

SciReasoner: Laying the Scientific Reasoning Ground Across Disciplines

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We present a scientific reasoning foundation model that aligns natural language with heterogeneous scientific representations. The model is pretrained on a 206B-token corpus spanning scientific text, pure sequences, and sequence–text pairs, then aligned via SFT on 40M instructions, annealed cold-start bootstrapping to elicit long-form chain-of-thought, and reinforcement learning with task-specific reward shaping, which instills deliberate scientific reasoning. It supports four capability families, covering up to 103 tasks across workflows: (i) faithful translation between text and scientific formats, (ii) text/knowledge extraction, (iii) property prediction, (iv) property classification, (v) unconditional and conditional sequence generation and design. Compared with specialist systems, our approach broadens instruction coverage, improves cross-domain generalization, and enhances fidelity. We detail data curation and training and show that cross-discipline learning strengthens transfer and downstream reliability. The model, instruct tuning datasets and the evaluation code are open-sourced at <https://huggingface.co/SciReason> and <https://github.com/open-science-lab/SciReason>.

Highlights

- **Adaptive Scientific Reasoning.** We observe not all scientific tasks necessitate explicit reasoning—for instance, property prediction tasks often admit direct answers, whereas retrosynthesis and design tasks require elaborate reasoning. Our model can exploit the robustness of answer-based matching to generate reliable CoT supervision only where reasoning is essential, which explicitly differentiates between two task modes: “instant” tasks, where the original supervised fine-tuning (SFT) data is preserved, and “thinking” tasks, where the data is fully replaced with CoT-augmented counterparts. This principled separation enables the model to adaptively allocate reasoning capacity, producing coherent CoT rationales for complex scientific tasks while preserving efficiency and accuracy on simpler, non-reasoning tasks.
- **Task Grouped Rewarding.** Typical reward functions for reinforcement learning on typical LLMs lack explicit signals for encouraging and correcting scientific reasoning patterns across diverse thinking tasks, e.g., knowledge extraction, property prediction and classification, sequence generation and design. To tackle these diverse scientific tasks, we propose to group various scientific rewards into three categories: distance-based reward functions for scientific predictions, matching-based reward functions for scientific retrieval and extraction, and scientific tooling-verified reward functions that are based on professional scientific tools. Such innovative grouping enables our model share the common knowledge among different tasks and simplifies the reinforcement learning framework.
- **Scientific Reward Softening.** Scientific tasks typically return True(1)/False(0), in which case we experimentally observe making the reinforcement learning difficult to converge. In this paper, we develop a method to continuously scale reward signals. Specifically, we transform task-specific

Aspect	SciReasoner	NatureLM	Bio-T5/T5+	UniGenX
Scientific Reasoning	✓	✗	✗	✗
<i>Scientific Task Coverage</i>				
Scientific Translation	10	3	2	0
Text/knowledge Extraction	6	0	0	0
Property Prediction	22	0	1	4
Property Classification	49	10	13	0
Generation and Design	16	17	5	18
Total	103	30	21	22
Pretraining corpus	206B diverse tokens: - Scientific text - Pure scientific sequences - Sequence-text interleaved pairs - Sequence-sequence interleaved pairs	140B sequence-centric tokens: - 90% sequence-based data - 10% general text	80B biochemical samples: - Completely composed of proteins and small molecules data - 99% protein-structure and materials data - 1% small molecule data	84.5M structural samples:
SFT corpus	40M QA samples	5M QA samples	2.8M QA samples	24M task-related samples
Reasoning corpus	570K answer-aligned long-form scientific CoT data and 72K difficulty-filtered RL data	NA	NA	NA

Table 1 | Comparison emphasizing **reasoning ability** and **coverage breadth**. Our model explicitly elicits scientific reasoning and supports **five** capability families with up to **103** tasks; While other methods either only emphasize cross-domain sequence-based discovery or support limited disciplines, they do not pay attention to scientific reasoning and end-to-end workflow coverage.

metrics, such as language-based scoring metrics (e.g., BERTScore) or quantitative measures (e.g., RMSE) for regression tasks, into a normalized [0, 1] range. This continuous reward signal effectively promotes stable training and significantly boosts the model’s performance on complex scientific reasoning tasks.

- **Comprehensive Scientific Capability.** Our model supports a broad scientific workflow, spanning five major families and encompassing up to 100 tasks:

- *Scientific Translation:* Bidirectional conversion between human text and scientific representations for interoperability.
- *Text & Knowledge Extraction:* Literature-aware modeling that turns unstructured text into structured evidence for read–reason–design cycles.
- *Property Prediction:* Accurate estimation of continuous scientific endpoints across chemistry, biology, and materials.
- *Property Classification:* Robust categorization of molecular, biological, and material properties into discrete classes.
- *Sequence Generation & Design:* Constraint-aware, controllable generation that reuses predictive structure for efficient design loops.

We obtain **state-of-the-art performance on 54 tasks** and **rank among top-2 on 101 tasks**, demonstrating that a single backbone integrating natural language with multi-representation scientific data can enable cross-domain generalization beyond fixed task menus and reduce the fragmentation seen in specialist pipelines. We highlight the superiority of our model in Tab. 1

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1. Introduction

Large foundation models (LFMs) have demonstrated tremendous potential in modeling natural language [1, 2, 3], vision [4, 5, 6, 7, 8], audio [9, 10, 11, 12] and multimodal [13, 14, 15, 16] tasks. Recent works such as GPT-5 [17], Qwen-3 [18], LLaMA-4 [19], DeepSeek-v3 [20], and Gemini-2.5 [21] have achieved remarkable performance across diverse domains, benefiting from advances in transformer architectures [22, 23, 24], large-scale pretraining [25], and instruction tuning [26, 27, 28]. While these models excel at general-purpose reasoning [29, 30, 31], summarization [32, 33, 34], and dialogue [35, 36, 37], their adaptation to scientific disciplines such as chemistry, biology, healthcare, and materials science remains an emerging frontier [38, 39, 40, 41, 42, 43, 44]. Scientific problems often involve diverse, domain-specific representations [45, 46, 47], ranging from molecular representation (e.g., SMILES [48], SELFIES [49]) and protein sequences (e.g., FASTA [50]) to genomic data, which differ fundamentally from natural language in structure and semantics. Bridging this gap requires foundation models capable of integrating symbolic, numerical, and sequence-based knowledge with natural language understanding, enabling applications such as molecular property prediction [51, 52, 53, 54], biomolecule engineering [55, 56, 57, 58, 59], and the interpretation of complex experimental data [60, 61, 62, 63, 64].

Existing works on scientific large models can be generally classified into two parts:

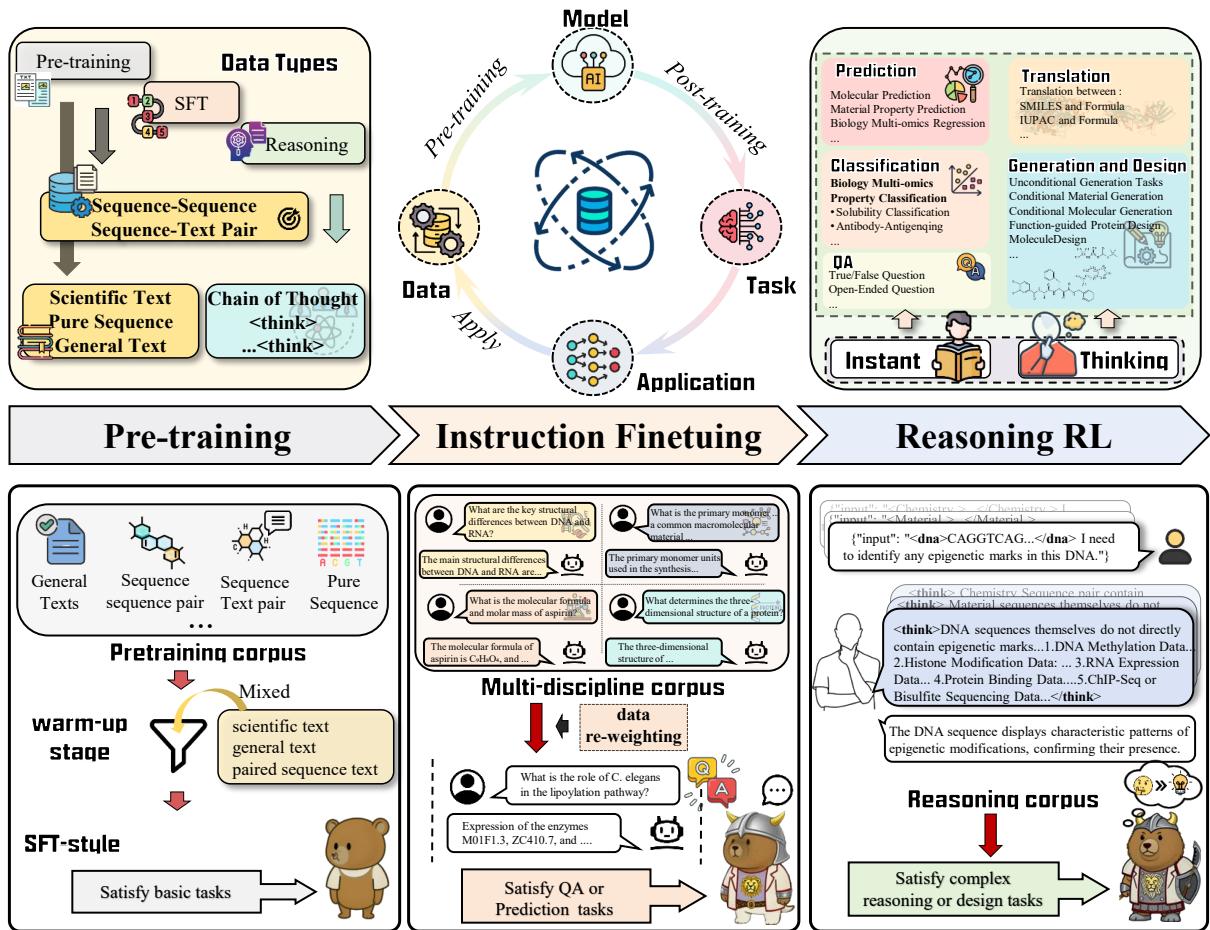


Figure 1 | We present a unified scientific LLM framework organized into three stages (Pre-training, SFT, and Reasoning). In the pre-training stage, a mixed “warm-up” corpus aligns the base model with scientific syntax and sequences, combining scientific and general text with pure sequences and paired sequence-text / sequence-sequence data spanning DNA/RNA, proteins, small molecules, and materials. The SFT stage aggregates more than 100 curated scientific sub-tasks across these domains to adapt the model to actionable research objectives such as property prediction and sequence-text transformations. The reasoning stage introduces a rationale-augmented corpus and supports two usage modes—Instant (fast answers) and Thinking (step-by-step deliberation)—to solve complex problems.

- **Specialist Large Models.** Bio-T5 families [65, 66], ChemLLM [67], ChemVLM [68], ChemMLLM [69], Chem3DLM [70], ProLlama [71], BioReason [72] adopt pretrained large language models (e.g., T5 [73], LLaMA-2 [74], Qwen-3 [18], InternLM [3]) to solve the discipline-specific tasks [75, 76, 77]. They typically collect *curated, domain-specific corpora* [78, 79, 80] and *task-aligned instruction data* [81], e.g., *sequence–property pairs; protein/DNA/RNA sequences with structural or functional annotations; reaction and synthesis records; and multi-form molecular representations* (e.g., SMILES/IUPAC/SELFIES).
- **Multi-discipline Large Models.** NatureLM [82] and UniGenX [83] adopt a pretrain-then-finetune scheme to learn a shared model for both life science and materials science. Galactica [84] is designed to support scientific knowledge mining from massive academic literatures. Biology-Instructions [85] collects a large-scale dataset to comprehend multi-omics biology.

Although these methods and other homologous techniques [86, 70, 87, 88, 68, 89, 90, 91] demonstrate the large models can successfully handle scientific tasks, *key gaps remain in cross-domain generalization, grounding to physical and experimental constraints, and systematic coverage of heterogeneous scientific modalities.* For specialist models, their narrow scope and customized pipelines limit transfer outside the target subfield, fragment the model ecosystem, and, more importantly, require retraining to support unseen tasks or modalities. For multi-discipline large models [82, 83], they typically focus on limited tasks (e.g., NatureLM supports only 30 tasks) and therefore fail to cover the long tail of scientific problems or generalize compositionally beyond a pre-specified task list. Furthermore, they still produce shallow pattern-based predictions rather than explicit multi-step reasoning traces that mirror how scientists derive conclusions from data and theory. We therefore aim to *close these gaps by unifying multi-representation scientific data with natural language in a single backbone, scaling instruction coverage to a substantially broader and more diverse task mixture, and grounding reasoning via long-form thinking process to ensure fidelity and verifiability.*

In this work, we propose the first scientific reasoning large language model that couples multi-representation pretraining with instruction-driven alignment and reasoning-inducing post-training. Our model ingests natural language alongside scientific sequences (DNA/RNA/protein), molecular strings (e.g., SMILES/IUPAC/SELFIES) and material representation through task-aware tokenization mapped into a shared backbone. Our training process involves pretraining, SFT-based post-training and RL-based post-training. Pretraining first aligns heterogeneous corpus (e.g., sequence-structure-text), while instruction tuning abstracts diverse tasks into a small set of consistent input-output schemas that encourage compositional generalization. Finally, a *reasoning-inducing* phase equips the model with deliberate and *verifiable* problem solving: we bootstrap long-form rationales via an annealed cold-start procedure, and finish with reinforcement learning using physics- and task-aware rewards (factuality, stoichiometry consistency, constraint satisfaction), yielding reliable chain-of-thought solutions. Our method supports a broad range of the following tasks. We organize capabilities into five families that align with the scientific workflow and enable cross-domain generalization beyond prior systems (e.g., limited task menus as in NatureLM), as follows:

- **Scientific Translation.** Ensures interoperability between human-readable text and machine-oriented scientific representations, enabling faithful bidirectional conversion that preserves semantics and physical meaning. Compared with earlier systems confined to a few format mappings, this category scales to many representations and thus supports data augmentation, tool chaining, and transparent human–AI collaboration.
- **Text and Knowledge Extraction.** Focuses on natural language understanding and reasoning tasks that operate directly on diverse scientific text. This evaluates the model’s ability to identify scientific entities, extract structured knowledge, and answer domain-specific questions from literature. By isolating linguistic comprehension from sequence modeling, it probes whether the model can capture the semantics of scientific discourse, resolve complex entity relations, and deliver accurate answers across diverse contexts.
- **Scientific Property Prediction.** Provides a unified interface for estimating continuous endpoints (e.g., biochemical, materials), producing continuous signals that can be used for screening and prioritization. Unlike prior models tied to a small set of benchmarks, our formulation flexibly accommodates heterogeneous continuous targets across disciplines, enhancing transfer and compositional generalization.
- **Scientific Property Classification.** Handles categorical endpoints (binary, multi-class, and hierarchical) such as solubility, stability, functional annotations, or phase labels. It delivers high-fidelity and domain-general capabilities over categorical properties, facilitating practical applications such as candidate triage, property screening, and informed design decisions across scientific domains.

- **Scientific Sequence Generation and Design.** Closes the loop from inference to actionable design under multi-objective and constraint-aware settings (e.g., synthesizability, stability, safety). This family goes beyond template matching by supporting controllable, cross-domain generation that reuses learned structure from prediction tasks, yielding better sample efficiency than siloed, single-discipline models.

The overall illustration of this work is shown in Fig. 1. In summary, we introduce a unified scientific LLM that couples scaled multi-representation pretraining with instruction-aligned I/O schemas and a *verifiable* reasoning stage. Task-aware tokenization aligns heterogeneous sequences and notations; a solve–check protocol with retrieval and domain tools, followed by reinforcement learning with physics- and task-aware rewards, enforces unit/stoichiometry and constraint consistency. The resulting single backbone supports prediction, design, translation, and literature-grounded extraction within a *read–reason–design* loop, delivering strong cross-domain generalization across chemistry, proteins, genomics, and materials; the following sections detail data, training, and evaluation.

2. Pre-Training

2.1. Pretraining Data Types

To ensure downstream results on scientific sequence generation, property prediction, and sequence-manipulation tasks, we design our pretraining strategy around four complementary types:

1. **Scientific Text.** We harvest long and short prose from PubMed [92], PubChem [93], textbooks, and materials databases (e.g., crystal-structure annotations), as well as solution threads from StackExchange for a specific discipline. This corpus grounds the model’s understanding of domain-specific reasoning and terminology needed for scientific Q&A and context-aware property inference.
2. **Pure Sequence.** To capture the contextual dependencies of biomolecular and chemical sequences, we collect:
 - *DNA/RNA*: Serving as the fundamental blueprint of genetic information, pure nucleotide sequences allow the model to directly learn base-level patterns and long-range dependencies without being influenced by external structural or functional annotations.
 - *Protein*: As the direct products of gene expression, amino acid sequences encode the full spectrum of structural and functional diversity in proteins, enabling the model to capture residue-level motifs and evolutionary conservation signals.
 - *Small Molecules*: We collect Simplified Molecular Input Line Entry System (SMILES) strings from PubChem. Furthermore, to ensure that the model can learn various representations of molecules beyond SMILES, we also adopt International Union of Pure and Applied Chemistry (IUPAC) and Self-Referencing Embedded Strings (SELFIES) names to achieve enhanced molecule representations. For SMILES sequences, we warp them with the <SMILES>...</SMILES> tags.
3. **Sequence–Sequence and Sequence–Text Pairs.** Beyond standard sequence collections, we enrich the training data with cross-discipline examples drawn from life sciences (e.g. protein structure), materials chemistry, and scientific literature. We hope this hybrid strategy preserves broad language fluency while instilling deep domain-specific proficiency. To simulate the diversity of cross-disciplinary queries, we develop:
 - *Intra-discipline pairs*: e.g. multi-protein homology judgment based on sequence patterns. Such data enhances the model’s ability to discern subtle evolutionary and structural relation-

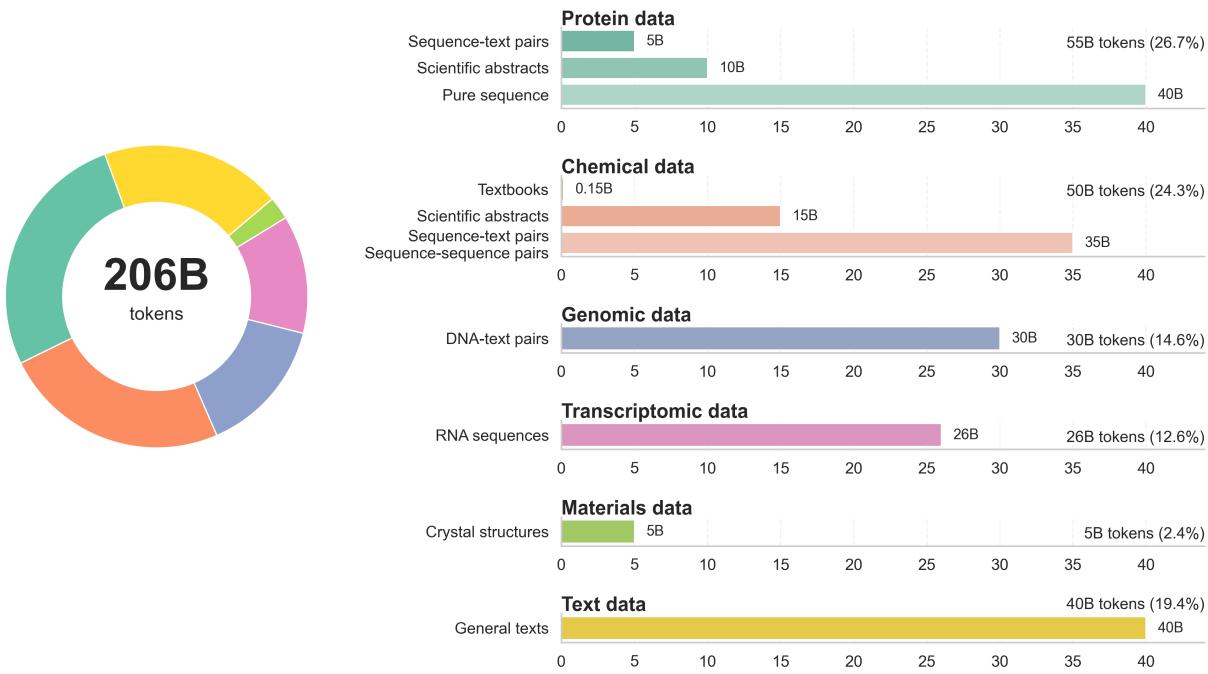


Figure 2 | Composition of the 206B-token scientific pretraining corpus across five scientific domains: protein data, chemical data, genomic data, transcriptomic data and materials data.

ships within a single domain, improving performance in specialized sequence comparison and classification.

