	17.6	13.8
C2	6.3	4.7	5.1	3.8	3.4	7.2	13	12.6	12.4	17.4	14
C3	6.9	4.2	3.4	4.2	5	7	12.9	10.8	12.9	17	15.7
C4	7.5	3.9	3.4	4.5	5.1	6.6	14.2	9.9	14.2	17.1	13.4
avg	6.9	4.1	4	4.2	4.6	7.1	13.5	11.4	12.8	17.3	14.2

Similarly, for the query: *'Find intracellular signaling proteins containing SH3 domains that localize to the plasma membrane upon phosphorylation to regulate actin cytoskeleton remodeling.'* the top 3 results were explicitly actin cytoskeleton-regulatory proteins, and the remaining 7 contained SH3 domains. Notably, 9 of the top 10 results are localized to the plasma membrane. These findings demonstrate that the embedding space effectively encodes multi-faceted biological constraints, including domain architecture, subcellular localization, and specific signaling pathways.

3.5 Protein-Search Benchmark

To quantitatively evaluate Protein-STORY's zero-shot retrieval capabilities, we curated a benchmark dataset titled *Protein-Search*. The benchmark consists of 5,000 query-response pairs, categorized into four groups (C1–C4) of 1,250 queries each. These categories represent search tasks requiring the identification of proteins based on 1, 2, 3, or 4 distinct biological attributes, respectively.

We utilized `Qwen2.5-32B-Instruct` (Qwen et al., 2025) to generate realistic natural language queries by providing it with 1–4 InterPro feature descriptions in random combinations (see Appendix). Following the pipeline described in Section 3.4, we performed similarity searches and measured the success rate. On average, Protein-STORY retrieves $>= 5$ correct hits (out of 10) in 76.3% of cases. Detailed results are presented in Table 4, and the benchmark dataset is publicly available in our GitHub repository.

3.6 Case Study : Synthesizing Story from Noisy Data

While Protein-STORY primarily leverages structured, biologically enriched descriptions, a vast majority of protein knowledge resides in unstructured literature, such as PubMed abstracts. To evaluate how our model handles these noisier signals, we randomly selected 1000 protein pairs and retrieved their corresponding PubMed abstracts. Using our model, we generated protein embeddings and measured their correlation with functional similarity (funSim). We observed a correlation of 0.29, which, while lower than the performance on curated InterPro texts, remains superior to PLM-based baselines. This result demonstrates the potential for scaling Protein-STORY to incorporate millions of scientific publications, a key objective for our future work.

3.7 Ablation Study

We performed several ablation experiments and our primary findings are as follows:

- Removing Slot Attention harmed multi-view retrieval. Our initial experiments demonstrated strong bias towards closely related textual attributes.
- Replacing Slot-conditioned Q-Former with static learnable queries reduced contextual fidelity and representation diversity.
- Removing slot regularizers led to slot collapse and reduced retrieval performance.

Please refer to the Appendix for more details.

3.8 Model Interpretation

Please refer to the appendix.

4 Conclusion

In this work, we have developed Protein-STORY, a text-guided representation learner for proteins. While existing self-supervised methods are highly competitive, they often neglect decades of rich biological knowledge stored in textual formats. Our comprehensive analyses demonstrate that integrating textual narratives as features significantly enhances protein representations, bridging the gap between raw sequences and established functional insights. These results underscore the potential of text-aligned models to capture a more holistic understanding of biological systems.

Moving forward, we intend to explore a broader range of textual sources to further enrich the semantic depth of protein representations. Furthermore, we plan to evaluate the generalizability of the framework in domains beyond biology.

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Limitations

The primary limitation of this work is the restricted scope of protein-associated textual data. Currently, we utilize only family, domain, and superfamily annotations, omitting critical metadata such as biochemical properties, metabolic pathways, and scientific literature. Incorporating these multi-faceted sources would likely enhance the semantic robustness and versatility of the resulting embeddings.

Additionally, our methodology simplifies text into fixed-length vectors via sentence transformers. While effective for broad conceptual alignment, this 'bottleneck' may overlook fine-grained semantic nuances and token-level relationships. Future work should explore using Large Language Models (LLMs) to operate directly on raw text, enabling a more sophisticated synthesis of complex protein-text interactions.

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A Appendix

A.1 Experimental Setup

All the experiments were performed in a linux server equipped with AMD EPYC 7313P 16-Core Processor, 128 GB Ram and 2x NVIDIA RTX A6000, 48 GB GPUs.

A.2 Model Parameter

Our model has a total of 19.42M parameters and requires 0.5–1.0 GFLOPs.

A.3 Code Availability

The model design, data processing, training, and experimental code were developed by the authors. The implementation is based on PyTorch v2.2.0+cu121. The code will be released under the GPL license.

A.4 Dataset Description

We collect text descriptions of protein from the InterPro database, which is a compilation of 13 databases dealing with various functional and structural features of proteins. The most useful benefit of using InterPro database is that they provide rich text description with literature evidence for the different protein features.

For our work, we considered 3 primary features of proteins:

1. Domain : Domains are independent structural or functional modules within a protein. Each domain typically executes a specific interaction or task, collectively supporting the protein's overall biological activity. Notably, these units are versatile, nearly identical domains are frequently identified across a wide range of proteins with otherwise unrelated functions.

2. Family : A protein family is a group of proteins that are evolutionarily linked. Because they descend from a common ancestor, they usually share similar amino acid sequences, three-dimensional shapes, and biological roles. Families can be further divided into subfamilies when certain members develop even more specific specialized functions.

3. Homologous Superfamily : A protein superfamily is a broader category that sits above the family level. It contains multiple protein families that are distantly related. While the proteins in a superfamily might not look very similar at a sequence level anymore, they still share a common structural 'fold' or a fundamental functional mechanism that proves they share an ancient common ancestor.

In the current version of the InterPro (Release 107.0, 16th October 2025), there are a total of 17,951 domains, 26,829 families and 3,511 homologous superfamilies. We collected text descriptions of all these entries from:

https://ftp.ebi.ac.uk/pub/databases/interpro/current_release/interpro.xml.gz

Once downloaded these text abstracts were sanitized and there embeddings were computed using the neuml/pubmedbert-base-embeddings sentence transformer, which is optimized on pubmed abstracts.

Next, we collect all the precomputed features of 11.29 million proteins from https://ftp.ebi.ac.uk/pub/databases/interpro/current_release/protein2ipr.dat.gz. The consist of 312,517 combinations of the aforementioned features. The distribution protein features are shown in Fig. 3

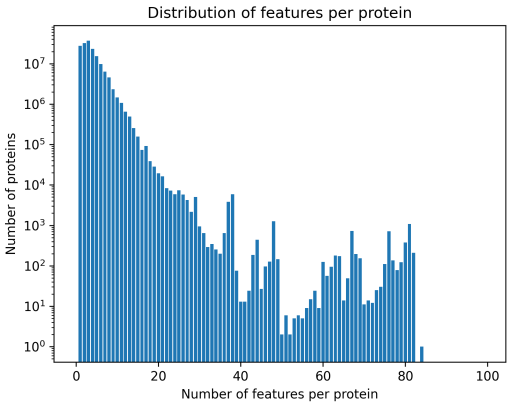

Figure 3: Distribution of features per protein

Since, well-curated proteins from SwissProt dataset are commonly used in benchmarks, we remove proteins having similar features. This reduces the dataset to 6.59 million proteins and 309,930 feature combinations.

A.5 Architecture Overview

Here we provide pseudocodes for our model implementation.

Algorithm 1: Protein-STORY Model

Input: InterPro feature tokens $T \in Z^{B\times N}$, mask $M \in \{0,1\}^{B\times N}$, optional slot count K

Output: Dictionary of embeddings and attention weights

/* 1. Embedding Extraction */

$\mathbf{E} \leftarrow$ Sentence-Transformer(T)

// Frozen pre-trained llm embeddings

$X \leftarrow \text{Linear}_{in}(\mathbf{E})$ // Project to internal dimension D

/* 2. Feature Disentanglement */

$K \leftarrow (K > 0)\ ?\ K$: self.num_slots // Default number of slots

$S, Attn_{slot} \leftarrow$ SlotAttention(X, K, M)

/* 3. Slot Grounding */

$S_g, Attn_{ground} \leftarrow$ SlotConditionedQFormer(S, X, M)

/* 4. Aggregation */

$e_{pool}, wgt_{pool} \leftarrow$ AttentionPooling(S_g)

$e_{mean} \leftarrow$ MeanPooling(S_g)