- *Cross-discipline pairs:* e.g. prediction of small-molecule binding to a protein segment. By bridging cross-disciplinary representations, these pairs could improve the capacity to integrate different knowledge for tasks such as drug discovery and biomolecular engineering.
 - *Multi-representation of the same entity:* concurrent IUPAC, SELFIES, and SMILES representations of a molecule. This could promote translation and reasoning between complementary notations, enabling robust understanding and cross-format interoperability.
 - *Text–data pairs:* combined prompts and labels for molecular, nucleic, or protein properties. Pairing natural language descriptions with scientific sequences enables rich bidirectional interaction, empowering downstream natural language understanding (e.g., protein or molecule interpretation) and language-driven generation of scientific sequences.
4. **General Text.** In order to maintain the language capabilities of the model itself, we adopt C4 dataset as our general text corpus. Compared with the existing methods [82], the pre-training data they use contains only about 10% of natural text, and almost entirely relies on pure sequence data; therefore, they lack coherent conversation capabilities and cross-domain reasoning abilities.

Data Preparation Details

DNA. We retrieve about 200 billion bases from NCBI [94], sampling at an average of 1,000 bp fragments per organism to produce 30 billion < dna > /< /dna >-tagged tokens and is represented by the FASTA format. Essential metadata (e.g., organism name and genomic coordinates) is included to anchor the model’s interpretation of each sequence’s context.

RNA. We collect about 20 billion RNA tokens from RNACentral [95], reflecting diverse transcriptomic contexts. Then, we warp the collected RNA sequence (FASTA format) with the <rna></rna> tag. The basic information of the RNA sequence (e.g., Family) is also retrieved and is used to guide the model’s understanding of sequence context.

Protein. We collect protein sequences from UniRef50 and UniRef90 (mammalia) and warp the raw sequence with <protein></protein> tag, this yields about 40 billion protein tokens. We also pair sequence fragments with concise natural-language descriptions, and sample pure text abstracts from PubMed for additional context.

Small Molecules. To ensure reliable representation and alignment of small molecules, we curate diverse textual resources, construct multiple molecular encodings, and implement rigorous token validation.

- *Text:* abstracts from PubChem and “long-form” chemistry Q&A from StackExchange.
- *Multi-Representations:* To ensure comprehensive molecular characterization, we utilize multiple chemical representations. These are obtained either directly from established databases (e.g., SMILES-to-IUPAC from PubChem) or generated via specialized toolkits (e.g., SMILES-to-SELFIES using the SELFIES library [49]).
- *Tagging:* We apply a multistage filter: regex based on RDKit [96] / SELFIES [49] toolkits, small LLM validation and manual review to eliminate ambiguous tokens (e.g., “In”, “Is”) and ensure high-fidelity tagging.

Materials. We collect raw material data from publicly available material databases, including Material Projects [97], GNoME [47], SNUMAT [98], etc. The fields of raw data include the crystal structure files (Crystallographic Information File, CIFs), chemical composition, space-group and crystal-system information, material type (e.g., bulk or slab), thermodynamic metrics (formation energy, energy above hull), electronic and mechanical properties (band gap, density, elastic moduli), magnetic properties, per-site coordination details, bond-length descriptions, etc.

To convert the raw data into the pretraining corpus, we generate task-specific templates by prompting an LLM to convert structural annotations into natural-language descriptions, then score and select the best templates for large-scale synthetic data generation.

Fig. 2 summarizes the composition of our training corpus across five scientific domains and their internal subdivisions. Specifically, protein sequences account for the largest share (55 billion tokens, 33.1%), followed by chemistry data (50 billion tokens, 30.1%), DNA genome fragments (30 billion tokens, 18.1%), RNA transcripts (26 billion tokens, 15.7%), and materials-science texts (5 billion tokens, 3.0%).

2.2. Training Protocol

We train the model for one epoch using bfloat16 mixed-precision. The base models are Qwen3 [18] 1.7B and 8B, respectively. Training batches consisted of 16 and 32 sequences per device for 1.7B model and 8B model, respectively. We set the initial learning rate to 2×10^{-4} and accumulated gradients over two steps, applying a linear warm-up over the first 1% of total steps. We especially arrange the data for the following training stages:

- At the warm-up stage, we adopt a mixed form of scientific text, general text and paired sequence

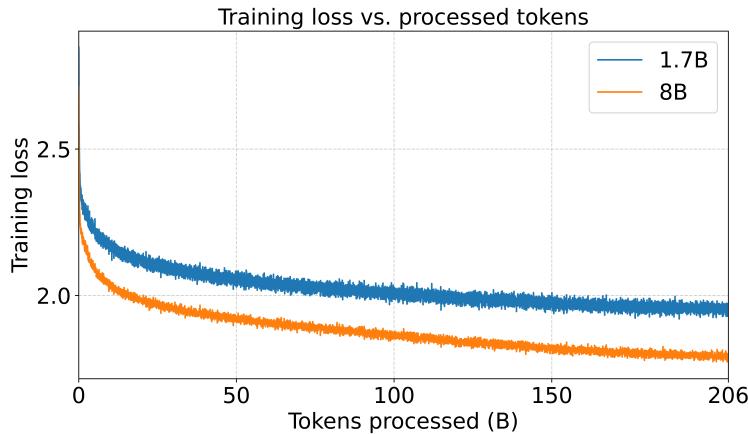


Figure 3 | Training loss over train tokens for the 1.7B and 8B models. The model does not exhibit any saturation phenomenon during the training process.

text data. This could help the model rapidly adapt to both domain-specific and general linguistic patterns before the main training phase.

- At the end of the training, we include SFT-style training data to refine the model's capability to follow complex, domain-specific instructions and produce task-aligned outputs. This stage serves to align the model's generative behavior with SFT-like reasoning and formatting standards, thereby enhancing its utility in real-world scientific applications.

For the training system, we use 128 A800 GPUs for 1.7B model and 256 A800 GPUs for 8B model. The training loss curves are shown in Fig. 3.

3. Post-Training

3.1. Supervised Fine-tuning

3.1.1. Data

In the supervised fine-tuning (SFT) stage, we integrated about 100 scientific sub-tasks spanning multiple disciplines, including chemistry (Mol-Instructions [81], ChemData [67], USPTO50k [99], SMolInstruct [100], etc.), DNA, RNA, proteins (Biology-Instructions [85], PEER [101], OPI [102], GUE [103], BEACON [104], etc.), materials (LLM4Mat [105], Material Projects [97]) and general instruction texts from OIG [106]. Moreover, cross-sequence interaction tasks and natural language-based scientific question answering are categorized within the cross-domain corpus. To warp the scientific sequences with discipline-related tags (i.e., <SMILES>...</SMILES>, <dna>...</dna>, <rna>...</rna>, <protein>...</protein>, etc.), the data preparation pipeline involved:

- Extracting scientific sequences from chemistry, DNA, RNA, protein, and macromolecule datasets via rule-based scripts tailored to each dataset format.
- Conducting secondary annotation using domain-specific checkpoints from pre-trained single-discipline models.
- Filtering and adding scientific tags with the assistance of small LLMs.
- Converting all data into a unified dialogue format for SFT training.

We show the data distribution of supervised finetuning stage in Tab. 2.

Category	Training samples (M)	Proportion
Materials	8.278	20.79%
General Text	10.873	27.30%
DNA&RNA	5.476	13.75%
Protein	2.473	6.21%
Molecule	12.556	31.53%
Cross Domain	0.168	0.42%
Total	39.824	100.00%

Table 2 | Distribution of supervised fine-tuning (SFT) training samples across five major scientific domains and additional general text data, reported in millions and proportions. Each domain undergoes tailored preprocessing, domain-specific annotation, and tagging (e.g., <SMILES>...</SMILES>, <dna>...</dna>, <protein>...</protein>) before being converted into a unified dialogue format for SFT. The corpus comprises 63.35 million samples.

3.1.2. Training Protocol

We train the model for five epochs using 16-bit bfloat16 precision. A per-device batch size of 32 is used, with gradient accumulation over two steps to achieve a larger effective batch size. The initial learning rate is set to 5×10^{-5} , and we apply a linear warm-up over the first 5% of total steps. Inputs are tokenized lazily with right-side truncation to a maximum sequence length of 8192 tokens, and the Liger-kernel [107] is enabled for efficiency. The training process is accelerated using DeepSpeed ZeRO Stage 2 [108] and FlashAttention implementation [109].

Based on the SFT dataset, we train four single-discipline models in DNA/RNA, protein, materials science, and chemical molecules. However, during multi-disciplinary joint training, we observe substantial performance degradation in certain sub-tasks due to data imbalance after dataset merging. To address this, we adopt two strategies: (1) we conduct large-scale pre-training followed by augmentation with additional SFT data—with materials science receiving further data expansion—and (2) data re-weighting, which adjusts task-level proportions to mitigate the impact of low-quality instructions or underrepresented tasks. This re-weighting approach effectively alleviates performance decline in mixed-dataset training.

3.2. Reasoning-based Reinforcement Learning

3.2.1. Data

Cold Start Before reinforcement learning (RL), we construct a correct-only chain-of-thought (CoT) corpus as a cold-start prior. For each sub-task, we use *DeepSeek-R1-Distill-Qwen-32B* to generate CoT, answer pairs and target $T=500$ correctly answered items under a hard evaluation budget of $C=50,000$ prompts. We first draw 6,000 random prompts, evaluate correctness, and retain the CoT attached to correct answers. If after N evaluated items the tally is $S < T$, we estimate the additional sample size via the empirical accuracy $\hat{p}=S/N$ as $n_{\text{add}} = \lceil (T - S) / \max(\hat{p}, \epsilon) \rceil$ (with small $\epsilon > 0$ for numerical stability), then repeat sampling-generation-adjudication until either $S \geq T$ or $N \geq C$; if the cap is reached, we keep all accumulated correct examples. Correctness is adjudicated by direct comparison of the generator’s final answer to SFT ground truth for auto-gradable tasks (exact match or task-specific tolerance), and by an external *GPT-3.5-turbo* judge for semantic equivalence on free-form tasks (e.g., protein descriptions). This adaptive, budgeted, correct-only harvesting mitigates rationale noise and yields a reliable initialization for subsequent RL.

Reinforcement Learning We curate reinforcement learning (RL) data at the level of each sub-task using an empirical solve-rate filter that targets medium-difficulty instances.

Let D_k^{train} denote the k-th sub-task's training set. For every example $x \in D_k^{\text{train}}$:

1. **Stochastic rollouts.** We generate $N = 8$ independent rollouts from M_0 on x using stochastic decoding with `do_sample=True`. To balance output diversity against format fidelity, we adopt an *adaptive temperature* T tuned once per sub-task prior to collection: we initialize at $T = 0.9$ (the DAPO default setting) and *increase* T if the eight-way samples show insufficient diversity (e.g., low uniqueness of normalized responses or highly repetitive content); conversely, if outputs become overly diffuse and induce frequent format non-compliance or invalid parses, we *decrease* T . During the final eight rollouts for each x , we hold T fixed and vary only the random seed, keeping all other decoding parameters constant.
2. **Empirical solve rate.** For rollout i , compute a correctness indicator $f_i(x) \in \{0, 1\}$ using the sub-task's canonical metric (e.g., exact match or a thresholded score), and aggregate

$$\hat{p}(x) = \frac{1}{8} \sum_{i=1}^8 f_i(x). \quad (1)$$

3. **Mid-difficulty filter.** Retain examples with partial success:

$$S = \{x \in D_k^{\text{train}} \mid 0.125 < \hat{p}(x) < 0.875\}. \quad (2)$$

This removes items that are nearly always solved ($\hat{p} \approx 1$) or nearly always failed ($\hat{p} \approx 0$), which typically yield weaker gradients for policy improvement.

4. **Sampling.** Uniformly sample without replacement $K = 1000$ examples from S . If $|S| < 1000$, include all of S and *top up* to $K = 1000$ by uniformly sampling from $D_{\text{train}} \setminus S$.

The resulting 1,000-example set serves as the RL training pool for that sub-task.

Focusing RL on neither-trivial-nor-impossible instances yields stronger and more stable improvement: items with $\hat{p} \in (0.125, 0.875)$ (i) expose the policy to cases where exploration can flip outcomes, (ii) avoid vanishing advantages on saturated positives, and (iii) reduce uninformative gradients from uniformly failed cases.

3.2.2. Training Protocol

Cold Start Before reinforcement learning, we apply an *annealed cold-start* (ACS) adaptation to a the model after SFT stage to (i) endow it with the ability to produce long, coherent chains of thought (CoT) on tasks that genuinely require stepwise reasoning, while (ii) preserving concise, direct-answer behavior on tasks that do not. We therefore partition the SFT task suite into *thinking* and *instant* categories. For thinking tasks, we **replace** the original SFT samples with their CoT-augmented counterparts (teacher-forced rationales followed by the final answer). For instant tasks, we retain the original direct-answer SFT data unchanged. Moreover, we have observed that **task-level replacement** outperforms within-task *mixing* of CoT and non-CoT targets. Mixing presents inconsistent sequence lengths, styles, and termination signals for near-identical instructions, weakening the model's calibration about when to elaborate. Replacement yields a cleaner conditional distribution, i.e., inputs from thinking tasks consistently map to CoT-style trajectories, thereby improving both the incidence and quality of generated rationales without confusing non-reasoning behavior.

To minimize behavioral drift from SFT while shaping rationale production where appropriate, the model is trained with a *reduced learning rate* and a short schedule relative to SFT (i.e., small-step updates). This “low-temperature” adjustment biases the model toward emitting structured reasoning *only* when the input distribution indicates a reasoning task.



Figure 4 | Scientific reward during DAPO training progress.

Reinforcement Learning. We adopt DAPO [110] as the RL algorithm to optimize the policy on heterogeneous scientific tasks. For each prompt we draw G candidates from the old policy $\pi_{\theta_{\text{old}}}$, compute group-standardized advantages:

$$r_{i,t}(\theta) = \frac{\pi_\theta(o_{i,t} | q, o_{i,<t})}{\pi_{\theta_{\text{old}}}(o_{i,t} | q, o_{i,<t})}, \quad \hat{A}_{i,t} = \frac{R_i - \text{mean}(\{R_i\}_{i=1}^G)}{\text{std}(\{R_i\}_{i=1}^G)}. \quad (3)$$

and maximize the PPO-style clipped objective:

$$\begin{aligned} \mathcal{J}_{\text{DAPO}}(\theta) = & \mathbb{E}_{(q,a) \sim \mathcal{D}, \{o_i\}_{i=1}^G \sim \pi_{\theta_{\text{old}}}(\cdot | q)} \\ & \left[\frac{1}{\sum_{i=1}^G |o_i|} \sum_{i=1}^G \sum_{t=1}^{|o_i|} \min \left(r_{i,t}(\theta) \hat{A}_{i,t}, \text{clip} \left(r_{i,t}(\theta), 1 - \varepsilon_{\text{low}}, 1 + \varepsilon_{\text{high}} \right) \hat{A}_{i,t} \right) \right] \\ \text{s.t. } & 0 < \left| \{o_i \mid \text{is_equivalent}(a, o_i)\} \right| < G, \end{aligned} \quad (4)$$

with the asymmetric *Clip-Higher* schedule to preserve exploration, together with *Dynamic Sampling* that filters degenerate groups with identical rewards and a token-level policy-gradient reduction. Unlike the original rule-based binary reward, many of our tasks (free-form semantic judgment, information extraction, and numeric regression) do not admit a single exact-match criterion. We therefore replace the binary signal with a *reward softening* scheme that maps the grouped metrics to a common $[0, 1]$ scale:

$$R_i^{\text{soft}} = g(m_i(q, o_i, \mathcal{A}(q))) \quad (5)$$

where $g(\cdot)$ is a monotone calibration ensuring comparable reward magnitudes across tasks and m_i is a *group-specific* quality metric. For grouping scheme, we employ distance-based rewards for scientific prediction tasks, matching-based rewards for retrieval and extraction tasks, and tool-verified rewards leveraging professional scientific software.

We show the training dynamics of scientific reward in Fig 4.

4. Evaluation and Application

4.1. Task Overview

Translation. The tasks in this group involve converting information between different scientific formats or representations, for example translating between IUPAC names and SMILES, generating descriptive text from molecular structures, or performing the inverse transformation. These capabilities are essential to ensure interoperability within the scientific data ecosystem and to enable effective human-machine communication.

Text and Knowledge Extraction/Question Answering. Applying natural language processing to scientific literature, these tasks include chemical entity recognition, interaction extraction, and various formats of question answering (multiple-choice, open-ended, true/false). They integrate AI methods with literature analysis to facilitate rapid extraction of knowledge from scientific texts.

Property Prediction and Classification. These tasks span a wide range of predictive challenges, from molecular properties (e.g., solubility, toxicity) to materials characteristics (e.g., MP classification, properties derived from JARVIS-DFT), DNA/RNA predictions (e.g., epigenetic markers, transcription factor binding in human), and protein functions (e.g., catalytic activity, stability). Their scope—encompassing chemistry, materials, nucleic acids, and proteins—highlights the universal demand for accurate predictive models in scientific discovery.

Generation and Design. This category focuses on the unconditional generation tasks and the conditional generation tasks. It includes unconditional generation of molecules, proteins, RNA, and materials, as well as targeted design challenges such as rational antibody design (RAbD) and programmable RNA switches. Progress in this domain is critical for accelerating the discovery of new compounds and biomolecules.

4.2. Baseline

For general-purpose closed-source models, we compare against **Gemini-2.5-pro*** and **GPT-o3^{†‡}**; for general-purpose open-source models, we use **GPT-oss-120B**. As specialist baselines, we consider two categories: (i) non-language models, represented by Transformer encoder-based architectures (denoted as *non-LLM Experts*); and (ii) language models, represented by the best-performing specialist large language model on this task (denoted as *Specialist LLMs*). Please refer to the Appendix for details.

4.3. Scientific Translation Tasks

Scientific translation evaluates whether a model preserves scientific semantics while mapping across modalities—symbolic encodings and formulae, natural-language text, and biological sequences. The goal is not to invent new facts but to produce an equivalent rendering that remains invertible and respects domain constraints (e.g., stoichiometry, valence, sequence–function coherence). This suite

*Gemini-2.5-pro version: 2025-06-17

†GPT-o3 version: 2025-04-16. Results are provided in Appendix Table. 10 to Table 15.

‡Since some test tasks involve extremely large-scale test sets, to avoid substantial testing costs, for closed-source models, we randomly sampled 1,000 samples from tasks with a test set size exceeding 1,000 for testing. Meanwhile, we also present the performance of our models on these 1,000 samples for comparison.

Task	Metric	Gemini 2.5-pro	GPT- OSS	Non-LLM Experts	Specialist LLMs	SciReasoner-1.7B	SciReasoner-8B
Molecular Representation Translation							
SMILES to IUPAC	Top1 Split Match ↑	4.70%†	0.17%	—	29.00%	<u>49.52%</u> 50.20%†	56.63% 57.10%†
SMILES to Formula	Top1 Element Match ↑	55.20%†	19.88%	—	93.20%	<u>95.92%</u> 87.1%†	96.39% 96.00%†
IUPAC to SMILES	Top1 Split Match ↑	38.20%†	7.58%	—	70.10%	<u>78.85%</u> 86.50%†	84.40% 90.70%†
IUPAC to Formula	Top1 Element Match ↑	88.50%†	33.24%	—	87.90%	<u>91.81%</u> 88.10%†	92.65% 93.00%†
Natural Language Translation of Molecule							
Molecular Description	ROUGE-L ↑	0.23	0.05	<u>0.75</u>	0.29	<u>0.75</u>	0.78
Molecular Captioning	MENTOR ↑	0.42†	0.15	—	0.45	<u>0.59</u> 0.59†	0.60 0.58†
Protein Functional Translation							
CASPSimilarSeq	ROUGE-L↑	0.01	0.02	—	0.74	<u>0.83</u>	0.85
IDFFilterSeq	ROUGE-L↑	0.01	0.03	—	0.70	<u>0.77</u>	0.82
UniProtSeq	ROUGE-L↑	0.01	0.03	—	0.71	<u>0.84</u>	0.88
Mol-Instructions	ROUGE-L↑	0.21†	0.07	0.68	0.44	<u>0.83</u> 0.82†	0.99 0.98†

Table 3 | Evaluation results of scientific translation tasks. **Bold** indicates the best performance, and underline indicates the second best. The names of expert models and specialist LLMs for each task are provided in Appendix Table. 10. † denotes that only randomly sampled 1000 test samples were utilized for evaluation in the corresponding task. This measure is adopted because extremely large-scale test sets exist for certain tasks, which would lead to substantial testing costs.

therefore probes compositional reasoning, ontology grounding, and robustness to notation/paraphrase as a modality-agnostic measure of semantic fidelity. The results are shown in Tab. 3.

Molecular Representation Translation. Following SMolInstruct [100], we evaluate the model’s ability to convert faithfully among common chemical representations, i.e., SMILES strings, IUPAC names, and empirical formulae. The tasks cover SMILES↔IUPAC, SMILES↔Formula, and IUPAC↔Formula, with performance judged by exact-match accuracy and structure-level equivalence after canonicalization.

- **SMILES to IUPAC Translation.** This task takes a molecule’s SMILES string as input and converts it into its corresponding IUPAC name. This is a fundamental challenge in cheminformatics, as it requires the model to interpret a simplified linear notation of a chemical structure and convert it into the standardized naming convention used by chemists.
- **SMILES to Formula Translation.** This task takes a molecule’s SMILES string as input and converts it into its corresponding molecular formula. The model receives a SMILES string as input and generates the complete molecular formula, which specifies the number of atoms for each element in the molecule. This task is crucial for computational chemistry, as it bridges the gap between a structural representation and the molecule’s elemental composition.
- **IUPAC to SMILES Translation.** This task converts a chemical name into its corresponding SMILES string. The model takes a molecule’s IUPAC name as input and generates the SMILES string, which is a concise text-based representation of the molecule’s chemical structure. This task is fundamental for many cheminformatics applications, as it allows for the conversion of human-readable names into a format that computers can process.
- **IUPAC to Formula Translation.** This task takes a molecule’s IUPAC name as input and converts it into its corresponding molecular formula. The model’s output is a list of all elements and the number of atoms for each element in the molecule. This task is crucial for chemical informatics, as it links a molecule’s systematic name to its elemental composition.

Molecular Captioning Case

Input

Please provide a brief introduction to this molecule. <SMILES>
CCCCCC/C=C\CCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(C)=O
</SMILES>

Reference	The molecule is a 1,2-diacyl-sn-glycero-3-phosphocholine in which the acyl groups at positions 1 and 2 are specified as (9Z)-hexadecenoyl and acetyl respectively. It has a role as a mouse metabolite. It derives from a palmitoleic acid.
Our model	The molecule is a 1,2-diacyl-sn-glycero-3-phosphocholine in which the 1- and 2-acyl groups are palmitoleoyl and acetyl respectively. It has a role as a mouse metabolite . It is functionally related to a palmitoleic acid .
GPT-5	This molecule is an unsaturated analog of platelet-activating factor (PAF), consisting of a glycerol backbone esterified at the sn-1 position with hexadec-9-enoic acid , acetylated at the sn-2 position , and linked at the sn-3 position to a phosphocholine group . The presence of a cis double bond in the long acyl chain introduces unsaturation, which may influence its membrane dynamics and biological activity. As a member of the PAF family, it is potentially involved in inflammatory signaling and immune modulation.

Figure 5 | Comparison of molecular captioning outputs.

Evaluation Metric. We evaluate performance using two metrics: *Top-1 Split Match* and *Top-1 Element Match*.

- **Split Match.** This metric assesses correctness by parsing the predicted formula P and the ground-truth formula G into structured components according to a predefined splitting rule. Let $\text{judge_string_split_match}(P, G)$ denote a Boolean function that returns true if P and G are equivalent under this split-based comparison. The metric is computed as

$$M_{\text{split}} = \frac{1}{N} \sum_{i=1}^N \mathbb{I}(\exists j \text{ judge_string_split_match}(P_i, G_{i,j})) ,$$

where $\mathbb{I}(\cdot)$ is the indicator function, P_i the i -th prediction, and $\{G_{i,j}\}$ the corresponding set of references.

- **Element Match.** This metric provides a more permissive comparison by disregarding element order and only checking whether the predicted and reference formulas contain identical counts of each element. For example, C5H8 and H8C5 are considered equivalent. Define $C(F)$ as the function that maps a formula F to its multiset of element counts. The metric is given by

$$M_{\text{element}} = \frac{1}{N} \sum_{i=1}^N \mathbb{I}(\exists j \text{ } C(P_i) = C(G_{i,j})) .$$

SMILES: CC1=NC=C[N-]1.CC1=NC=C[N-]1.[Zn+2]
 Reference: zinc;2-methylimidazol-3-ide
 Our output: **zinc;2-methylimidazol-3-ide**
 GPT-5: zinc bis(5-methylpyridin-2-ide)
 LLaSMol: 2-[*(E*)-2-[2-hydroxy-2-(dimethylamino)acetyl]-3-oxocyclopent-3-en-1-ylidene]acetic acid
 Gemini2.5-Pro: bis(2-methylimidazolato)zinc(II)

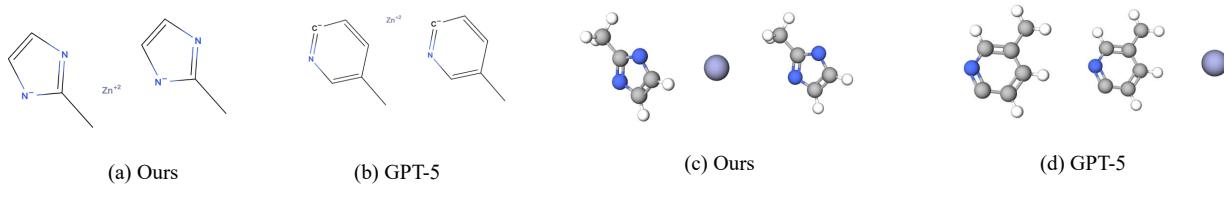


Figure 6 | Case study of “ZIF-8” in Metal Organic Framework (MOF).

Natural Language Translation of Molecule. To bridge the gap between chemical representations and human-readable knowledge, we evaluate tasks that translate molecular structures into natural language descriptions.

- **Molecular Description.** This is a generative task designed to describe a molecule based on its chemical structure. The model takes a molecule’s SMILES string as input. Its goal is to generate a natural language description that includes the molecule’s properties, functions, and a summary of its effects. This task is crucial for making complex chemical information accessible and understandable to a broader audience. This task comes from Mol-Instructions [81].
- **Molecular Captioning.** Similar to the Molecular Description task, this task requires the model to output the SMILES string’s explanation, using data from SMolInstruct [100].

Evaluation Metric. We use ROUGE-L and Metric for Evaluation of Translation with Explicit ORdering (MENTOR) as metrics.

As shown in Fig. 5, our model matches the reference on every core fact while avoiding unsupported inferences. It correctly identifies the lipid class as a 1,2-diacyl-sn-glycero-3-phosphocholine, specifies the exact acyl substituents (palmitoleoyl at sn-1 and acetyl at sn-2), reproduces the biological role (mouse metabolite), and links it to palmitoleic acid—all with normalized terminology and no embellishment.

As shown in Fig. 6, we visualize the generated 2D chemical structure and 3D ball-and-stick model for $\text{CC1=NC=C[N-]1.CC1=NC=C[N-]1.[Zn+2]}$, which is called “ZIF-8” in Metal Organic Framework (MOF). Since MOF is a coordination compound, there is a “Coordinate bond” in MOF. Our method generates the IUPAC name of ZIF-8 successfully, while GPT-5 could not. Moreover, LLaSMol and Gemini2.5-Pro generate IUPAC names without meaningful 2D chemical structures. In addition to “Coordinate bond”, we also evaluate our model for generating molecules with only “covalent bonds”. As depicted in Fig. 7, our method is able to successfully translate SMILES to IUPAC name. However, the IUPAC name generated by GPT-5 yields the opposite chiral isomer, and the IUPAC names generated by LLaSMol and Gemini2.5-Pro are not consistent with the SMILES.

Protein Functional Translation. For the given protein sequence, we prompt the model to describe the function of the protein in a clear and coherent manner within the context of the natural language domain. It thus tests both the model’s reasoning when inferring functional roles from sequence data

Create Date: 2025-07-28

SMILES: C[C@H](C(=O)N[C@H](CC1=CC=CC=C1)C(=O)C(=O)NCC2=CC=CC=N2)NC(=O)C3=CC(=C(C=C3)Cl)Cl

Reference: 3,4-dichloro-N-[(2R)-1-[(2R)-3,4-dioxo-1-phenyl-4-(pyridin-2-ylmethylamino)butan-2-yl]amino]-1-oxopropan-2-yl]benzamide

Our output: **3,4-dichloro-N-[(2R)-1-[(2R)-3,4-dioxo-1-phenyl-4-(pyridin-2-ylmethylamino)butan-2-yl]amino]-1-oxopropan-2-yl]benzamide**

GPT-5: (2S)-2-[(2S)-2-benzyl-3-(pyridin-2-ylmethylcarbamoyl)propanoyl]amino]-N-(3,4-dichlorophenyl)propanamide

LLaSMol: (2Z,5Z)-2-chloro-5-[2-[(2Z,5Z)-2-chloro-5-[(2-methyl-3-oxo-3-phenylpropanoyl)amino]penta-2,4-dienoyl]-3-oxo-3-phenylpropanoyl]penta-2,4-dienoic acid

Gemini2.5-Pro: (4S)-4-{(2S)-2-(3,4-dichlorobenzamido)propanamido}-4-phenyl-N-(pyridin-2-ylmethyl)-2,3-dioxobutanamide

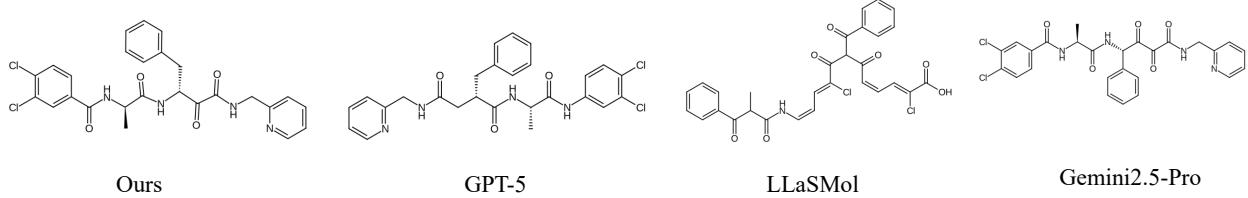


Figure 7 | Case study of SMILES→IUPAC from latest PubChem data. Given the input SMILES (top), our model generates the exact reference IUPAC name (*shown in blue*), preserving the 3,4-dichloro-benzamide core, the pyridin-2-ylmethylamino 1,3-dicarbonyl motif, and the (2R)/(2R) stereochemistry; the reconstructed structure (bottom left) is therefore congruent with the input. In contrast, competing LLMs (GPT-5, LLaSMol, Gemini-2.5-Pro) yield chemically inconsistent names that alter substituents, lose halogens, change chain length, or flip chirality, leading to mismatched reconstructions.

and its proficiency at producing accurate, fluent text. These tasks include four different data for testing, **(i)** CASPSimilarSeq: the sequences that are similar to the sequences released by CASP14. **(ii)** IDFiltSeq: this version uses ID-filtered sequences to reduce redundancy. **(iii)** UniProtSeq: this version’s protein sequences are from the UniProt database. **(iv)** Mol-ins: The protein sequence of this version is derived from the Mol-Instructions [81] benchmark. Additionally, this test set requires the model to also output subcellular localization information. We therefore consider the above four data sources are four sub-tasks of Protein Functional Translation.

Summary of Evaluation Results. Our models consistently outperform baselines. The SciReasoner-8B model achieves near-ceiling accuracy in formula recovery (>93%), markedly improves challenging SMILES-IUPAC translations, and delivers the highest scores in molecular captioning (MENTOR 0.61) and protein functional translation (ROUGE-L up to 0.98). These results highlight strong semantic fidelity and scalability, establishing a new frontier for scientific translation tasks.

4.4. Scientific Knowledge Extraction and Question Answering

Unlike our sequence-based tasks that require models to process structured biological inputs such as DNA, RNA, protein sequences, or SMILES strings, the tasks grouped under Scientific Knowledge Extraction and QA focus purely on natural language understanding and reasoning. They evaluate our model’s ability to extract scientific knowledge, recognize scientific entities, and answer domain-specific questions directly from unstructured text. Furthermore, this isolates linguistic comprehension from sequence modeling, allowing us to probe whether models can capture the semantics of scientific literature, resolve complex entity relations, and deliver accurate answers across diverse contexts. The results are listed in Tab. 4.

Chemical Entity Recognition. This task entails detecting textual mentions of chemical substances from the inputs and assigning them to specific entities (e.g., chemical compounds). This poses chal-

Task	Metric	Gemini 2.5-pro	GPT- OSS	Non-LLM Experts	Specialist LLMs	SciReasoner 1.7B	SciReasoner 8B
Scientific Knowledge Extraction and QA							
Chemical Entity Recognition	F1 ↑	0.71	0.55	—	0.75	<u>0.81</u>	0.92
Chemical–Protein Interaction Extraction	F1 ↑	0.12	0.05	—	0.22	<u>0.46</u>	0.83
Chemical–Disease Interaction Extraction	F1 ↑	0.35	0.23	—	0.40	<u>0.66</u>	0.97
General Multiple Choice Question	ACC ↑	0.94	0.87	—	0.65	<u>0.92</u>	0.99
True/False Question	ACC ↑	0.62	<u>0.67</u>	—	0.55	0.64	0.68
Open-Ended Question	BertScore ↑	<u>0.84</u>	0.80	—	<u>0.84</u>	0.83	0.87

Table 4 | Evaluation results of scientific knowledge extraction and QA tasks. **Bold** indicates the best performance, and underline indicates the second best. The names of expert models and specialist LLMs for each task are provided in Appendix Table. 11.

lenges for models since the heterogeneity of chemical nomenclature. Accordingly, the performance of this task provides a sensitive probe of an LLM’s domain competence in biomedical text understanding.

Chemical-Protein Interaction Extraction This task evaluates language models on chemical–protein interaction (CPI) annotation: given biomedical text snippets, the model must (i) detect mentions of chemical entities and protein/gene targets, (ii) link candidate pairs, and (iii) assign an interaction label that captures mechanism and polarity (e.g., binding). The task requires grounding each prediction to supporting evidence spans and correctly handling context , thereby probing biochemical and pharmacological knowledge under realistic nomenclature variability.

Chemical-Disease Interaction Extraction This task probes extraction of chemical-induced disease (CID) relations from biomedical literature. For the input, the model must (i) detect mentions of chemicals and diseases, (ii) link candidate pairs, and (iii) decide whether the passage asserts a causal, adverse relation in which exposure to the chemical induces or exacerbates the disease, citing the supporting span. Accurate CID extraction enables downstream applications in toxicology, pharmacovigilance, and disease-mechanism mapping.

General Multiple Choice Question The task is to select the correct option for each question, probing factual knowledge, conceptual understanding, and applied reasoning relevant to biology, chemistry, and other relevant fields.

True/False Question Following the practice in Mol-Instructions [81], this task requires the language models to answer research questions with positive/negative/uncertain results, without being given the references from PubMed.

Open-Ended Question Open-ended questions require free-form responses to input content related to biomedicine, without following a fixed format. Open-ended QA tests genuine biomedical understanding, demands clear self-contained explanations, mirrors real use.

Summary of Evaluation Results Scaling from **SciReasoner-1.7B** to **SciReasoner-8B** yields consistent gains across scientific knowledge extraction and QA. The **SciReasoner-8B** model surpasses prior Specialist LLMs on every tasks. The most pronounced improvements appear on relation extraction (chemical–protein and chemical–disease), reflecting stronger entity linking, synonym/acronym disambiguation, and evidence grounding; chemical entity recognition also benefits, indicating sharper

Task	Metric	Gemini 2.5-pro	GPT oss	Non-LLM Experts	Specialist LLMs	SciReasoner 1.7B	SciReasoner 8B
Molecular Property Regression							
ESOL	RMSE ↓	1.28	3.45	—	1.04	1.21	<u>1.08</u>
LIPO	RMSE ↓	1.21	1.65	—	1.01	<u>0.94</u>	<u>0.82</u>
Physicochemical Prediction	MAE ↓	0.027	1.329	—	0.013	<u>0.003</u>	0.002
Material Property Regression							
MPRegression		1.32†	0.95	5.32	0.76	4.98 4.67†	<u>5.12</u> 5.21†
SNUMATRegression		1.07†	1.00	1.83	1.16	2.18 2.18†	<u>1.96</u> 2.22†
JARVISDFT		1.09†	0.88	4.10	0.70	<u>5.11</u> 5.28†	<u>5.21</u> 5.59†
JARVISQETB		0.53†	0.50	59.44	1.05	138.59 148.71†	<u>126.61</u> 137.61†
GNoME	$\frac{MAD}{MAE} \uparrow$	1.28†	0.73	15.60	0.50	<u>19.05</u> 18.46†	22.03 21.81†
hMOF		0.65†	0.67	1.48	0.66	<u>1.05</u> 1.04†	0.99 0.99†
Cantor-HEA		0.77†	0.45	8.40	0.87	<u>7.40</u> 7.38†	7.18 7.02†
QMOF		1.24†	0.86	2.05	0.93	8.55 8.76†	<u>8.07</u> 7.94†
OQMD		1.20†	0.65	6.02	1.16	5.29 5.50†	<u>5.43</u> 5.67†
OMDB		0.82†	0.93	1.55	1.01	<u>1.40</u> 1.41†	1.39 1.42†
Biology Multi-omics Property Regression							
Fluorescence	Spearman ↑	-0.43†	3.20	<u>69.00</u>	2.57	69.36 70.82†	66.24 68.49†
Stability_Biology-Instructions	Spearman ↑	-9.15†	-7.79	79.00	60.25	63.25 55.67†	<u>64.41</u> 59.03†
Thermostability	Spearman ↑	5.47†	6.29	78.00	45.07	56.25 53.17†	<u>58.55</u> 54.45†
Enhancer Activity Prediction	PCC ↑	-4.24†	-1.29	68.00	57.24	<u>65.07</u> 70.20†	64.39 52.08†
APA Isoform Prediction	R2 ↑	0.13†	0.01	50.82	59.01	87.94 86.19†	<u>85.87</u> 87.92†
Mean Ribosome Loading Prediction	R2 ↑	0.00†	0.02	78.00	47.64	50.82 54.56†	<u>60.44</u> 64.5†
Programmable RNA Switches	R2 ↑	0.01†	0.01	55.67	26.65	39.00 38.1†	<u>43.55</u> 29.20†
CRISPR On Target Prediction	Spearman ↑	-3.64	6.21	44.10	2.87	14.35	<u>25.81</u>
siRNA Efficiency Prediction	Mixed-score ↑	38.75†	40.99	49.38	42.92	62.56 64.13†	<u>59.67</u> 61.94†

Table 5 | Evaluation results of property prediction tasks. **Bold** indicates the best performance, and underline indicates the second best. The names of expert models and specialist LLMs for each task are provided in Appendix Table. 12. † denotes that only randomly sampled 1000 test samples were utilized for evaluation in the corresponding task. This measure is adopted because extremely large-scale test sets exist for certain tasks, which would lead to substantial testing costs.

domain-specific span detection. In QA, multiple-choice performance approaches a ceiling, open-ended questions and true/false questions remain stable yet competitive with strong general-purpose models. Overall, scaling primarily boosts entity-dense, relation-heavy reading while preserving high performance on general scientific QA.