$e_{protein} \leftarrow \text{Linear}_{llm}(e_{pool} + e_{mean})$

// Project back to LLM dimension

$S_{grounded} \leftarrow \text{Linear}_{llm}(S_g)$

return begin

- "protein_emb" : $e_{protein}$
- "slots" : S
- "grounded_slots" : $S_{grounded}$
- "slot_attn" : $Attn_{slot}$
- "pool_weights" : wgt_{pool}

end

Algorithm 2: Slot Attention Module

Input: Input features $X \in R^{B\times N\times D}$, number of slots K, mask $M \in \{0,1\}^{B\times N}$

Output: Refined slots $S \in R^{B\times K\times D}$, attention weights A_{raw}

/* 1. Initialization */

$X \leftarrow$ LayerNorm(X)

$k \leftarrow XW_k, \quad v \leftarrow XW_v$ // Project inputs to keys and values

$\mu, \sigma \leftarrow$ learnable parameters $\in R^D$

$S \sim \mathcal{N}(\mu, \sigma^2)$ // Sample K slots from Gaussian prior

/* 2. Iterative Refinement */

for $t = 1$ **to** T_{iter} **do**

- $S_{prev} \leftarrow S$
- $q \leftarrow$ LayerNorm$(S)W_q$
- $logits \leftarrow \frac{1}{\sqrt{D}} qk^\top$ // competitive attention (softmax over slots)
- **if** M *is provided* **then**
  - $logits \leftarrow$ MaskFill$(logits, M, -INF)$
- **end**
- $A_{raw} \leftarrow$ Softmax$(logits, \text{dim} = \text{slots})$ // Shape: (B, K, N)
- **if** M *is provided* **then**
  - $A \leftarrow A_{raw} \cdot (\neg M)$ // Ignore masked inputs
  - $A \leftarrow A/(\sum_{j=1}^{N} A_{i,j} + \epsilon)$
- **end**
- **else**
  - $A \leftarrow A_{raw}/(\sum_{j=1}^{N} A_{i,j} + \epsilon)$
- **end**
- /* 3. Slot Update via GRU and MLP */
- $updates \leftarrow Av$
- $S \leftarrow$ GRUCell(flatten$(updates)$, flatten(S_{prev}))
- $S \leftarrow S +$ MLP(LayerNorm(S))

end

return S, A_{raw}

Algorithm 3: SlotConditioned QFormer

Input: Slots $S \in R^{B\times K\times D}$, input features $X \in R^{B\times N\times D}$, mask $M \in \{0,1\}^{B\times N}$

Output: Grounded slots $S_g \in R^{B\times K\times D}$, attention weights $\mathbf{A}$

/* 1. Linear Projections */

$q \leftarrow SW_q$ `// Queries derived from slots`

$k \leftarrow XW_k, \quad v \leftarrow XW_v$ `// Keys and values derived from input sequence`

/* 2. Attention Score Computation */

$\text{logits} \leftarrow \frac{qk^\top}{\sqrt{D}}$ `// Dot-product affinity` (B, K, N)

/* 3. Masking and Normalization */

if M *is provided* **then**

  $\text{logits} \leftarrow \text{MaskFill}(\text{logits}, M, -INF)$ `// Mask keys/values`

end

$\mathbf{A} \leftarrow \text{Softmax}(\text{logits}, \text{dim} = \text{sequence})$ `// Normalize over sequence dimension` N

/* 4. Context Projection */

$S_g \leftarrow \mathbf{A}v$ `// Weighted sum of values`

return $S_g, \mathbf{A}$

Algorithm 4: Attention Pooling

Input: Grounded slots $S \in R^{B\times K\times D}$

Output: Pooled embedding $\mathbf{e}_p \in R^D$, attention weights $\mathbf{w} \in R^K$

/* 1. Multi-Head Self-Attention (MHSA) among slots */

$H \leftarrow$ number of heads, $\quad d_h \leftarrow D/H$

$q, k, v \leftarrow SW_q, SW_k, SW_v$ `// Project to` (B, K, H, d_h)

$q, k, v \leftarrow \text{Transpose}(q, k, v)$ `// Reshape to` (B, H, K, d_h)

$\text{logits} \leftarrow \frac{qk^\top}{\sqrt{d_h}}$ `// Compute inter-slot affinity` (B, H, K, K)