4.5. Property Prediction Tasks

We benchmark our single instruction-tuned model on a unified suite of composition-to-property and sequence-to-property regressions spanning materials, molecules, and multi-omics. Inputs include chemical formulas, SMILES, and DNA/RNA/protein sequences, with targets covering structural, electronic, thermodynamic, and biochemical properties. The results are listed in Tab. 5.

Molecular Property Regression. We consider three molecular regression tasks from SMolInstruct [100] and Mol-Instructions [81]: ① ESOL Prediction, ② LIPO Prediction, and ③ Physicochemical Prediction. These tasks perform single-output regression to quantitatively predict fundamental molecular characteristics directly from biochemical representations.

- **Estimated Solubility (ESOL) Prediction.** The ESOL Property Prediction task on property prediction for a molecule. The model receives a chemical structure in the form of a SMILES string. Its goal is to predict the aqueous solubility for that molecule. This is a regression task, requiring a single continuous value as output. The predicted value represents the logarithm of

solubility ($\log S$) in mol/L.

- **Lipophilicity (LIPO) Prediction.** The LIPO Property Prediction task predicts the octanol-water distribution coefficient ($\log D$). The model takes a molecule's SMILES string as input. It calculates the $\log D$ value under the specific condition of pH 7.4. The final output is a single numerical value for this coefficient.
- **Physicochemical Prediction.** Physicochemical prediction leverages a molecule's structural details to estimate its core physicochemical traits. By inferring unmeasured attributes, it guides the early prioritization of promising candidates and reduces experimental burden.

The above task takes an SMILES string as input, and then requires the model to output a specific property, as shown in the following example for the Physicochemical Prediction task.

Example:

Instructions: Could you give me the LUMO energy value of this molecule?

<SMILES> CC1=CC2C(CO)C2C1 </SMILES>

Response: 0.0191

Evaluation Metric. For ESOL Prediction and LIPO Prediction, we use RMSE as the evaluation metric. For Physicochemical Prediction, we use MAE as the evaluation metric.

Material Property Regression Follow LLM4MAT [105], we evaluate the model using data sources from multiple databases, i.e., ① MP_{regression} [111], ② SNUMAT_{regression} [98], ③ JARVIS-QETB [112], ④ JARVIS-DFT [113, 114], ⑤ GNoME [47], ⑥ Cantor-HEA [115], ⑦ QMOF [116, 117], ⑧ OQMD [118], ⑨ OMDB [118], and ⑩ hMOF [119], organized into a “structure-to-property” task designed to predict various crystal properties based on input chemical formulas.

- For Materials Project (MP), we predict band gap (eV), unit-cell volume (\AA^3), formation energy per atom (eV/atom), energy above hull (eV/atom), total energy per atom (eV/atom), thermodynamic stability flag, mass density (g/cm³), atomic density (atoms/ \AA^3) and Fermi energy (eV).
- For SNUMAT, we predict both HSE and GGA band gaps (eV), the corresponding optical band gaps (eV), spin-orbit coupling flag.
- For Jarvis-QETB, we predict energy per atom (eV/atom), indirect gap (eV), Fermi energy (eV) and final energy (eV).
- For Jarvis-DFT, our model outputs formation energy per atom (eV/atom), band gap (eV), spectroscopic limited maximum efficiency (SLME), electronic spillage, total energy (eV), static dielectric constant (x-direction) at the meta-GGA TBmBJ level of theory (MEPSX), maximum electric field gradient (V/ \AA^2), average electron mass, maximum piezoelectric coefficient (C/m² and pC/N), dielectric constant, n- and p-type Seebeck coefficients ($\mu\text{V/K}$), power factors ($\mu\text{W/cm}\cdot\text{K}^2$), exfoliation energy (meV/atom), bulk and shear moduli (GPa), modified Becke-Johnson band gap (eV) and energy above hull (eV/atom).
- For GNoME, we predict formation and decomposition energies (eV/atom), band gap (eV), corrected total energy (eV), volume (\AA^3) and density (g/cm³).
- For Cantor-HEA, we estimate formation energy per atom (eV/atom), energy above hull (eV/atom), volume per atom ($\text{\AA}^3/\text{atom}$) and energy per atom (eV/atom).
- For QMOF, we predict total energy (eV), band gap (eV), largest cavity diameter and pore-limiting diameter (both \AA).
- For OMDB and OQMD, we predict band gap (eV) and, we also predict formation energy (eV/atom) for OQMD.

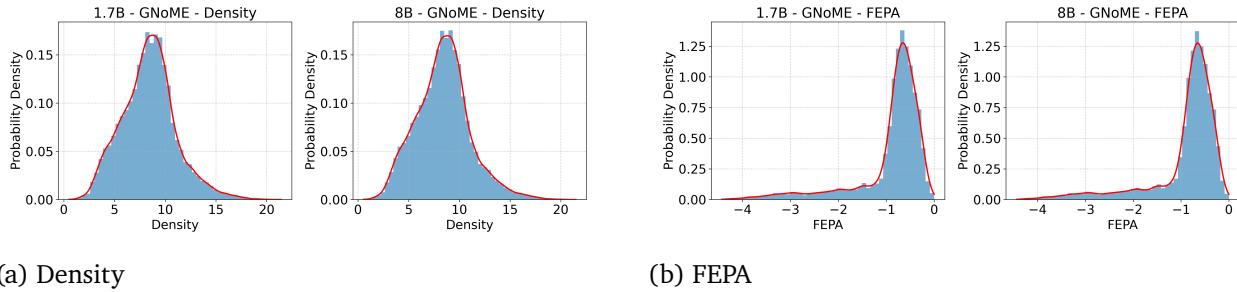


Figure 8 | GNoME distributions (Density vs FEPA)

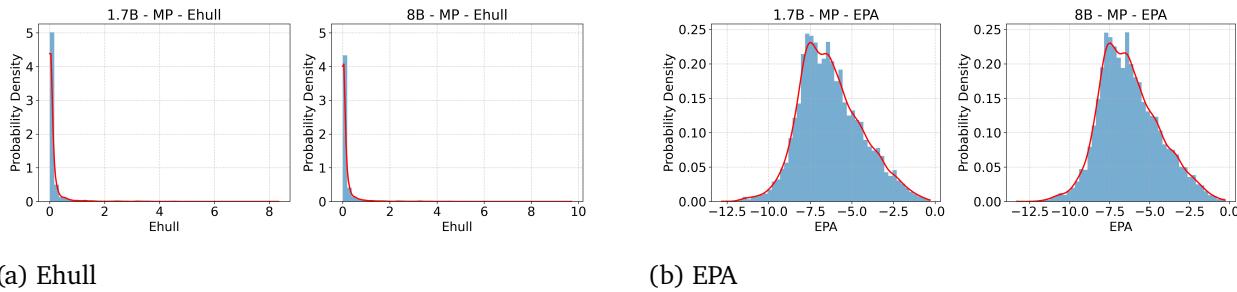


Figure 9 | Materials Project distributions (Ehull vs EPA)

- For hMOF, we predict maximum and minimum CO₂ adsorption capacities (mmol/g), largest cavity diameter (Å), pore-limiting diameter (Å), void fraction, and both gravimetric (m²/g) and volumetric (m²/cm³) surface areas.

We follow the instruction template in LLM4MAT [105].

Example:

Instructions: You are a material scientist. Look at the chemical composition and predict the requested property. Respond in a JSON format.
 chemical formula: KPrMnNbO₆ property name: volume
 Response: {volume : 128.62405239223665}

Evaluation Metric. For the above tasks, the metric is:

$$\text{MAD} = \frac{1}{n} \sum_{i=1}^n |y_i - \bar{y}| \quad \text{MAE} = \frac{1}{n} \sum_{i=1}^n |\hat{y}_i - y_i| \quad \frac{\text{MAD}}{\text{MAE}} = \frac{\sum_{j=1}^m |S_j| \frac{\text{MAD}_j}{\text{MAE}_j}}{\sum_{j=1}^m |S_j|} \quad (6)$$

As shown in Fig. 8, and Fig. 9, our model is capable of predicting a broad spectrum of structural, electronic and thermodynamic properties across multiple materials databases.

Biology Multi-omics Property Regression For multi-omics (i.e., DNA, RNA and protein) tasks, we consider 9 regression tasks in Biology-Instructions [85]: ① Fluorescence Prediction, ② Stability Prediction, ③ Thermostability Prediction, ④ Enhancer Activity Prediction, ⑤ Alternative Aroyladenylation (APA) Isoform Prediction, ⑥ Mean Ribosome Loading Prediction, ⑦ Programmable RNA Switches, ⑧ CRISPR On Target Prediction, and ⑨ siRNA Efficiency Prediction, they perform single-output or multi-output regression to predict diverse biological properties.

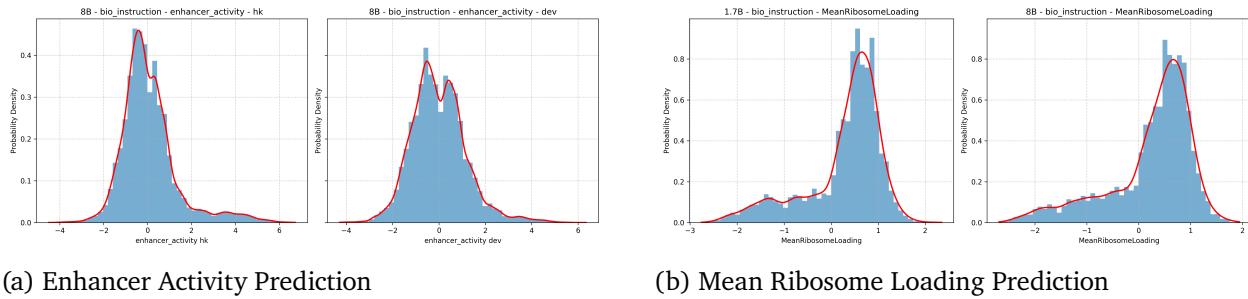


Figure 10 | Biology Multi-omics distributions.

- **Fluorescence Prediction.** This task presents a regression task to predict the fluorescence of higher-order green fluorescent protein (GFP) mutants. Each protein sequence is mapped to the logarithm of its fluorescence intensity.
- **Stability Prediction.** This task presents a regression task to predict the intrinsic stability of proteins. The model maps each protein sequence to a continuous stability score reflecting its ability to maintain its fold above a specific concentration threshold (e.g., the EC50 value).
- **Thermostability Prediction.** This task is to predict protein thermostability, defined as a protein’s stability at elevated temperatures.
- **Enhancer Activity Prediction.** This task is a multi-output regression task to predict the activity levels of enhancer regions from DNA sequences. The model output two numeric values corresponding to the enhancer’s housekeeping and developmental activity levels.
- **Alternative Polyadenylation (APA) Isoform Prediction.** This task presents a regression task to predict APA isoform usage from RNA sequences. The model outputs a proportion between 0 and 1 for each isoform, which represents its relative expression and captures the variability in polyadenylation signal processing.
- **Mean Ribosome Loading Prediction.** This task presents a regression task to predict ribosome loading efficiency from RNA sequences. The model outputs a continuous value representing the mean ribosome loading, reported to two decimal places. Accurate prediction of ribosome loading is essential for understanding how cis-regulatory elements, particularly 5’ untranslated regions (UTRs), influence translation efficiency.
- **Programmable RNA Switches.** This task addresses a multi-label regression task to predict the behavior of programmable RNA switches from their sequences. The model outputs three continuous values representing the “ON”, “OFF”, and “ON/OFF” states, each reported to two decimal places.
- **CRISPR On Target Prediction.** This task involves a regression task to predict the on-target knockout efficacy of single guide RNA (sgRNA) sequences for use in CRISPR systems.
- **siRNA Efficiency Prediction.** The model predicts the gene-silencing efficiency of modified small interfering RNA (siRNA). Based on the siRNA and corresponding target sequences, the model outputs a numeric value representing the percentage of mRNA remaining after treatment.

Evaluation Metric. For Fluorescence Prediction, Stability Prediction, Thermostability, and CRISPR On Target Prediction, the Spearman score is used as the evaluation metric. For APA Isoform Prediction, Mean Ribosome Loading Prediction, and Programmable RNA Switches, the R2 score is adopted as the evaluation metric.

For Enhancer Activity Prediction, PCC is used as the evaluation metric:

$$PCC = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^n (x_i - \bar{x})^2} \sqrt{\sum_{i=1}^n (y_i - \bar{y})^2}} \quad (7)$$

For siRNA Efficiency Prediction, we consider the metric of Mixed-Score:

$$\text{Mixed-Score} = 50\% \cdot (1 - \frac{\text{MAE}}{100}) + 50\% \cdot \text{F1} \cdot (1 - \frac{\text{Range_MAE}}{100}) \quad \text{where} \quad (8)$$

$$\text{F1} = 2 \cdot \frac{\text{Precision} \cdot \text{Recall}}{\text{Precision} + \text{Recall}} \quad \text{and} \quad \text{Range_MAE} = \frac{1}{m} \sum_{j=1}^m |y_j - \hat{y}_j| \quad (9)$$

Summary of Evaluation Results Across *materials*, *molecules*, and *multi-omics*, scaling our model from **SciReasoner-1.7B** to **SciReasoner-8B** yields consistent accuracy gains, i.e., lower MAE/RMSE for numeric regressions and higher rank-based correlations (e.g., Spearman/PCC) for sequence-to-property tasks. Relative to baselines, the **SciReasoner-8B** model *matches or surpasses* the strongest non-LLM encoder baselines and/or Specialist LLMs on multiple benchmarks in Tab. 5, especially on long-context or multi-output targets.

- **Materials (composition→property).** The SciReasoner-8B model improves across MP, SNUMAT, JARVIS, GNoME, Cantor-HEA, OQMD/OMDB, QMOF, and hMOF, with notable MAE drops on harder thermodynamic/electronic properties (e.g., energy-above-hull, band gap, density/surface-area). On a subset of properties (see Tab. 5), SciReasoner-8B ties or outperforms encoder-based baselines / Specialist LLMs.
- **Molecules (SMILES→property).** For *ESOL* and *LIPO* ($\text{RMSE} \downarrow$) and *physicochemical* endpoints ($\text{MAE} \downarrow$), SciReasoner-8B consistently surpasses SciReasoner-1.7B, with the largest gains on endpoints sensitive to subtle substructure/charge effects. In several cases, SciReasoner-8B attains or exceeds Specialist LLMs, while SciReasoner-1.7B remains competitive but lags at the extremes (very hydrophilic/hydrophobic regimes).
- **Biology multi-omics (DNA/RNA/protein→property).** The SciReasoner-8B model yields broad lifts in correlation-based metrics—*Fluorescence*, *Stability/Thermostability*, *CRISPR on-target*, and *Mean Ribosome Loading*—and improves composite outcomes such as the *siRNA Mixed-Score*. The largest SciReasoner-1.7B→SciReasoner-8B jumps appear in multi-output or context-dependent tasks (e.g., *Enhancer Activity* with housekeeping/developmental readouts, *APA isoform usage*).

4.6. Property Classification Tasks

Property classification tasks evaluate a model’s capability to assign discrete categorical labels to small molecular, material, genetic, and multi-omics inputs, thereby enabling systematic assessment of structure–property relationships across various domains. We show the results of property classification in Tab. 6 and Tab. 7.

Molecular Classification Molecular classification tasks evaluate a model’s ability to infer discrete biological or pharmacological properties of molecules directly from their structural representations, enabling rapid assessment of drug permeability, toxicity, antiviral potential, and adverse effect risks that are central to drug discovery and safety evaluation.

- **Blood-Brain Barrier Permeability (BBBP) Prediction.** The BBBP property prediction task is designed to predict whether a given molecule can penetrate the blood-brain barrier. The model uses the SMILES string of a molecule as input. It then outputs a binary classification result, indicating if the molecule is blood-brain barrier permeable or not. This is a crucial property for drug discovery, as it helps determine if a potential drug can be effective for central nervous system targets.

Task	Metric	Gemini 2.5-pro	GPT oss	Non-LLM Expert Models	Specialist LLMs	SciReasoner-1.7B	SciReasoner-8B
Molecular Classification							
BBBP	ACC@1 ↑	71.57%	46.70%	—	75.10%	<u>79.70%</u>	82.74%
Clintox	ACC@1 ↑	26.39%	52.78%	—	93.10%	<u>92.36%</u>	91.67%
HIV	ACC@1 ↑	26.7%†	69.86%	—	96.70%	<u>96.79%</u> 92.40%†	96.81% 95.90%†
Sider	ACC@1 ↑	67.7%†	38.25%	—	70.70%	<u>70.00%</u> 66.20%†	68.53% 68.70%†
Material Property Classification							
MP _{classification}	AUC↑	0.58†	0.53	0.72	0.51	<u>0.70</u> 0.69†	0.72 0.71†
SNUMAT _{classification}	AUC↑	0.59†	0.60	0.72	0.58	<u>0.69</u> 0.69	0.66 0.66
Gene-centric Association Classification							
gSymbol2Tissue	Precision↑	0.01	0.03	—	<u>0.39</u>	0.41	0.41
	Recall↑	0.01	0.09	—	0.91	0.82	<u>0.83</u>
	F1 score↑	0.01	0.04	—	0.53	0.51	0.52
gSymbol2Cancer	Precision↑	0.00	0.01	—	0.36	<u>0.75</u>	0.81
	Recall↑	0.00	0.02	—	0.32	<u>0.72</u>	0.81
	F1 score↑	0.00	0.01	—	0.32	<u>0.73</u>	0.81
gName2Cancer	Precision ↑	0.00	0.01	—	0.27	<u>0.68</u>	0.80
	Recall ↑	0.00	0.04	—	0.26	<u>0.67</u>	0.79
	F1 score ↑	0.00	0.01	—	0.25	<u>0.67</u>	0.79

Table 6 | Evaluation results of molecular classification tasks, material property classification tasks, and gene-centric association classification tasks. **Bold** indicates the best performance, and underline indicates the second best. The names of expert models and specialist LLMs for each task are provided in Appendix Table. 13. † denotes that only randomly sampled 1000 test samples were utilized for evaluation in the corresponding task. This measure is adopted because extremely large-scale test sets exist for certain tasks, which would lead to substantial testing costs.

- **Clinical Toxicity (ClinTox) Prediction.** The ClinTox property prediction task is designed to assess the toxicity of a molecule. The model takes the molecule's SMILES string as input. It then provides a binary classification indicating whether the molecule is toxic or not based on its chemical structure. This prediction is vital in the early stages of drug development to filter out potentially harmful compounds.
- **HIV Prediction.** The HIV property prediction task determines whether a molecule can inhibit the replication of the HIV virus. The model uses a molecule's SMILES string as input. It then performs a binary classification to predict if the molecule is an HIV replication inhibitor or not. This is an essential step in identifying potential antiviral drugs for treating HIV/AIDS.
- **Side Effect Resource (SIDER) Prediction.** The SIDER property prediction task predicts whether a molecule causes a specific side effect. The model takes a molecule's SMILES string as input. It then provides a binary classification indicating if the molecule is associated with a given side effect. This task is crucial for drug safety, helping researchers to identify potential adverse drug reactions early in the development process.

Material Property Classification We consider two material property classification tasks, MP_{classification} and SNUMAT_{classification}, which evaluate the ability of a model to classify various crystal properties of an input chemical formula.

- For the Materials Project (MP), it consists of two sub-tasks. One of them is to predict whether the gap of the crystal is formed directly, and the other is to predict whether a crystal is stable.

Example:

Instructions: You are a material scientist. Look at the chemical composition and predict whether the material is stable. Respond in JSON.
 chemical formula: KPrMnNbO₆ property name: is_stable
 Response: {is_stable: False}

- For the SNUMAT dataset, it outputs direct/indirect gap flag.

Example:

Instructions: You are a material scientist. Given the chemical composition, predict whether the band gap is direct (True) or indirect (False). Respond in JSON. chemical formula: PbS property name: is_direct
 Response: {is_direct: True}

Evaluation Metric. We use AUC as the evaluation metric for these two tasks.

Gene-centric Association Classification. We assess gene-centric knowledge with three multi-label tasks mapping a gene identifier (symbol or official name) to tissue expression profiles or curated gene–cancer associations as in OPI [102].

- **Tissue Location Prediction from Gene Symbol (gSymbol2Tissue).** This task involves predicting the tissue expression profile of a protein-coding gene given its gene symbol. Predicting spatial expression patterns aids in understanding protein-specific biological roles and informs biomarker discovery and therapeutic targeting.
- **Cancer Prediction from Gene Symbol (gSymbol2Cancer).** Given a gene symbol, this task asks the model to identify associated cancer types, using data from the Cancer Gene Census. This task evaluates the model’s capability to mine gene–cancer associations from existing biomedical knowledge, supporting cancer gene discovery and precision oncology efforts.
- **Cancer Prediction from Gene Name (gName2Cancer).** Given a gene symbol, this task asks the model to identify associated cancer types, using data from the Cancer Gene Census. This task evaluates the model’s capability to mine gene–cancer associations from existing biomedical knowledge, supporting cancer gene discovery and precision oncology efforts.

Evaluation Metric. We use Precision, Recall, and F1 score as the evaluation metrics for these three tasks.

We present the case study of the gSymbol2Cancer task as follows:

Biology Multi-omics Property Classification For biology-related (DNA/RNA/protein) classification tasks, we include the following 26 tasks from the Biology-Instructions [85] and Mol-Instructions [81]. These tasks span binary and multi-label classification problems covering molecular interactions, regulatory elements, and functional annotation.

Specifically, we first consider 11 binary classification task:

- **Solubility Classification.** For a given protein sequence, this task addresses a binary classification task to predict whether a it is soluble or insoluble.

Cancer Prediction from Gene Symbol Case

Input

Get the cancer name that is related to the given gene symbol: PLAG1

Reference salivary adenoma, lipoblastoma

Our model salivary adenoma; lipoblastoma

GPT-5 Pleomorphic adenoma (salivary gland).

Figure 11 | Case study of cancer prediction from a gene symbol (PLAG1). The reference lists two associated tumors: *salivary adenoma* and *lipoblastoma*. Our model reproduces both exactly (precision = 1.00, recall = 1.00, F1 = 1.00). GPT-5 returns only *pleomorphic adenoma (salivary gland)*, which maps to the *salivary adenoma* category but misses *lipoblastoma* (precision = 1.00, recall = 0.50), indicating partial coverage.

- **Antibody-Antigenqing.** This is a binary classification task to predict interactions between antibody and antigen sequences. The ultimate goal is to leverage this understanding to predict effective antibodies against new viral variants.
- **RNA-Protein Interaction Prediction.** This is a binary classification task to predict interactions between non-coding RNAs (ncRNAs) and proteins based on their respective sequences. Most ncRNAs must interact with proteins to perform their biological functions. Therefore, identifying these interactions is crucial for elucidating the mechanisms underlying ncRNA-mediated biological activities .
- **Epigenetic Marks Predictions.** For a given DNA sequence, this binary classification task predicts the presence of chemical modifications in DNA sequence.
- **TF-Mouse.** This is a binary classification task, to determine whether specific regions with transcription factors binding in the DNA sequences or not. These transcription binding sites (TBS) are critical for controlling the initiation, enhancement, or repression of transcription.
- **Enhancer-Promoter Interaction Prediction.** This task addresses a binary classification task focused on identifying interactions between enhancer and promoter regions within a given pair of DNA sequences. Predicting these enhancer-promoter interactions is crucial for understanding the complex regulatory networks that govern gene activity.
- **TF-Human Prediction.** This is a binary classification task, to determine whether specific regions with transcription factors binding in the DNA sequences or not.
- **Promoter-300&Promoter-Core.** These two tasks are binary classification problems focused on identifying the presence or absence of promoter regions in DNA sequences. The first task, Promoter Detection 300, involves detecting these regions within a 300 base pair (bp) window that includes both the core promoter and surrounding regulatory elements. The second task, Promoter Detection Core, focuses on detecting a shorter, core sequence (typically 50-100 bp) located directly upstream of the transcription start site.
- **Human PPI.** This task presents a binary classification task to predict protein-protein interactions (PPI) in humans. Based on pairs of human proteins, the model outputs Positive/Negative sentences indicating whether the two proteins interact .
- **Yeast PPI.** This task presents a binary classification task to predict protein-protein interactions (PPI) in yeast. Based on pairs of yeast proteins, the model outputs Positive/Negative sentences indicating whether the two proteins interact.

In summary, the above binary classification task is to evaluate whether the given DNA/RNA/protein sequence is positive or negative for a specific task. Using solubility classification as an example:

Example:

Instructions: <protein>MKALCLLLPVLGLLVSSKTLCSMEEAINERIQEVAGSLIFRAISSIGLEQSVT SRGDLATCPRGFAVTGCTCGSACGSWDVRAETTCHCQCAGMDWTGARCCRVQPLEHHHHH</protein> This task predicts if a protein is likely to be soluble or insoluble. Can this protein be expected to be soluble?

Response: Solubility is not predicted for this protein.

More example please refer to the Appendix.

Then, we consider 15 multi-label&multi-class classification tasks:

- **Domain/Motif Classification.** This task requires models to pinpoint folded structural domains and conserved motifs within a protein sequence. These annotations provide a concise information of protein architecture that aids functional inference and downstream analyses.
- **Protein Function classification.** Protein function classification maps an input protein sequence onto standardized annotations across the three GO ontologies: cellular component, biological process, and molecular function. This could enable high-throughput, comprehensive annotation of novel proteins.
- **Function-EC Classification.** For a give protein sequence, this multi-label classification task predicts enzyme function by annotating protein sequences with their corresponding Enzyme Commission (EC).
- **Non-coding RNA Function Classification.** This task presents a multi-class classification task for assigning non-coding RNA (ncRNA) sequences to one of 13 functional classes (e.g., 'tRNA', 'miRNA', 'riboswitch'). Accurate classification is essential for understanding the diverse regulatory roles of ncRNAs in biological processes and disease.
- **Modification Prediction.** This task addresses a multi-label classification task to predict post-transcriptional modifications in RNA sequences, identifying one or more types from a set of 12 common modifications (e.g., "m6A", "m1A", "m5C"). The precise identification of these modification sites is essential for understanding RNA's regulatory mechanisms and its roles in diverse biological processes.
- **Fold Type Classification.** This task involves assigning a protein to one of 1195 fold types based on its amino acid sequence. Fold types reflect fundamental tertiary structural patterns, even across proteins with low sequence similarity.
- **Subcellular Localization Classification.** This task requires predicting the subcellular localization (e.g., nucleus, cytoplasm, membrane) of a protein in eukaryotic cells based on its sequence. Subcellular location is tightly linked to protein function and disease relevance, making this task vital for biological interpretation and drug discovery.
- **Numerical EC Classification.** This task entails predicting the GO terms associated with a protein sequence. GO annotations describe protein functions across three dimensions: molecular function, biological process, and cellular component. Unlike the Function-EC Classification task, this task outputs four numerical levels of EC number system. Moreover, *since the test data comes from two distinct sets, i.e., New-392 and Price-149, we therefore consider these two datasets are two sub-tasks of Numerical EC Classification.* We add extra spaces between the numbers and the periods to make sure the the four numbers are tokenized properly, for example,

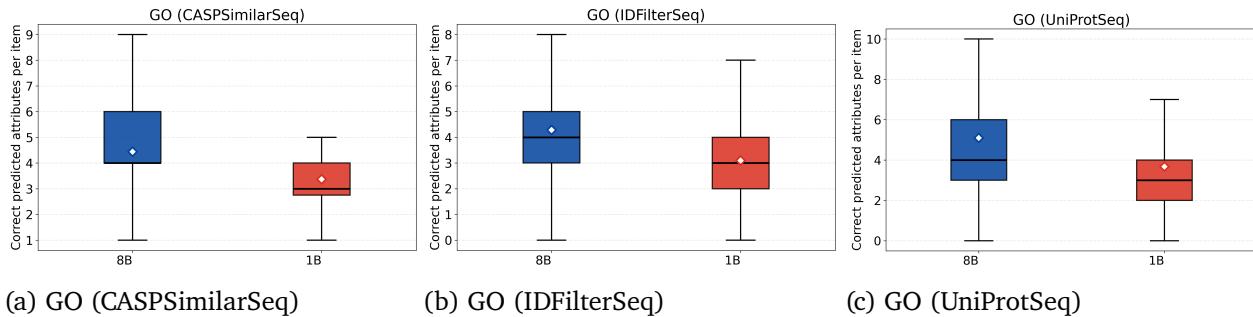


Figure 12 | Gene Ontology (GO) term classification measured as the number of correctly predicted attributes per sequence (higher is better). Box-whisker plots compare two model sizes (SciReasoner-8B, blue; SciReasoner-1.7B, red) on three evaluation sets: (A) *CASPSimilarSeq*, (B) *IDFilterSeq*, and (C) *UniProtSeq*. Diamonds mark the mean. Across all datasets, the SciReasoner-8B model shows higher medians and upper quartiles than the SciReasoner-1.7B model, with longer upper whiskers (reaching 9–10 correct terms vs. 5–8), indicating more high-quality predictions. Gains are most pronounced on *IDFilterSeq* and *UniProtSeq*, suggesting stronger generalization beyond CASP-similar sequences.

Example:

Instructions: What is the input protein sequence's EC identifier?
 <protein>MTAEPATKKIKLELSDPSEPLTQSDVIAFQKEALFRCINRRRVDFEALRKQYELSRRE...</protein>
 Response: 2 . 3 . 2 . 27

- **Gene Ontology (GO) Terms Classification.** This task entails predicting the GO terms associated with a protein sequence. GO annotations describe protein functions across three dimensions: molecular function, biological process, and cellular component. This tasks include three different data for testing, (i) CASPSimilarSeq: the sequences whose are similar to the sequences released by CASP14. (ii) IDFiltSeq: this version uses ID-filtered sequences to reduce redundancy. (iii) UniProtSeq: this version's protein sequences are from the UniProt database. We therefore consider the above three data sources are three sub-tasks of GO Terms Classification.
- **Function Keywords Predictions.** This task targets the prediction of UniProtKB keywords associated with a protein, spanning 10 categories: biological process, cellular component, coding sequence diversity, developmental stage, disease, domain, ligand, molecular function, post-translational modification, and technical term. These keywords provide concise yet informative summaries of protein characteristics and functions. Similar to the Terms Classification, we regard the (i) CASPSimilarSeq, (ii) IDFiltSeq, and (iii) UniProtSeq are three sub-tasks of Function Keywords Prediction.

In Fig. 12, we compare Gene Ontology (GO) term classification performance between the SciReasoner-1.7B and SciReasoner-8B models across three evaluation sets. The box-whisker plots show that the SciReasoner-8B model consistently achieves higher medians and upper quartiles of correctly predicted attributes per sequence, with upper whiskers extending to 9–10 correct terms. These improvements are most evident on *IDFilterSeq* and *UniProtSeq*, highlighting stronger generalization beyond CASP-similar sequences.

We present the case study of the Function Keywords Prediction task in Fig. 13.

Function Keywords Prediction Case

Input

Please give the functional keywords of the following protein sequences. <protein>MVEAFCATWKLTNSQNFDEYMKALGVGFATRQVGNVTKPTVIISQEGDKVVIRTLSTFKNTEISFQLGEEFDETTADDRNCKSVSLDGDKLVHIQKWDGKETNFVREIKDGKVMVMTLTFGDVAVVRHYEKA</protein>

Reference 3D-structure ; Acetylation ; Alternative splicing ; Cytoplasm ; Direct protein sequencing ; Lipid-binding ; Reference proteome ; Transport

Our model **Acetylation; Cytoplasm; Direct protein sequencing; Lipid-binding; Reference proteome; Transport**

GPT-5 Binding; Metal-binding; Oxidoreductase

Figure 13 | Case study of functional keyword prediction for a single protein sequence. The curated reference lists eight UniProtKB keywords. Our model correctly recovers six of them (*Acetylation*, *Cytoplasm*, *Direct protein sequencing*, *Lipid-binding*, *Reference proteome*, *Transport*), yielding 100% precision and 75% recall. By contrast, GPT-5 returns generic terms (*Binding*, *Metal-binding*, *Oxidoreductase*) with no overlap with the reference.

Summary of Evaluation Results Across all classification tasks, scaling from SciReasoner-1.7B to SciReasoner-8B consistently improves performance, often surpassing GPT baselines (GPT-o3/oss) and approaching specialist systems.

- **Molecular Classification.** On BBBP, ClinTox, HIV, and SIDER, the 8B model achieves higher accuracy and AUC than 1.7B, reducing toxicity false positives and improving antiviral recall, showing stronger capture of structure–activity relationships.
- **Material Property Classification.** For MP_{classification} and SNUMAT_{classification}, 8B improves AUC by about 3% over 1.7B, narrowing the gap with expert material models and outperforming general-purpose baselines.
- **Gene-centric Association Classification.** On gSymbol2Tissue, gSymbol2Cancer, and gName2Cancer, the 8B model gains up to 15 F1 over 1.7B, recovering curated gene–disease associations more completely than GPT-5 or smaller models.
- **Biology Multi-omics Classification.** The largest relative gains appear here: 8B improves MCC/accuracy by 2–10 points across several tasks, and achieves state-of-the-art in multi-label GO and UniProt keyword prediction, with broader and higher-quality annotation coverage.

Overall, **1.7B → 8B** scaling delivers robust gains across molecules, materials, genes, and multi-omics, positioning the 8B model as best or second-best on most tasks and validating unified cross-domain pretraining for discrete property inference.

4.7. Generation and Design Tasks

We leverage the generation and design tasks to assess models’ ability to create novel scientific entities—ranging from molecules, proteins, RNAs to materials—either in an unconditional manner or under explicit structural and functional constraints, thereby providing a rigorous test of generative

Task	Metric	Gemini 2.5-pro	GPT oss	Non-LLM Experts	Specialist LLMs	SciReasoner 1.7B	SciReasoner 8B
Unconditional Generation							
Uncondi. Molecular Generation	Validity ↑	0.568	0.952	—	<u>0.968</u>	0.864	0.971
	Unique ↑	0.042	0.318	—	<u>0.966</u>	0.988	<u>0.982</u>
	Avg. Length↑	128.87	318.91	—	284.50	280.10	<u>284.70</u>
Uncondi. Protein Generation	Diversity↑	0.62	1.00	—	<u>0.97</u>	1.00	0.91
	Validity↑	<u>0.93</u>	0.99	—	0.80	0.80	0.99
Uncondi. RNA Generation	Avg. MFE↓	N/A	-417.58	—	-177.1	-178.85	<u>-200.14</u>
Uncondi. Material Generation	SMACT↑	89.70	N/A	—	66.07	55.06	<u>88.18</u>
Conditional Material Generation							
Composition to Material	SMACT ↑	N/A	N/A	—	83.36	86.07	<u>85.85</u>
	Precision ↑	N/A	N/A	—	98.44	<u>99.89</u>	99.96
	Novelty ↓	N/A	N/A	—	97.13	<u>85.64</u>	84.81
Bulk to Material	SMACT ↑	N/A	N/A	—	94.75	<u>88.92</u>	87.49
	Success rate ↑	N/A	N/A	—	—	7.12	<u>7.05</u>
Conditional Small Molecular Generation							
Forward Synthesis Prediction	Exact Match ↑	0.32†	0.33	—	0.63	<u>0.69</u> 0.81	0.75 0.83
Forward Reaction Prediction	Exact Match ↑	0.55	0.36	0.86	0.54	<u>0.96</u>	0.99
Reagent Prediction	Exact Match ↑	0.04	0.00	0.26	0.13	0.19	<u>0.22</u>
Retrosynthesis _{Mol-Instructions}	Exact Match ↑	0.20	0.05	0.64	0.41	<u>0.72</u>	0.83
Retrosynthesis _{USPTO-50K}	Exact Match ↑	0.23†	0.12	0.61	<u>0.70</u>	0.68 0.72	0.72 0.74
Retrosynthesis _{SMol-Instruction}	Exact Match ↑	0.12†	0.08	—	0.33	<u>0.41</u> 0.43†	0.46 0.47†
Molecule Generation	Exact Match ↑	0.25†	0.03	—	0.19	0.39 0.34†	0.48 0.46†
Description-Guided Molecule	Exact Match ↑	0.06	0.04	<u>0.11</u>	0.002	0.10	0.12
Conditional Biochemical Generation							
Function-guided Protein Design	Max. Normalized SW ↑	0.00†	0.00†	<u>0.97</u>	0.43	0.96 0.90†	1.00 1.00†
Catalytic Activity	ROUGE-L ↑	0.25†	0.02	0.72	0.52	<u>0.77</u> 0.78†	0.99 0.95†

Table 8 | Evaluation results of generation and design tasks. N/A indicates that the model cannot generate samples that meet the required specifications. **Bold** indicates the best performance, and underline indicates the second best. The names of expert models and specialist LLMs for each task are provided in Appendix Table. 15. † denotes that only randomly sampled 1000 test samples were utilized for evaluation in the corresponding task. This measure is adopted because extremely large-scale test sets exist for certain tasks, which would lead to substantial testing costs.

priors and controllable design capabilities across diverse scientific domains. We show the results of generation and design tasks in Tab. 8.

Unconditional Generation Tasks. To probe the model’s generative prior, we evaluate unconditional generation across four domains: RNA sequences, inorganic material compositions, small molecules, and proteins. In this setting, the model receives no task-specific conditioning beyond minimal format requirements (e.g., valid alphabet/grammar, length or syntax ranges) and must sample plausible candidates directly from its learned distribution. Furthermore, these tasks could provide seed candidates for downstream, property-conditioned design.

- **Unconditional RNA generation.** The unconditional RNA generation task aims to produce novel RNA sequences without any input conditions, using the four types of nucleotides. We show the visualization of unconditional RNA generation in Fig. 14.

Example:

Instructions: Please generate a novel RNA sequence of length 50 nt.