$\mathbf{A} \leftarrow \text{Softmax}(\text{logits}, \text{dim} = -1)$

$o \leftarrow \mathbf{A}v$

$S_{attn} \leftarrow \text{Reshape}(\text{Transpose}(o))$ `// Back to` (B, K, D)

/* 2. Norm-Based Importance Pooling */

for *each slot* $i \in \{1, \ldots, K\}$ **do**

  $n_i \leftarrow \|s_{attn,i}\|_2$ `// Compute` L_2 `norm of refined slot`

end

$\mathbf{w} \leftarrow \text{Softmax}([n_1, \ldots, n_K])$ `// Normalize weights across` K `slots`

/* 3. Aggregation */

$\mathbf{e}_p \leftarrow \sum_{i=1}^{K} w_i \cdot s_{attn,i}$ `// Weighted sum of attended slots`

return $\mathbf{e}_p, \mathbf{w}$

A.6 Loss Functions

A.6.1 Primary Loss

Since the effectiveness of our system depends on how well the synthesized embedding can retrieve the input embedding components, we train the model with retrieval objective as the primary loss function. The popular SupCon loss was used for that purpose. SupCon loss has two variants, dealing with sum *outside* and *inside* of the log operation.

$$\mathcal{L}_{out}^{sup} = \sum_{i\in I} \frac{-1}{|P(i)|} \sum_{p\in P(i)} \log \frac{\exp\left(\boldsymbol{z}_i \cdot \boldsymbol{z}_p/\tau\right)}{\sum_{a\in A(i)} \exp\left(\boldsymbol{z}_i \cdot \boldsymbol{z}_a/\tau\right)}$$

$$\mathcal{L}_{in}^{sup} = \sum_{i\in I} -\log \left\{ \frac{1}{|P(i)|} \sum_{p\in P(i)} \frac{\exp\left(\boldsymbol{z}_i \cdot \boldsymbol{z}_p/\tau\right)}{\sum_{a\in A(i)} \exp\left(\boldsymbol{z}_i \cdot \boldsymbol{z}_a/\tau\right)} \right\}$$

Empirically, the *out* loss performs better and it is intuitive as well. The *out* loss focuses on satisfying the overall constraints, whereas the *in* loss handles each constraint independently and then combine them. Therefore, we can consider the *out* and *in* losses as global and local losses, respectively. In order to balance these two aspects, we consider our retrieval loss as follows:

$$\mathcal{L}_{retrieval} = \mathcal{L}_{out}^{sup} + 0.2 \times \mathcal{L}_{in}^{sup} \quad (1)$$

Moreover, we optimized the $\mathcal{L}_{retrieval}$ both ways, i.e., from protein to text retrieval and from text to protein retrieval.

It should be noted that the baseline methods were also trained with the same loss function.

A.6.2 Slot Regularizer

To ensure the model learns a meaningful set of latent representations in the slots, that map effectively to input features (tokens), we employ a composite set of slot regularizer.

- Coverage loss : This loss penalizes if some input tokens don't receive sufficient attention

$$L_{coverage} = (1 - slot\_attn.sum(dim = 1))^2$$

- Activity loss : This loss penalizes lazy or less active slots

$$L_{activity} = (avg\_attn - slot\_attn)^2$$

- Orthogonality loss : This loss compels the slots to learn different concepts.

$$L_{orthogonality} = (I - slot@slot.T)^2$$

- De-uniform loss : This loss prevents the slots from following a uniform pattern by minimizing negative entropy

$$L_{de-uniform} = -entropy(slot\_attn)$$

The combined slot regularizer loss is as follows:

$$\mathcal{L}_{slot} = L_{coverage} + L_{activity} + L_{orthogonality} + L_{de-uniform}$$