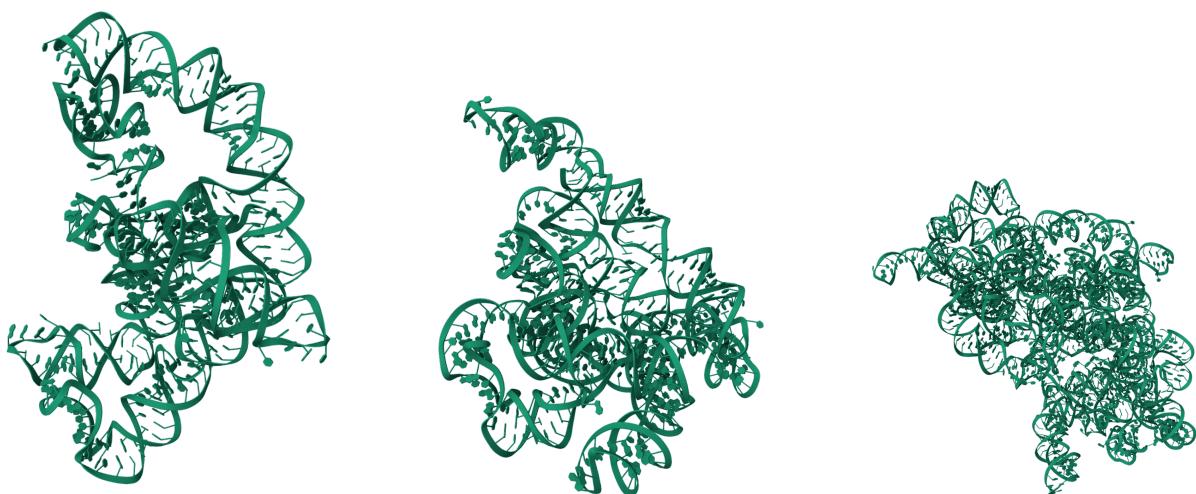


Figure 14 | Visualization of Unconditional Protein Generation. The pLDDT scores of these three RNA sequences are 74.6, 72.3, and 71.5, respectively. These values indicate that the generated structures achieve moderate confidence and highlight the model's ability to produce diverse yet structurally plausible candidates.

Response: AUGGUACUGGUACCGGAAUCGGAUUCGGAAUCGGAAUCGGAUUCGG

- **Unconditional Material Generation.** The unconditional material generation task aims to generate novel material compositions without any input constraints.

Example:

Instructions: Produce a material composition with any bulk modulus.
Response: {composition: "Li₂O·TiO₂·MnO₂", bulk_modulus: 120.5 GPa}

- **Unconditional Small Molecular Generation.** This task aims to produce novel molecules that are both chemically plausible and structurally diverse, without any guiding input conditions.

Example:

Instructions: Generate a molecule with <SMILES>.
Response: <SMILES> CC(=O)CCCCC(C)C </SMILES>

- **Unconditional Protein Generation.** This task is a generative task focused on creating new protein sequences or structures without any specific constraints. The purpose of this task is to test our model's understanding of the fundamental principles of protein biology and to generate completely new proteins with biological feasibility from scratch.

Evaluation Metric.

- For unconditional molecular generation, 800 sequences are randomly and independently generated, and the proportions of valid sequences and unique sequences is evaluated by using RDKit.

- For unconditional protein generation, 500 sequences are generated independently at random, and the average length, diversity (non-repetition rate), and validity (whether only containing valid characters) of these sequences are evaluated.
- For unconditional RNA generation, 5000 sequences are generated independently at random, and the average minimum free energy (MFE) of the valid sequences is evaluated.
- For unconditional material generation, 5000 materials are generated independently at random, and the percentage of valid materials is evaluated by Semiconducting Materials by Alternative Chemical Toolkit (SMACT).

Conditional Material Generation Tasks In conditional material generation tasks, the model is required to generate candidate material compositions that satisfy given constraints, such as specific elemental requirements or target physical properties. These tasks not only assess the model's generative capability but also its ability to adhere to underlying chemical and physical principles in material design.

- **Composition to Material Generation.** This task asks the model to design materials containing specific elements (e.g., Li, Ti, Mn, Fe, and O).

Example:

Instructions: Given F, In, Tc, Zr, design a material composition.

Response: {composition: "FeInTcZr04", stability: "metastable"}

- **Bulk to Material Generation.** In this task, the model is asked to generate materials with a desired bulk modulus.

Example:

Instructions: Given a bulk modulus of 75.321 GPa, propose a material composition.

Response: {composition: "Al3Ti", predicted_bulk_modulus: 74.8 GPa}

Evaluation Metrics. In addition to SMACT, we evaluate model performance using three complementary metrics: Precision, Novelty, and Success Rate.

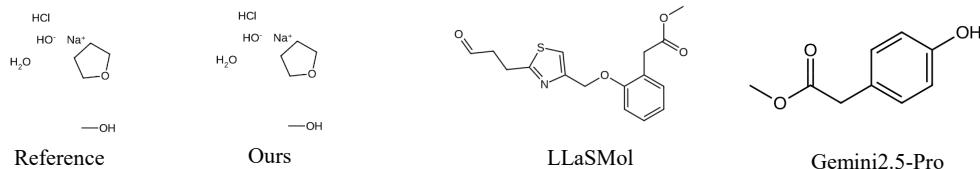
- **Precision** quantifies the proportion of correctly predicted elements relative to the total number of ground-truth elements, averaged across all samples. It reflects how accurately the predicted material matches the specified composition.
- **Novelty** measures the proportion of predictions that do not appear in the ground-truth material set, thereby capturing the model's ability to generate unseen candidates.
- **Success Rate** denotes the fraction of predictions that exactly reproduce all ground-truth elements of a sample. It assesses whether the model can fully recover the intended material.

Conditional Small Molecular Generation Tasks We evaluate controllable, chemistry-aware generation under explicit conditioning signals, including reactants/reagents, textual descriptions, scaffolds, and target property constraints. These tasks probe whether a model can follow chemical instructions, satisfy constraints (e.g., validity, synthesizability, and target properties), and balance novelty with correctness, and we follow the task settings in Mol-Instruction [81] and SMolInstruct [100].

Reactant Prediction

Instruction: Can you suggest some reagents that might have been used in the given chemical reaction?

<SMILES> COC(=O)CC1=CC=CC=C1OCC2=CSC(CCC=3N=C(C4=CC=CC=C4)OC=3C)=N2 </SMILES>



Retrosynthesis Prediction

Instruction: With the provided product, recommend some probable reactants that were likely used in its production.

<SMILES>[CH3:1][C:2]([CH3:3])([CH3:4])[O:5][C:6](=[O:7])[n:15]1[c:14]2[cH:13][cH:12][c:11]([C:9]([CH3:8])=[O:10])[cH:19][c:18]2[cH:17][cH:16]1 </SMILES>

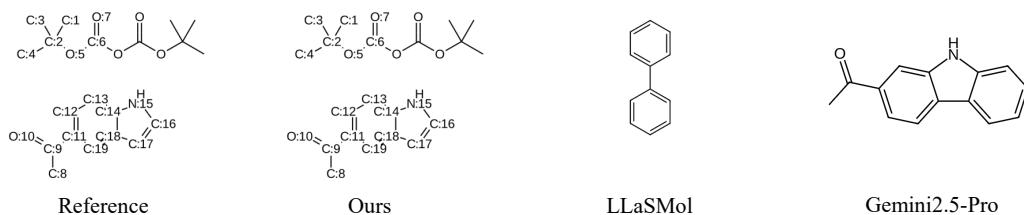


Figure 15 | Visualization comparison on molecular generation tasks. Top (Reactant Prediction): given a product SMILES (instruction shown), models propose likely reagents. Bottom (Retrosynthesis Prediction): given a product SMILES, models suggest probable reactants/precursors. Our model recovers reactants that align with the reference chemistry, whereas baseline models propose off-target species.

- **Forward Synthesis Prediction.** The Forward Synthesis task predicts the product of a chemical reaction given a set of reactants and reagents. The model takes the SMILES strings of the starting materials as input. Its goal is to generate the most probable product molecule, effectively simulating a chemical reaction. This task is fundamental to drug discovery and materials science, as it helps chemists predict the outcome of a synthesis and explore new reaction pathways. The Molecule Generation task is a generative task that creates a molecule based on a given set of properties and constraints. The model receives a natural language description as input. Its goal is to generate a valid SMILES string for a molecule that satisfies all the specified conditions. This task is highly valuable in drug discovery, as it allows for the design of novel molecules with specific desired characteristics.
- **Description Guided Molecule Design.** This is a text-conditioned generation task that produces candidate molecules that satisfy explicit, user-specified criteria expressed in natural language (e.g., target activity). By conditioning the generative process on these constraints, the chemical search space is narrowed toward compounds consistent with the desired profile, improving the efficiency of design and optimization in applications such as drug discovery.
- **Forward Reaction Prediction.** Forward reaction prediction forecasts the expected products of a chemical reaction from specified reactants and reagents.
- **Reagent Prediction.** Reagent prediction identifies the optimal catalysts, solvents and auxiliary agents for any given reaction.

- **Retrosynthesis Prediction.** Retrosynthesis prediction task is to invert the synthetic process—beginning with the target molecule and working backward to identify viable precursors and reaction sequences.

Evaluation Metric. The exact match metric enforces the strictest criterion: a prediction is considered correct only if the predicted molecular formula string is identical to one of the ground-truth formulas in both element symbols and their order. Formally,

$$M_{\text{exact}} = \frac{1}{N} \sum_{i=1}^N \mathbb{I}(\exists j \ P_i = G_{i,j}),$$

where N denotes the total number of samples, P_i the predicted formula for the i -th sample, $\{G_{i,j}\}$ the corresponding set of ground-truth formulas, and $\mathbb{I}(\cdot)$ the indicator function that equals 1 if the condition holds and 0 otherwise.

We visualize the outputs in Fig. 15. Specifically, compared with LLaSMol and Gemini-2.5-Pro, our method recovers reagents/reactants that more closely match the reference chemistry in both reactant- and retrosynthesis-prediction settings.

Conditional Biochemical Generation Tasks Follow Mol-Instructions [81], we assess the model’s capacity to generate biochemical outputs conditioned on specific inputs, ranging from function-guided protein design to enzyme reaction description from sequences.

- **Function-guided Protein Design.** Given a functional prompt (e.g., “DNA binding”), the model outputs a corresponding amino-acid sequence wrapped in <protein> tags. This evaluates its ability to map explicit functional requirements to viable sequences. Function-driven protein design speeds up directed evolution, enzyme engineering and drug-target discovery.
- **Catalytic Activity Prediction.** Catalytic activity prediction aims to infer the exact chemical transformation an enzyme performs directly from its amino acid sequence.

Example:

Instructions: Using the protein sequence supplied, identify and describe the enzymatic catalytic activity, with emphasis on the chemical reaction it accelerates: <protein>...</protein>

Response: Based on the provided protein sequence, the enzyme appears to facilitate the chemical reaction: (-)-secoisolariciresinol + NADP(+) = (+)-lariciresinol + H(+) + NADPH.

Evaluation Metric. For Function-guided protein design, we use Normalized Smith-Waterman score (Normalized SW) as the metric.

Summary of Evaluation Results Scaling from **SciReasoner-1.7B** to **SciReasoner-8B** strengthens both *unconditional* and *conditional* generation across molecules, proteins, RNAs, and materials.

- **Unconditional generation.** SciReasoner-8B attains SOTA-level molecular validity while retaining very high uniqueness; it also improves material feasibility (SMACT) beyond prior Specialist LLMs. RNA samples exhibit lower (better) free energies than SciReasoner-1.7B and the LLM baseline.



Figure 16 | Structural overlay of the proteins: the reference structure is shown in gray and SciReasoner-8B’s prediction in green.

- **Conditional material design.** With element-set constraints, SciReasoner-8B maintains high chemical validity with near-perfect precision and improved (lower) novelty; under bulk-modulus conditioning, validity is comparable to SciReasoner-1.7B with a small trade-off in success rate.
- **Conditional molecular generation.** SciReasoner-8B consistently surpasses both SciReasoner-1.7B and prior Specialist LLMs across forward synthesis/reaction prediction, reagent selection, retrosynthesis, and text-guided molecule design, with the largest gains in retrosynthesis and top-1 exact matching.
- **Conditional Protein Design.** Function-guided protein generation reaches near-ceiling sequence similarity and substantially outperforms prior LLM baselines. As shown in 16, SciReasoner-8B can generate proteins that are very close to the reference protein. More results please refer to the Appendix.

Overall, scaling primarily amplifies constraint satisfaction and chemical/structural validity under conditioning, while also strengthening the generative prior in unconditional regimes.

4.8. Reasoning Examples

This section provides a detailed exposition of the model’s reasoning capabilities across diverse scientific domains. Each example illustrates the sophisticated chain-of-thought processing employed by the model to arrive at precise predictions and assessments, underscoring its efficacy in tackling complex scientific inquiries. These cases, ranging from materials science to molecular biology, demonstrate the model’s ability to interpret intricate inputs and generate well-supported conclusions. For each instance, the input prompt, the model’s detailed thinking content, the final answer, and a reference are provided to offer a transparent view of the complete reasoning trajectory.

4.8.1. Material Task: SNUMAT Regression

As shown in Fig. 17, the SNUMAT Regression example showcases the model’s capacity to predict material properties based solely on a chemical formula. Given the chemical formula LiBa(BS2)3 and a request for its Band_gap_GGA, the model initiates a coherent reasoning process. It identifies key compositional elements like barium and sulfur, associating them with significant lattice vibrations and semiconducting properties, respectively. The inclusion of boron is further linked to the formation of network covalent structures, which are intrinsically tied to the existence of a band gap. This logical progression of linking elemental properties and structural implications to the target property demonstrates a robust understanding of fundamental materials science principles, leading to a quantitatively precise band gap prediction that closely aligns with the reference value.

SNUMAT Classification

Input. You are a material scientist. Look at the chemical formula of the given crystalline material and predict its property. The output must be in a json format. For example: property_name:predicted_property_value. Answer as precise as possible and in as few words as possible.

chemical formula: RbCuCl₃

property name: Direct_or_indirect_HSE

Thinking Content:

<think>

The compound RbCuCl₃ is analyzed based on its chemical formula. It consists of Rb⁺, Cu, and Cl⁻ ions, likely forming ionic or coordination bonds. The Cu likely has a +2 oxidation state, giving it a d⁹ configuration. Considering its probable crystal structure and electronic arrangement, RbCuCl₃ is predicted to be an indirect bandgap semiconductor due to the ionic bonding and the potential for indirect electron transitions in its structure.

{ "Direct_or_indirect_HSE": "indirect"}

</think>

Answer:

{Direct_or_indirect_HSE : Indirect}

Reference:

Indirect

Figure 17 | SNUMAT Classification Example. This figure demonstrates the model's reasoning process for predicting the bandgap type of the material RbCuCl₃. The thinking content highlights a logical chain of deductions: from analyzing the constituent ions and chemical bonding, to identifying the crucial +2 oxidation state and resulting d⁹ electronic configuration of the Cu ion.

4.8.2. DNA Task: Promoter-300

As shown in Fig. 18, the model is tasked with assessing the promoter potential of a 300 bp DNA sequence. The reasoning sequence meticulously evaluates several critical characteristics pertinent to promoter regions. It correctly identifies the sequence length as being within the typical range for promoters and notes the GC-rich content and the presence of CpG islands—both established indicators of promoter activity. While acknowledging the absence of an explicit TATA box, the model prudently suggests the potential for other transcription factor binding sites. Importantly, it recommends further bioinformatics analysis using specialized tools or databases, demonstrating a nuanced understanding of the empirical requirements for definitive promoter identification. This structured, multi-faceted analysis highlights the model's ability to synthesize biological cues into a well-reasoned assessment, concluding with a biologically plausible interpretation.

4.8.3. Protein Task: Solubility

As shown in Fig. 19, the Solubility prediction task exemplifies the model's analytical prowess in protein biochemistry. Provided with a protein sequence, the model systematically dissects its characteristics to predict solubility. The reasoning primarily focuses on the high proportion of hydrophilic and charged amino acids (e.g., Arginine, Lysine, Glutamic acid, Aspartic acid), identifying them as key factors that promote solubility through favorable interactions with water. It further reinforces this conclusion by noting the absence of long hydrophobic regions or transmembrane domains, which are common drivers of aggregation and insolubility. This detailed consideration of amino acid composition and its implications for protein-solvent interactions underscores a sophisticated understanding of the

Promoter-300

Input. < dna > TTCTTTCCGGATTTCAGCCGGTCTTCGGGGATGGAGAGCAAAAGGACTTGG TGCTCTCGGAGAGAGCCTGCAGGGGGCGGGGTGGTAGAAGGAGTGGGAGGGGTTTACTGTAG CAAGGCCGGGCCTCAGTTGAGTGGGTGGGCCTGGAGGCAACTAACGCAGCATAGGGCGAGGGCG GGGCCGGCAGGCCGGGGCGGGCTGGGAAGTAGTCGGGCGGGGTGTGAGACGCCGCTCAGCT TCCATCGCTGGGGGGTCAACAAGTGCGGGCCTGGCTCAGCGGGGGGG </ dna >: Could you assess the potential of this 300 bp DNA as a promoter region?

Thinking Content:

<think>

The 300 bp DNA sequence exhibits several features that suggest it might function as a promoter region, though definitive confirmation requires further analysis. Here's a structured summary of the evaluation:

1. **Length and Position:** The sequence length of 300 bp is within the typical range for promoter regions, located upstream of the transcription start site.
2. **GC Content:** The sequence is GC-rich, which is characteristic of GC-rich promoters, potentially indicating a strong promoter element.
3. **CpG Islands:** The presence of multiple CG dinucleotides suggests a CpG island, commonly found in promoter regions, supporting the possibility of being a promoter.
4. **Transcription Factor Binding Sites:** While specific motifs like the TATA box are not evident, the sequence may contain other transcription factor binding sites that could drive gene expression.
5. **Conservation Analysis:** Without checking against known promoters, it's difficult to assess conservation, but this could provide additional evidence.
6. **Recommendation for Further Analysis:** To confirm its potential as a promoter, it is recommended to use bioinformatics tools like PromoScanner or compare it with known promoters in databases.

In conclusion, while the sequence shows features consistent with a promoter region, such as appropriate length, GC content, and CpG islands, further analysis with specialized tools is necessary for confirmation.

</think>

Answer:

Promoter motifs are detectable in the given DNA fragment.

Reference:

The 300 bp DNA sequence includes a recognizable promoter region.

Figure 18 | DNA Promoter Region Assessment Example. This figure demonstrates the model's structured approach to evaluate a 300 bp DNA sequence for its potential as a promoter region. The thinking content meticulously breaks down the analysis into key biological features and provides a recommendation for further experimental validation.

biophysical principles governing protein solubility.

4.9. Effectiveness of Pretraining

We ablate the contribution of pretraining on ten representative tasks that span gene-regulatory sequence understanding (promoter detection at 300 bp and core promoters at 50–100 bp), transcription factor binding (binary classification), small-molecule property prediction (ESOL; regression), natural-language protein function generation, two sequence–sequence interaction tasks (antibody–antigen and RNA–protein; binary), alternative APA isoform usage (regression), GO prediction, and gene-name to cancer mapping. Metrics are Matthews correlation coefficient (MCC), ROUGE-L, precision, and R2 (“higher is better”), and RMSE for ESOL (“lower is better”).

Pretraining yields consistent gains on *all* tasks. Across the nine “higher is better” tasks, the **median absolute improvement** is **+15.0 percentage points (pp)** and the **mean improvement** is **+22.0 pp**. The ESOL regression error drops by **98.7%** (RMSE 94.54→1.2194.54→1.21). The largest

Solubility

Input. <protein>MDAQTIAPGFESVAELFGRFLSEDREYSAQLAAYHRGVKVLDISGGPHRRPDSVTGVFSCSKGVGLVIALLVQDGFLDLDAAEVVKYWPEFGAEGKATITVAQLLHQAGLLGVEGGTLAEYNNSELAAAALQMRPLWKPGTAFGYHALTIGVFMEELCRRITGSTLQEIQIYEQRIRSVTGAHFGLGLPESEEPRYATLRWAADPSQPWIDPASHFGLSANSAGVDILDLPNLREVRAAGLSSAAGVASAEGMARVYAAALTGLAANGDRAAVAPLLSEETIQTVAEQVFGIDRVFGETSCFGTVFMKSHARSPYGSYRAFGHDGASASLGFDPVYELAFGYVPQQAEPEGGAGCRNLELSAAVRKAVTELAQ</protein> [Solubility Prediction Binary Classification] Will the protein generated from this sequence be soluble?

Thinking Content:

<think>

Based on the analysis of the provided protein sequence, the protein is likely soluble. Here's a concise summary of the reasoning:

1. Amino Acid Composition: The sequence contains a significant number of hydrophilic and charged amino acids such as Arginine (R), Lysine (K), Glutamic acid (E), and Aspartic acid (D). These residues promote solubility by interacting with water.