The overall loss is computed as a weighted combination:

$$\mathcal{L} = \mathcal{L}_{retrieval} + 0.3 \times \mathcal{L}_{slot}$$

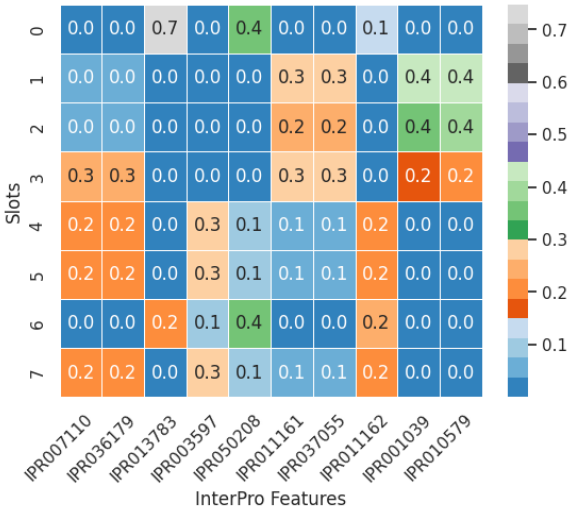

Figure 4: Slot attention weights for the protein 1A01_GORGO

A.7 Model Interpretation

A primary motivation behind our model design is interpretability, which is facilitated by our choice of Slot Attention and the Q-former architecture. As previously discussed, protein-related text features can often be redundant and inter-correlated. In such cases, a uniform pooling mechanism may over-emphasize repetitive content and fail to capture granular details. Slot Attention, however, is designed to disentangle these overlapping features.

We demonstrate this capability by analyzing the slot attention patterns for a specific protein in Fig. 4. In this visualization, slots are arranged along the y-axis and input text features along the x-axis. For example, IPR007110 and IPR036179 both correspond to immunoglobulin-like domains; across all slots, the features of these two inputs are highly correlated, suggesting the model recognizes their similarity and treats them as a unified concept. Similarly, IPR011161, IPR037055, IPR001039, and IPR010579, all related to MHC class I, exhibit correlation within the attention space. More specifically, while IPR011161 and IPR037055 relate to MHC class I-like antigen recognition, IPR011162 recognizes both MHC class I/II-like antigens, leading to shared attention across in some slots.

A.8 Ablation Study

A.8.1 Contribution of the individual components

The contribution of our individual components can be assessed by comparing the full model against the specific baselines. By removing Slot Attention and

the Q-former, the model reverts to an architecture similar to Attention Pooling or a standard Multi-Head Self-Attention (MHSA) model. Furthermore, if we omit Slot Attention and utilize a standard Q-former with learned global queries, the architecture becomes equivalent to a Set Transformer. Consequently, the results presented in Table 1 serve as a sufficient ablation study of our model components.

A.8.2 Impact of retrieval loss

As retrieval loss, we considered a combination of $\mathcal{L}_{out}^{sup}$ and $\mathcal{L}_{in}^{sup}$. Empirically, $\mathcal{L}_{out}^{sup}$ performs much better than $\mathcal{L}_{in}^{sup}$, as it focuses on the global context and thus manages to satisfy majority of the constraints while also being less sensitive to outliers. On the contrary, $\mathcal{L}_{in}^{sup}$, focuses on the individual constraints and specific patterns and thus is more susceptible to noise. In our experiment we observed this interesting outcome as well. When, we trained the model with only $\mathcal{L}_{in}^{sup}$, during retrieval, it managed to extract a few hits in much earlier rank, but at the same time missed a good amount of candidates. On the other extreme, training the model with only $\mathcal{L}_{in}^{sup}$ improved overall recall, but the hits started coming at later ranks. Therefore, as a mean to balance this two opposing behavior we considered a weighted sum of the two losses.

A.8.3 Impact of slot regularizer

The selection of slot regularization functions proved to be particularly interesting and significant. Omitting the coverage and activity losses resulted in the under-representation of certain tokens and the inactivity of specific slots, respectively. Similarly, training the model without an orthogonality loss led to highly correlated and redundant slot features. The de-uniform regularizer was another critical component; without it, the attention patterns became almost entirely flat—exhibiting a uniform focus across all inputs—which effectively caused the attention mechanism to collapse. Only by incorporating these slot regularizers into the objective function were we able to achieve the meaningful attention patterns illustrated in Fig. 4.

A.8.4 Dependence of number of slots

The number of slots (K) to consider, is an important hyperparameter for our pipeline. We have observed that for our current set of inputs, the representation gets saturated after $K = 8$ and further increasing slots marginally changes the performance despite the added computational complexity. However, for less than 8 slots, the performance falls, as shown in Fig 5.

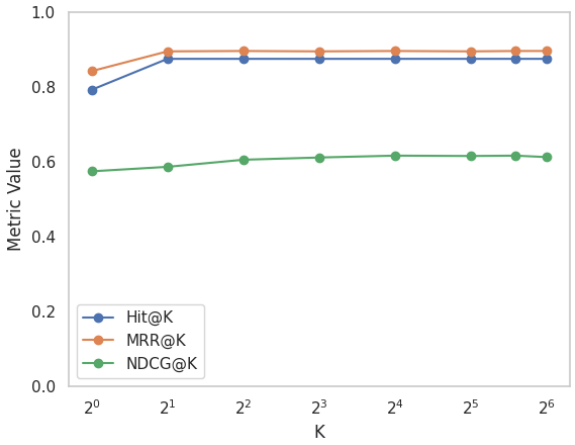

Figure 5: Retrieval Metrics vs K

A.9 Details on Linear Probing Experiment

We conducted two linear probing experiments using the Swiss-Prot database. The tasks included Enzyme Commission (EC) number prediction and CATH class prediction, representing a functional and a structural task, respectively. Our dataset consisted of 7 EC classes and 5 CATH classes. In cases where a protein possessed multiple class memberships, we assigned the majority class label. Following this preprocessing, we obtained 270,689 proteins with EC annotations and 477,027 proteins with CATH classifications. We then performed 3-fold stratified cross-validation using a scikit-learn logistic regression model and reported the results using macro F1 scores.

A.10 Details on PROBE benchmark

The PROBE benchmark assesses the how functionally informative protein representations are. A list of 20,000 human proteins are provided by the benchmark, and users need to submit embeddings for those proteins. We considered 3 tasks from this benchmark.

1. **Semantic Similarity Inference**: This task measures the degree of functional semantic similarity of the protein representations, i.e., which representation vectors capture functional information by comparing the pairwise similarity of protein feature vectors (using Manhattan, Cosine, and Euclidean distances) against ground-truth functional similarities derived from Gene Ontology (GO) annotations

Table 5: Impact of retrieval loss

Loss	hit@1	MRR	MAP	Recal@|R|
$\mathcal{L}_{out}^{sup}$	0.68	0.791	0.519	0.495
$\mathcal{L}_{in}^{sup}$	0.821	0.889	0.421	0.416
$\mathcal{L}_{out}^{sup} + 0.2 \times \mathcal{L}_{in}^{sup}$	0.686	0.797	0.512	0.492

through Lin similarity score. For the final evaluation Manhattan distance is considered.

2. **Ontology-based Protein Function Prediction (PFP)**: A supervised classification task where representations are used to predict specific GO terms across three categories: Molecular Function (MF), Biological Process (BP), and Cellular Component (CC). There are a total of 117 GO terms in this benchmark and they are annotated with experimental evidence. The representations are used as features to a linear classifier and 5 fold cross-validation is performed. The weight F1 score is metric considered in this task.

3. **Drug Target Protein Family Classification**: This task assesses the representation's capacity to identify structural and functional protein families (e.g., enzymes, membrane receptors, ion channels) crucial for drug discovery. MCC is the primary metric for this evaluation.

We downloaded the benchmark from https://github.com/kansil/PROBE and ran the experiments locally using Protein-STORY embeddings.

For the sake of simplicity we only considered the best performing method against each metric. To the best of our knowledge, the best performing methods in this benchmark, i.e., PROBE-best are:

- Semantic Similarity
  1. MF : ProtT5-XL
  2. BP : Mut2Vec
  3. CC : PFAM
  4. Avg : Mut2Vec
- Protein Function Prediction
  1. MF : Domain-PFP
  2. BP : Domain-PFP
  3. CC : Domain-PFP
  4. Avg : Domain-PFP
- Drug Target Protein
  1. Random : ProtT5-XL
  2. 50% : ProtT5-XL
  3. 30% : ProtT5-XL
  4. 15% : ProtT5-XL

A.11 Protein-Search Benchmark Construction

In order to systemitically evaluate the text-based protein retrieval capability, we curated the Protein-Search benchmark dataset. This dataset comprises 5000 query and responses. It is divided into 4 categories:

1. C1 : Query asking about biological attribute related to 1 InterPro feature. Example Query: *Search for cytoplasmic and membrane-bound proteins that have been implicated in antiproliferative activities and are part of the broader stomatin superfamily, including those found in both eukaryotic and prokaryotic organisms.* Targets : proteins having feature = **IPR036013**.