2. Absence of Long Hydrophobic Regions: While there are some hydrophobic residues, they do not form extensive stretches that could lead to aggregation or membrane insertion, which might reduce solubility.

3. No Obvious Transmembrane Domains: The sequence lacks regions indicative of transmembrane domains, which are typically hydrophobic and contribute to insolubility.

4. Presence of Charged Residues: The abundance of charged residues suggests potential for ionic interactions with water, enhancing solubility.

5. Aromatic Residues: While aromatic residues can sometimes reduce solubility, their distribution in this sequence does not appear to be a significant issue. Given these factors, the protein is predicted to be soluble.

Conclusion: The protein is likely soluble based on its composition and sequence analysis.

</think>

Answer:

The solubility task forecasts a protein's ability to dissolve in solution. This protein is highly soluble.

Reference:

This task evaluates if a protein will dissolve in a solution. Yes, this protein is soluble.

Figure 19 | Protein Solubility Prediction Example. This figure illustrates the model's reasoning for predicting protein solubility. The thinking content details an analysis of key factors, such as the high proportion of hydrophilic and charged amino acids and the absence of long hydrophobic regions or transmembrane domains, which collectively lead to the prediction of a **soluble** protein.

absolute gains appear on sequence-sequence *interaction* and *regulatory* tasks (APA, RNA-protein, antibody-antigen), indicating that pretraining most strongly enhances representations that require long-range dependencies, cross-sequence compatibility, and motif composition. Promoter detection at 300 bp benefits more than core-promoter detection at 50–100 bp, consistent with the hypothesis that broader context amplifies the value of pretraining. Language-centric tasks (function generation; structured GO terms; gene-name→cancer) also improve steadily, showing transfer from pretrained biochemical/biomedical knowledge to text- and ontology-grounded outputs.

Tab. 9 summarizes per-task results. For proportion-like metrics reported in percent in the raw logs, we rescale to [0,1][0,1]. Absolute deltas are expressed in pp for those metrics and in raw units for RMSE; relative deltas follow the usual convention of (after-before)/before(after-before)/before for higher-is-better metrics and (before-after)/before(before-after)/before for RMSE.

Task	Metric	Before	After	Δ (pp / RMSE)	Relative Δ
Promoter Detection	MCC	0.451	0.719	26.8	\uparrow 59.4%
Core Promoter Detection	MCC	0.515	0.589	7.4	\uparrow 14.4%
TF-Human	MCC	0.447	0.529	8.2	\uparrow 18.3%
ESOL	RMSE ↓	94.54	1.21	-93.33-93.33	\downarrow 98.7%
Protein Function Generation	ROUGE-L	0.755	0.823	6.7	\uparrow 8.9%
Antibody–Antigen Interaction	MCC	0.129	0.416	28.7	\uparrow 221.9%
RNA–Protein Interaction	MCC	0.507	0.865	35.8	\uparrow 70.6%
APA Isoform Usage	R2	0.311	0.879	56.8	\uparrow 182.3%
GO (CASP-SimilarSeq)	Precision	0.690	0.840	15.0	\uparrow 21.7%
GeneName → Cancer	Precision	0.610	0.740	13.0	\uparrow 21.3%

Table 9 | Ablation of pretraining on 10 tasks. Larger is better for MCC/ROUGE-L/Precision/R; lower is better for RMSE. Values are on the [0,1][0,1] scale after rescaling percent-formatted entries; “pp” denotes percentage points.

Notes. (i) Percent-like entries in the raw results (e.g., 12.92) were rescaled to proportion (e.g., 0.12920.1292). (ii) “pp” = $100 \times (\text{after}-\text{before}) = 100 \times (\text{after}-\text{before})$ for non-RMSE metrics. (iii) Relative Δ is computed with respect to the “before” score; for RMSE we report relative reduction.

5. Conclusion

We introduced a scientific language foundation model that bridges general-purpose large language modeling with the heterogeneous data and reasoning workflows of the natural sciences. Our framework couples multi-representation pre-training with instruction-driven alignment and a reasoning stage that supports both fast responses and step-by-step deliberation. By mapping natural language, DNA/RNA/protein sequences, molecular strings, and materials representations into a shared backbone via task-aware tokenization and consistent input–output schemas, the model moves beyond narrow, discipline-specific solutions and limited task menus. This design enables a single system to support four core capability families central to scientific work—property prediction/classification, sequence generation and design under constraints, scientific translation across formats, and text/knowledge extraction—while grounding its outputs through retrieval and tool execution for improved fidelity and verifiability.

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Appendix

Task	Metric	Gemini 2.5-pro	GPT o3	GPT oss	Non-LLM Expert Models	Specialist LLMs	SciReasoner-1.7B	SciReasoner-8B
Molecular Representation Translation								
SMILES to IUPAC	Top1 Split Match ↑	4.70%†	1.50%†	0.17%	—	29.00%(LlaSMol-7B [100])	<u>49.52%</u> 50.20%†	56.63% 57.10%†
SMILES to Formula	Top1 Element Match ↑	55.20%†	64.81%†	19.88%	—	93.20%(LlaSMol-7B [100])	<u>95.92%</u> 87.1%†	96.39% 96.00%†
IUPAC to SMILES	Top1 Split Match ↑	38.20%†	21.82%†	7.58%	—	70.10%(LlaSMol-7B [100])	<u>78.85%</u> 86.50%†	84.40% 90.70%†
IUPAC to Formula	Top1 Element Match ↑	88.50%†	76.50%†	33.24%	—	87.90%(LlaSMol-7B [100])	<u>91.81%</u> 88.10%†	92.65% 93.00%†
Natural Language Translation of Molecule								
Molecular Description	ROUGE-L↑	0.23	0.07	0.05	<u>0.75</u> (BioT5+ [66])	0.29(Mol-Instructions-7B [81])	<u>0.75</u>	0.78
Molecular Captioning	MENTOR↑	0.42†	0.28†	0.15	—	0.45(LlaSMol-7B [100])	<u>0.59</u> 0.59†	0.60 0.58†
Protein Functional Translation								
CASPSimilarSeq	ROUGE-L↑	0.01	0.01	0.02	—	0.74 (OPI-Galactica-6.7B [102])	<u>0.83</u>	0.85
IDFilterSeq	ROUGE-L↑	0.01	0.01	0.03	—	0.70 (OPI-Galactica-6.7B [102])	<u>0.77</u>	0.82
UniProtSeq	ROUGE-L↑	0.01	0.02	0.03	—	0.71 (OPI-Galactica-6.7B [102])	<u>0.84</u>	0.88
Mol-Instructions	ROUGE-L↑	0.21†	0.08†	0.07	0.68(BioT5+ [66])	0.44(Mol-Instructions-7B [81])	<u>0.83</u> 0.82†	0.99 0.98†

Table 10 | Evaluation results of scientific translation tasks. **Bold** indicates the best performance, and underline indicates the second best. † denotes that only randomly sampled 1000 test samples were utilized for evaluation in the corresponding task. This measure is adopted because extremely large-scale test sets exist for certain tasks, which would lead to substantial testing costs.

Task	Metric	Gemini 2.5-pro	GPT o3	GPT oss	Non-LLM Expert Models	Specialist LLMs	SciReasoner-1.7B	SciReasoner-8B
Scientific Knowledge Extraction and QA								
Chemical Entity Recognition	F1 ↑	0.71	0.66	0.55	—	0.75(Mol-Instructions-7B [81])	<u>0.81</u>	0.92
Chemical–Protein Interaction Extraction	F1 ↑	0.12	0.06	0.05	—	0.22(Mol-Instructions-7B [81])	<u>0.46</u>	0.83
Chemical–Disease Interaction Extraction	F1 ↑	0.35	0.33	0.23	—	0.40(Mol-Instructions-7B [81])	<u>0.66</u>	0.97
General Multiple Choice Question	ACC ↑	0.94	0.71	0.87	—	0.65(Mol-Instructions-7B [81])	<u>0.92</u>	0.99
True/False Question	ACC ↑	<u>0.67</u>	0.62	0.66	—	0.55(Mol-Instructions-7B [81])	0.64	0.68
Open-Ended Question	BertScore ↑	0.84	0.82	0.80	—	0.84(Mol-Instructions-7B [81])	0.83	0.87

Table 11 | Evaluation results of scientific knowledge extraction and QA tasks. **Bold** indicates the best performance, and underline indicates the second best.

Task	Metric	Gemini 2.5-pro	GPT o3	GPT oss	Non-LLM Expert Models	Specialist LLMs	SciReasoner-1.7B	SciReasoner-8B
Molecular Property Regression								
ESOL	RMSE ↓	1.28	1.58	3.45	—	1.04 (LlaSMol-7B [100])	1.21	<u>1.08</u>
LIPO	RMSE ↓	1.21	1.44	1.65	—	1.01(LlaSMol-7B [100])	<u>0.94</u>	<u>0.82</u>
Physicochemical Prediction	MAE ↓	0.027	1.879	1.329	—	0.013(Mol-Instructions-7B [81])	<u>0.003</u>	<u>0.002</u>
Material Property Regression								
MPRegression		1.32†	1.22†	0.95	5.32 (MatBERT-109M [105])	0.76(Gemma 2-9b-it:5S [105])	4.98 4.67†	<u>5.12</u> 5.21†
SNUMATRegression		1.07†	1.14†	1.00	1.83(MatBERT-109M [105])	1.16(Llama 2-7b-chat:5S [105])	2.18 2.18†	<u>1.96</u> 2.22†
JARVISDFT		1.09†	1.2†	0.88	4.10(MatBERT-109M [105])	0.70(Llama 2-7b-chat:5S [105])	<u>5.11</u> 5.28†	<u>5.21</u> 5.59†
JARVISQETB		0.53†	0.53†	0.50	59.44(LLM-Prop-35M [105])	1.05(Llama 2-7b-chat:5S [105])	138.59 148.71†	<u>126.61</u> 137.61†
GNoME	^{MAD} ^{MAE} ↑	1.28†	1.19†	0.73	15.60(LLM-Prop-35M [105])	0.50(Llama 2-7b-chat:5S [105])	<u>19.05</u> 18.46†	<u>22.03</u> 21.81†
hMOF		0.65†	0.8†	0.67	1.48 (LLM-Prop-35M [105])	0.66(Llama 2-7b-chat:5S [105])	<u>1.05</u> 1.04†	0.99 0.99†
Cantor-HEA		0.77†	0.91†	0.45	8.40 (LLM-Prop-35M [105])	0.87(Llama 2-7b-chat:5S [105])	<u>7.40</u> 7.38†	7.18 7.02†
QMOF		1.24†	1.41†	0.86	2.05(MatBERT-109M [105])	0.93(Llama 2-7b-chat:5S [105])	<u>8.55</u> 8.76†	8.07 7.94†
OQMD		1.20†	1.25†	0.65	6.02 (LLM-Prop-35M [105])	1.16(Llama 2-7b-chat:5S [105])	5.29 5.50†	<u>5.43</u> 5.67†
OMDB		0.82†	0.89†	0.93	1.55 (MatBERT-109M [105])	1.01(Llama 2-7b-chat:5S [105])	<u>1.40</u> 1.41†	1.39 1.42†
Biology Multi-omics Property Regression								
Fluorescence	Spearman ↑	-0.43†	0.78†	3.20	69.00 (ShallowCNN [120])	2.57(ChatMultiOmics-8B [85])	69.36 70.82†	66.24 68.49†
StabilityBiology-Instructions	Spearman ↑	-9.15†	-7.96	-7.79	79.00 (Evoformer [121])	60.25(ChatMultiOmics-8B [85])	63.25 55.67†	<u>64.41</u> 59.03†
Thermostability	Spearman ↑	5.47†	15.00	6.29	78.00 (ESM-1v [122])	45.07(ChatMultiOmics-8B [85])	56.25 53.17†	<u>58.55</u> 54.45†
Enhancer Activity Prediction	PCC ↑	-4.24†	0.49†	-1.29	68.00 (DeepSTARR [123])	57.24(ChatMultiOmics-8B [85])	<u>65.07</u> 70.20†	64.39 52.08†
APA Isoform Prediction	R2 ↑	0.13†	0.24†	0.01	50.82(APARENT [124])	59.01(ChatMultiOmics-8B [85])	87.94 86.19†	<u>85.87</u> 87.92†
Mean Ribosome Loading Prediction	R2 ↑	0.00†	0.00†	0.02	78.00 (Optimus [125])	47.64(ChatMultiOmics-8B [85])	50.82 54.56†	<u>60.44</u> 64.5†
Programmable RNA Switches	R2 ↑	0.01†	0.15†	0.01	55.67 (MLP-O [126])	26.65(ChatMultiOmics-8B [85])	39.00 38.1†	<u>43.55</u> 29.20†
CRISPR On Target Prediction	Spearman ↑	-3.64	-2.21	6.21	44.10 (SCC [127])	2.87(ChatMultiOmics-8B [85])	14.35	<u>25.81</u>
siRNA Efficiency Prediction	Mixed-score ↑	38.75†	34.02	40.99	49.38(Meta-Biomol [128])	42.92(ChatMultiOmics-8B [85])	62.56 64.13†	<u>59.67</u> 61.94†

Table 12 | Evaluation results of property prediction tasks. **Bold** indicates the best performance, and underline indicates the second best. † denotes that only randomly sampled 1000 test samples were utilized for evaluation in the corresponding task. This measure is adopted because extremely large-scale test sets exist for certain tasks, which would lead to substantial testing costs.

Task	Metric	Gemini 2.5-pro	GPT o3	GPT oss	Non-LLM Expert Models	Specialist LLMs	SciReasoner-1.7B	SciReasoner-8B
Molecular Classification								
BBBP	ACC@1 ↑	71.57%	78.68%	46.70%	—	75.10%(LlaSMol-7B [100])	<u>79.70%</u>	82.74%
Clintox	ACC@1 ↑	26.39%	47.92%	52.78%	—	93.10% (LlaSMol-7B [100])	<u>92.36%</u>	91.67%
HIV	ACC@1 ↑	26.7%†	77.70%†	69.86%	—	96.70%(LlaSMol-7B [100])	96.79% 92.40%†	96.81% 95.90%†
Sider	ACC@1 ↑	67.7%†	70.50%†	38.25%	—	70.70% (LlaSMol-7B [100])	<u>70.00%</u> 66.20%†	68.53% 68.70%†
Material Property Classification								
MP classification	AUC↑	0.58†	0.56†	0.53	0.72 (MatBERT-109M [105])	0.51(Gemma 2-9b-it:5S [105])	<u>0.70</u> 0.69†	0.72 0.71†
SNUMAT classification	AUC↑	0.59†	0.63†	0.60	0.72 (LLM-Prop-35M [105])	0.58(Gemma 2-9b-it:5S [105])	<u>0.69</u> 0.69	0.66 0.66
Gene-centric Association Classification								
gSymbol2Tissue	Precision↑	0.01	0.38	0.03	—	0.39(OPI-Galactica-6.7B [102])	0.41	0.41
	Recall↑	0.01	0.68	0.09	—	0.91 (OPI-Galactica-6.7B) [102]	0.82	0.83
	F1 score↑	0.01	0.45	0.04	—	0.53 (OPI-Galactica-6.7B) [102]	0.51	0.52
gSymbol2Cancer	Precision↑	0.00	0.11	0.01	—	0.36(OPI-Galactica-6.7B [102])	<u>0.75</u>	0.81
	Recall↑	0.00	0.10	0.02	—	0.32(OPI-Galactica-6.7B [102])	<u>0.72</u>	0.81
	F1 score↑	0.00	0.10	0.01	—	0.32(OPI-Galactica-6.7B [102])	<u>0.73</u>	0.81
gName2Cancer	Precision ↑	0.00	0.11	0.01	—	0.27(OPI-Galactica-6.7B [102])	<u>0.68</u>	0.80
	Recall ↑	0.00	0.10	0.04	—	0.26(OPI-Galactica-6.7B [102])	<u>0.67</u>	0.79
	F1 score ↑	0.00	0.10	0.01	—	0.25(OPI-Galactica-6.7B [102])	<u>0.67</u>	0.79

Table 13 | Evaluation results of molecular classification tasks, material property classification tasks, and gene-centric association classification tasks. **Bold** indicates the best performance, and underline indicates the second best. † denotes that only randomly sampled 1000 test samples were utilized for evaluation in the corresponding task. This measure is adopted because extremely large-scale test sets exist for certain tasks, which would lead to substantial testing costs.

Task	Metric	Gemini 2.5-pro	GPT o3	GPT oss	Non-LLM Expert Models	Specialist LLMs	SciReasoner 1.7B	SciReasoner 8B
Keywords (CASPSimilarSeq)	Precision↑	0.04	0.21	0	-	0.81(OPI-Galactica-6.7B [102])	<u>0.83</u>	0.86
	Recall↑	0.03	0.19	0.02	-	0.74(OPI-Galactica-6.7B [102])	<u>0.80</u>	0.83
	F1↑	0.03	0.19	0.01	-	0.76(OPI-Galactica-6.7B [102])	<u>0.81</u>	0.84
Keywords (IDFilterSeq)	Precision↑	0.03	0.17	0	-	0.84(OPI-Galactica-6.7B [102])	<u>0.86</u>	0.89
	Recall↑	0.02	0.16	0.02	-	0.80(OPI-Galactica-6.7B [102])	<u>0.85</u>	0.89
	F1↑	0.01	0.16	0.01	-	0.82(OPI-Galactica-6.7B [102])	<u>0.85</u>	0.88
Keywords (UniProtSeq)	Precision↑	0.01	0.2	0.01	-	0.86(OPI-Galactica-6.7B [102])	<u>0.85</u>	0.92
	Recall↑	0	0.18	0.03	-	0.82(OPI-Galactica-6.7B [102])	<u>0.90</u>	0.91
	F1↑	0	0.18	0.01	-	0.83(OPI-Galactica-6.7B [102])	<u>0.88</u>	0.91
GO Terms (CASPSimilarSeq)	Precision↑	0	0	0	-	0.76(OPI-Galactica-6.7B [102])	<u>0.81</u>	0.86
	Recall↑	0	0	0	-	0.74(OPI-Galactica-6.7B [102])	<u>0.81</u>	0.86
	F1↑	0	0	0	-	0.75(OPI-Galactica-6.7B [102])	<u>0.80</u>	0.86
GO Terms (IDFilterSeq)	Precision↑	0	0	0	-	0.74(OPI-Galactica-6.7B [102])	<u>0.78</u>	0.83
	Recall↑	0	0	0	-	0.73(OPI-Galactica-6.7B [102])	<u>0.77</u>	0.82
	F1↑	0	0	0	-	0.72(OPI-Galactica-6.7B [102])	<u>0.77</u>	0.81
GO Terms (UniProtSeq)	Precision↑	0	0	0	-	0.76(OPI-Galactica-6.7B [102])	<u>0.84</u>	0.88
	Recall↑	0	0	0	-	0.74(OPI-Galactica-6.7B [102])	<u>0.82</u>	0.87
	F1↑	0	0	0	-	0.74(OPI-Galactica-6.7B [102])	<u>0.81</u>	0.86

Table 14 | Evaluation results of biology multi-omics property classification tasks. Dashed lines separate tasks that report multiple metrics (Precision/Recall/F1). **Bold** indicates the best performance, and underline indicates the second best.