2. C2 : Query asking about biological attribute related to 2 InterPro features. Example Query: *Identify multi-domain proteins containing a zinc-binding catalytic domain resembling thermolysin, along with an N-terminal beta-domain characteristic of aminopeptidases, and investigate their roles in peptide trimming and chemokine cleavage processes.* Targets : proteins having features = {**IPR014782, IPR042097**}.

3. C3 : Query asking about biological attribute related to 3 InterPro features. Example Query: *Proteins that integrate an immunoglobulin-like fold in their C-terminal domain, resembling the structure seen in NF-kB family members, and are involved in the regulation of immune responses through interactions with other Ig-like domains and DNA-binding activities.* Targets : proteins having features = {**IPR000451, IPR013783, IPR014756**}.

4. C4 : Query asking about biological attribute related to 4 InterPro features. Example Query : *Identify hexameric proteins with ATPase and helicase activities that possess a cold-shock domain and are involved in the termination of transcription by interacting with ribosome-free mRNA and facilitating the release of RNA from the DNA template.* Targets : proteins having features = {**IPR004665, IPR011112, IPR011129, IPR036269**}.

Each category has 1250 questions with intended target features and potential candidate proteins from SwissProt database. This benchmark dataset is generated by `Qwen2.5-32B-Instruct` LLM based on random combinations of InterPro textual descriptions with the following prompt:

SYSTEM_PROMPT

You are an expert in protein biology and bioinformatics.

Your task is to generate realistic natural language search queries that a scientist might use to retrieve proteins with a specific functional or structural property.

The queries must:

- Be biologically meaningful and scientifically accurate

- Reflect the functional, structural, or mechanistic aspects of the protein domain

- Avoid directly mentioning the InterPro domain name or ID

- Vary in specificity (broad $\rightarrow$ narrow)

- Be suitable for searching a protein database

You must NOT:

- Hallucinate functions not supported by the description

- Use vague phrases like "this protein" or "something like"

- Include irrelevant biological concepts

PROMPT_TEMPLATE

Given the following set of protein-related themes, generate a few search queries for proteins that exist at the intersection of these concepts.

The goal is to identify proteins that realistically embody a combination of all the provided themes.

Themes to Combine:

First theme: {{THEME1}}

Second theme: {{THEME2}}

Third theme: {{THEME3}}

Forth theme: {{THEME4}}

Guidelines:

- Each query must synthesize the provided themes into a single, biologically plausible description.

- Do NOT generate separate queries for each theme; instead, describe proteins where these themes overlap or interact.

- Vary the abstraction level across the combined queries:

- At least one high-level functional query (e.g., how these themes collaborate in a biological system).

- At least one domain/family-oriented query (e.g., structural intersections or multi-domain proteins).

- At least one mechanism- or process-specific query (e.g., a specific pathway where these themes converge).

- Queries should be written in natural language, not keywords only.

- Do NOT mention specific protein IDs or species unless implied by the themes.

- Keep each query concise (1-2 sentences max).

- Ensure biological coherence and realism.

- Avoid reusing exact phrases; paraphrase to show how the concepts are integrated.

A.12 Zero Shot Protein Search Hits

Table 6: Results of Zero Shot Protein Search

Query	Hits
Identify extracellular proteins involved in the regulation of blood coagulation that utilize specialized structural modules to bind to membrane phospholipids or other protein mediators.	MFAP4_HUMAN, FBCDA_XENLA, FCN2_MOUSE, FBCD1_HUMAN, FCN2_PIG, FBCD1_XENTR, FCNV3_CERRY, TLLP_PHONI, FGL2_HUMAN, FCN1B_XENLA
Find intracellular signaling proteins containing SH3 domains that localize to the plasma membrane upon phosphorylation to regulate actin cytoskeleton remodeling.	SLA1_SCHPO, SLA1_SCLS1, SLA1_MYCMD, SH3Y1_HUMAN, SH3Y1_RAT, SH3Y1_XENLA, SH3Y1_BOVIN, SH3Y1_MOUSE, SH3Y1_PONAB, LSB3_YEAS7
Identify proteins localized to the nucleolus (additional example)	NOL6_DROYA, NOL6_DROSI, UTP22_SCHPO, NOL6_HUMAN, UTP22_YEAST, NOL6_DROMO, NOL6_DROWI, NOL6_DROVI, NOL6_DROME, NOL6_DROPE