Task	Metric	Gemini 2.5-pro	GPT o3	GPT oss	Non-LLM Expert Models	Specialist LLMs	SciReasoner 1.7B	SciReasoner 8B
Unconditional Generation								
Unconditional Molecular Generation	Validity ↑	0.568	0.715	0.952	—	0.968(NatureLM-8B [82])	0.864	0.971
	Unique ↑	0.042	0.364	0.318	—	0.966(NatureLM-8B [82])	0.988	0.982
Unconditional Protein Generation	Avg. Length↑	128.87	153.56	318.91	—	284.50(NatureLM-8B [82])	280.10	<u>284.7</u>
	Diversity↑	0.62	<u>0.99</u>	1.00	—	0.97 (NatureLM-8B [82])	1.00	0.91
	Validity↑	0.93	<u>0.97</u>	0.99	—	—	0.80	0.99
Unconditional RNA Generation	Avg. MFE↓	N/A	-151.70	-417.58	—	-177.1(NatureLM-8x7B [82])	-178.85	-200.14
Unconditional Material Generation	SMACT↑	89.70	N/A	N/A	—	66.07(NatureLM-8x7B [82])	55.06	<u>88.18</u>
Conditional Material Generation								
Composition to Material Generation	SMACT ↑	N/A	N/A	N/A	—	83.36(NatureLM-8B [82])	86.07	<u>85.85</u>
	Precision ↑	N/A	N/A	N/A	—	98.44(NatureLM-8B [82])	<u>99.89</u>	99.96
	Novelty ↓	N/A	N/A	N/A	—	97.13 (NatureLM-1B [82])	<u>85.64</u>	84.81
Bulk to Material Generation	SMACT ↑	N/A	N/A	N/A	—	94.75 (NatureLM-8x7B [82])	<u>88.92</u>	87.49
	Success rate	N/A	N/A	N/A	—	—	<u>7.12</u>	<u>7.05</u>
Conditional Small Molecular Generation								
Forward Synthesis Prediction	Exact Match ↑	0.32†	0.27†	0.33	—	0.63(LlaSMol-7B [100])	<u>0.69</u> 0.81	0.75 0.83
Forward Reaction Prediction	Exact Match ↑	0.55	0.58	0.36	0.86(BioT5+ [66])	0.54(InstructMol-GS-6.9B [137])	<u>0.96</u>	0.99
Reagent Prediction	Exact Match ↑	0.04	0.01	0.00	0.26 (BioT5+ [66])	0.13(InstructMol-GS-6.9B [137])	0.19	<u>0.22</u>
Retrosynthesis _{Mol-Instructions}	Exact Match ↑	0.20	0.16	0.05	0.64(BioT5+ [66])	0.41(InstructMol-GS-6.9B [137])	<u>0.72</u>	0.83
Retrosynthesis _{USPTO-50K}	Exact Match ↑	0.23†	0.07†	0.12	0.61(EditRetro [138])	<u>0.70</u> (NatureLM-8B [82])	0.68 0.72	0.72 0.74
Retrosynthesis _{SMol-Instruction}	Exact Match ↑	0.12†	0.04†	0.08	—	0.33(LlaSMol-7B [100])	<u>0.41</u> 0.43†	0.46 0.47†
Molecule Generation	Exact Match ↑	0.25†	0.16†	0.03	—	0.19(LlaSMol-7B [100])	0.39 0.34†	0.48 0.46†
Description-Guided Molecule Design	Exact Match ↑	0.06	0.04	0.04	<u>0.11</u> (MolT5 [139])	0.002(Mol-Instructions-7B [81])	0.10	0.12
Conditional Biochemical Generation								
Function-guided Protein Design	Max. Normalized SW ↑	0.00†	0.00†	0.00†	<u>0.97</u> (BioT5+ [66])	0.43(Mol-Instructions-7B [81])	0.96 0.90†	1.00 1.00†
Catalytic Activity	ROUGE-L ↑	0.25†	0.09†	0.02	0.72(BioT5+ [66])	0.52(Mol-Instructions-7B [81])	<u>0.77</u> 0.78†	0.99 0.95†

Table 15 | Evaluation results of generation and design tasks. N/A indicates that the model cannot generate samples that meet the required specifications. **Bold** indicates the best performance, and underline indicates the second best.

Protein Generation



Figure 20 | Additional Visualization for Protein Generation task (a).

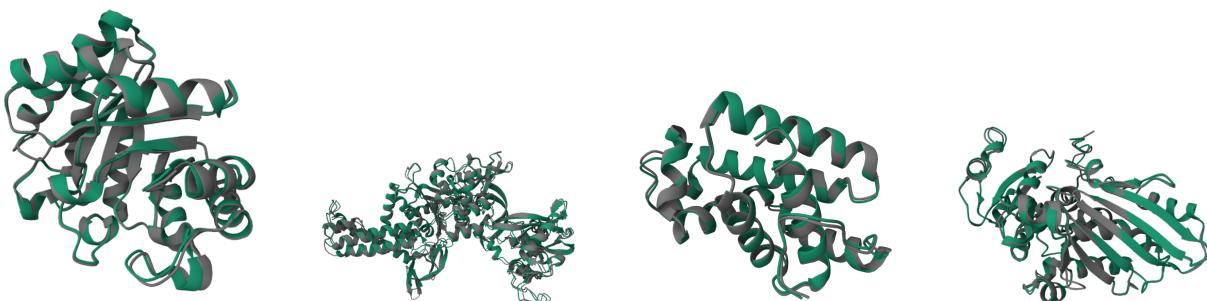


Figure 21 | Additional Visualization for Protein Generation task (b).

Translation between SMILES and IUPAC

Create Date: 2025-07-28

SMILES: C[C@H](C(=O)N[C@H](CC1=CC=CC=C1)C(=O)C(=O)NCC2=CC=CC=N2)NC(=O)C3=CC(=C(C=C3)Cl)Cl

Reference: 3,4-dichloro-N-[(2R)-1-[(2R)-3,4-dioxo-1-phenyl-4-(pyridin-2-ylmethylamino)butan-2-yl]amino]-1-oxopropan-2-yl]benzamide

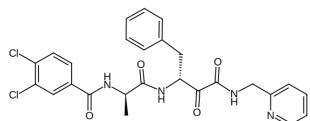
Our output: **3,4-dichloro-N-[(2R)-1-[(2R)-3,4-dioxo-1-phenyl-4-(pyridin-2-ylmethylamino)butan-2-yl]amino]-1-oxopropan-2-yl]benzamide**

GPT-5: (2S)-2-[[[(2S)-2-benzyl-3-(pyridin-2-ylmethylcarbamoyl)propanoyl]amino]-N-(3,4-dichlorophenyl)propanamide

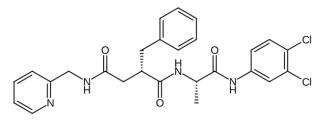
Mol-Instruct: (2Z,5Z)-2-chloro-5-[2-[(2Z,5Z)-2-chloro-5-[(2-methyl-3-oxo-3-phenylpropanoyl)amino]penta-2,4-dienoyl]-3-oxo-3-

phenylpropanoyl]penta-2,4-dienoic acid

Gemini2.5-Pro: (4S)-4-{(2S)-2-(3,4-dichlorobenzamido)propanamido}-4-phenyl-N-(pyridin-2-ylmethyl)-2,3-dioxobutanamide



Ours



GPT-5

Figure 22 | Additional Visualization for SMILES-to-IUPAC Translation task

Task Examples

Example 1:

Prompt: How soluble is <SMILES> CC(C)C1 </SMILES> ?

Response: Its log solubility is -1.41 mol/L.

ESOL This task has 112 test samples.

Example 1:

Prompt: Predict the octanol/water distribution coefficient logD under the circumstance of pH 7.4 for <SMILES> NC(=O)C1=CC=CC=C1O </SMILES> .

Response: 1.090

LIPO This task has 420 test samples.

Example 1:

Prompt: Is blood-brain barrier permeability (BBBP) a property of <SMILES> CCNC(=O)/C=C/C1=CC=CC(Br)=C1 </SMILES>?

Response: Yes

BBBP This task has 197 test samples.

Example 1:

Prompt: Is <SMILES> COC[C@H] (NC(C)=O)C(=O)NCC1=CC=CC=C1 </SMILES> toxic?

Response: No

Clintox This task has 144 test samples.

Example 1:

Prompt: Can <SMILES> CC1=CN(C2C=CCCC2)C(=O)NC1=O </SMILES> serve as an inhibitor of HIV replication?

Response: No

HIV This task has 4107 test samples.

Example 1:

Prompt: Are there any known side effects of <SMILES> CC1=CC(C)=C(NC(=O)CN(CC(=O)O)CC(=O)O)C(C)=C1Br </SMILES> affecting the heart?

Response: No

SIDER This task has 2860 test samples.

Example 1:

Prompt: You are a material scientist. Look at the chemical formula of the given crystalline material and predict its property. The output must be in a json format. For example: {property_name:predicted_property_value}. Answer as precise as possible and in as few words as possible.chemical formula: KPrMnNb06property name: volume
Response: {volume : 128.62405239223665}

MP_{regression} This task has 82241 test samples.

Example 1:

Prompt: You are a material scientist. Look at the chemical formula of the given crystalline material and predict its property. The output must be in a json format. For example: {property_name:predicted_property_value}. Answer as precise as possible and in as few words as possible.chemical formula: Na2Ti3Cl8property name: Band_gap_HSE
Response: {Band_gap_HSE : 1.583856}

SNUMAT_{regression} This task has 4152 test samples.

Example 1:

Prompt: You are a material scientist. Look at the chemical formula of the given crystalline material and predict its property. The output must be in a json format. For example: {property_name:predicted_property_value}. Answer as precise as possible and in as few words as possible.chemical formula: YReW208property name: formation_energy_peratom
Response: {formation_energy_peratom : -2.15925}

JARVISDFT This task has 54647 test samples.

Example 1:

Prompt: You are a material scientist. Look at the chemical formula of the given crystalline material and predict its property. The output must be in a json format. For example: {property_name:predicted_property_value}. Answer as precise as possible and in as few words as possible.chemical formula: BeMoRhproperty name: final_energy
Response: {final_energy : -169.1866374093}

JARVISQETB This task has 249596 test samples.

Example 1:

Prompt: You are a material scientist. Look at the chemical formula of the given crystalline material and predict its property. The output must be in a json format. For example: {property_name:predicted_property_value}. Answer as precise as possible and in as few words as possible.chemical formula: Yb3Eu7(TlPd2)2property name: Density
Response: {Density : 8.2778}

GNoME This task has 216455 test samples.

Example 1:

Prompt: You are a material scientist. Look at the chemical formula of the given crystalline material and predict its property. The output must be in a json format. For example: {property_name:predicted_property_value}. Answer as precise as possible and in as few words as possible.chemical formula: Zn4C84N16H22O17property name: max_co2_adsp
Response: {max_co2_adsp : 8.95639}

hMOF This task has 92925 test samples.

Example 1:

Prompt: You are a material scientist. Look at the chemical formula of the given crystalline material and predict its property. The output must be in a json format. For example: {property_name:predicted_property_value}. Answer as precise as possible and in as few words as possible.chemical formula: Al2Co1Cr1Mn1Ni2Si1property name: e_above_hull
Response: {e_above_hull : 0.4014893125}

Cantor-HEA This task has 33608 test samples.

Example 1:

Prompt: You are a material scientist. Look at the chemical formula of the given crystalline material and predict its property. The output must be in a json format. For example: {property_name:predicted_property_value}. Answer as precise as possible and in as few words as possible.chemical formula: Zn12C48H88O80property name: lcd
Response: {lcd : 3.40559}

QMOF This task has 3064 test samples.

Example 1:

Prompt: You are a material scientist. Look at the chemical formula of the given crystalline material and predict its property. The output must be in a json format. For example: {property_name:predicted_property_value}. Answer as precise as possible and in as few words as possible.chemical formula: Sm₂CuH₆property name: e_form
Response: {e_form : -0.3328793676}

OQMD This task has 192799 test samples.

Example 1:

Prompt: You are a material scientist. Look at the chemical formula of the given crystalline material and predict its property. The output must be in a json format. For example: {property_name:predicted_property_value}. Answer as precise as possible and in as few words as possible.chemical formula: C₄H₅(CH)₃(CH₂)₃C₅H₅NCH₃C₃NH₄H₃(CO)2C₄NH₄SO₂property name: bandgap
Response: {bandgap : 2.886436}

OMDB This task has 1213 test samples.

Example 1:

Prompt: Please evaluate the following protein sequence and provide an explanation of the enzyme's catalytic activity, including the chemical reaction it facilitates: <protein>MVKKRIAVIGAGISGLGAIKCCCLDEDLEPTCFERNDDIGGLWKFQKNASEKMPSIYRSVTINTSKEMMCFSDFPIPDPHFPNYMHNSKLMFYFRMYAKRFSLLDYIRFKTTVRSVRKPDFHIHGQWDVVVETDGKQESLVFDGVLCGSHHTDPHLPLKSFPGIEKFEGCYFHSREYKSPEDYVGKRIIVVGIGNSGVDIAVELGRVAKVFLSTRRGSWILHRVWNNGYPMDSSFFTRFHSFLQKILTTEAVNKYLEKTLNSRFNHAHYGLQPQHRLSQHPTISDDLPHIISGKVQVKPNKEFTGTDVHFDDGTVEENIDVVIFATGYSISFPFLGDLIAVTDNEVSLYKLMFPPDLEKPTLAVIDGLIQPLGIILPIAELQSRWAVRVFKGLSKLPSVKAMKADMDQRKKAMEKRYVKTARHTIQVDHIEYMDEIASLAGVKPNLLLFLSDPTLAMEVFFGPCTPYQYRLQGPGKWDGARRAILTQRERIIKPLKTRITSEKSRSAPGLFWIKMALGLAFLVPSLTYSYICQ</protein>
Response: Upon reviewing the provided protein sequence, the corresponding enzyme's catalytic activity is identified as the following chemical reaction: H(+) + hexan-3-one + NADPH + O₂ = ethyl butanoate + H₂O + NADP(+).

Catalytic Activity This task has 1601 test samples.

Example 1:

Prompt: Can you give me the energy difference between the HOMO and LUMO orbitals of this molecule? <SMILES> O=C1OCC2CC1C2 </SMILES>
Response: 0.2756

Physicochemical Prediction This task has 1999 test samples.

Example 1:

Prompt: <protein>SKGEELFTGVVPILVELGDVNGHKFSVSGEGEGDATYGKLTGKFICTTGKLPVPWPTLVTTLSYGVQCFSRYPDHMKQHDFFKSAMPEGYVQERTIFFKDDGNYKTRAEVRFEGDTLVNRIELKGIDFKEDGNLGHKLEYNYNSHNVYIMADKQKIGIKVNFRIRHNIEDGSVQLADHYQQNTPIGDGPVLLPDNHYLSTQSALSKDPNEKRDMVLLEFVTAAAGITHGMDELYK</protein> [Fluorescence Prediction Regression] What is the anticipated fitness of this green fluorescent protein mutant?

Response: The fluorescence intensity for this GFP mutant is calculated as 3.67.

Fluorescence This task has 27217 test samples.

Example 1:

Prompt: <protein>TTIKVNGQEYTVPLSPEQFAAKKRWPDYEVQIHGNTVKVTR</protein> What is the expected stability score for this sequence?

Response: The stability score determined for this sequence is 0.53.

Stability This task has nan test samples.

Example 1:

Prompt: <protein>MNYARFITAASAARNPSPIRTMTDILSRGPKSMISLAGGLPNPNMFPFKTAVITVENGKTIQFGEEMMKRALQYSPSAGIPELLSWLKQLQIKLHNPPTIHYPPSQGQMDLCVTSGSQQGLCKVFEMIINPGDNVLLDEPAYSGTLQSLHPLGCNIINVASDESGLIPDSLRDILSRWKPEDAKNPQKNTPKFLYTVPNGNNPTGNSLTSERKKEIYELARKYDFLIIEDDPYYFLQFNKFRVPTFLSMDVDGRVIRADFSKIISSGLRIGFLTGPKPPLIERVILHIQVSTLHPSTFNQLMISQLLHEWGEEGFMAHVDRVIDFYSNQKDAILAAADKWLTLGLAEWHVPAAGMFLWIKVKGINDVKELIEEKAVKMGVLMPLPGNAFYVDSSAPSPYLRASFSSASPEQMDVAFQVLAQLIKESL</protein> The task evaluates protein thermostability using mass spectrometry to measure melting points in human cells. How is the thermostability of this protein assessed?

Response: The task uses mass spectrometry to measure protein melting curves and predict thermostability in human cells. The thermostability measure recorded for this protein is 56.77

Thermostability This task has 1336 test samples.

Example 1:

Prompt: < dna > TGTGCGCTCCATTCTGTCATGTTGCGTGTAAATTGCGCTTCTGGCGGCTATTTTGTATTTGTTGCCGCTTACACTTCACATTTGCCCTCGGGGGCGTCGTTAAAAAAACGCACACACACACTCGCGCATTCACATATTATTTGGTTCTCCAACTTGTACGCTCTGCGTTCTTC</ dna > [Regression: Enhancer activity prediction] Please provide an enhancer activity prediction for this sequence.

Response: The enhancer activity prediction yields: HK -0.68, Dev -1.26

Enhancer Activity Prediction This task has 41186 test samples.

Example 1:

Prompt: <rna>CTGCTTGGAGTTACATTGAGGAAGCTGGTAAGTACGCTCAAAGCTAAAATATAAAAC
TATTGGAGTATGAAACGATGTCGTGACTGGTGTACCCCTATCCCTGTGACGTTGGCCTCTGACAATACTGGTA
TAATTGTAAATAATGTCAAACCTCCGTTTAGCAAGTATTAAGGGA</rna> [Isoform prediction]

What is the likelihood that this sequence ends in a proximal isoform?

Response: The processing of 3' UTR regions in the sequence results in a proximal isoform proportion of 0.33.

APA Isoform Prediction This task has 49755 test samples.

Example 1:

Prompt: <rna>TAATCGTTCTAAATACGATTAGTG</rna> What ribosome loading rate is expected from the sequence?

Response: The sequence impacts ribosome loading during translation initiation with an efficiency of 0.63

Mean Ribosome Loading Prediction This task has 7600 test samples.

Example 1:

Prompt: <rna>GGGCTTGGGAAAGTGGACAGAGATGATTATTAAACCAAACACAAACGCACAA
TCATCTCTGCCACTTCCCCAAGAACAGAGAGACTTGGATGAGTGGACAGAACCTGGCGGC
AGCGCAAAAGATGCGTAAAGGAGAA</rna> [Programmable RNA switches prediction] How does the sequence influence the ON and OFF states of the RNA switch?

Response: The RNA switch with this sequence is predicted to have an ON state of 0.02, an OFF state of 0.47, and an ON/OFF ratio of 0.06

Programmable RNA Switches This task has 9154 test samples.

Example 1:

Prompt: <rna>TTCACTGCGCAGCCTGGCATTGG</rna> What gene disruption success rate is associated with the sequence?

Response: The predicted gene disruption level for this sequence is 0.26.

CRISPR On Target Prediction This task has 416 test samples.

Example 1:

Prompt: <sirna>a Af a c u Uf g a a u g a a Af c Gf a c u u c u c</sirna>
<rna>ACGTACCTGAGATCTACGGGGCTGGAGCACCTGAAGACTCAAGACCAAAAGACTGTCAGGA
AGGCAGAGTCAGAGCAATCCACTGTCCAAGACCACACGACTTCGAGAACGGGAATACTGGCCCCGGTCTCCCTACTAC
AATGTGAGTGATGAGATCTCTTCCACTGCTATGACGGTTACACTCTCCGGGGCTCTGCCAATCGCACCTGCCAAGTGAA
TGGCCGATGGAGTGGCAGACAGCGATCTGTGACAACGGAGCGGGGACTGCTCCAACCCGGCATCCCCATTGGCACAA

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GGAAGGTGGCAGCCAGTACCGCCTTGAAGACAGCGTCACCTACCCTGCAGCCGGGGCTTACCCCTGCGTGGCTCCCAG
CGCGAACGTGTCAGGAAGGTGGCTTGGAGCGGGACGGAGCCTCCTGCCAAGACTCCTCATGTACGACACCCCTCA
AGAGGTGGCCGAAGCTTCCTGTCTCCCTGACAGAGACCATAGAAGGAGTCGATGCTGAGGATGGCACGGCCCAGGGG
AACAAACAGAAGCGGAAGATCGTCCCTGGACCCCTCAGGCTCCATGAACATCTACCTGGTCTAGATGGATCAGACAGCATT
GGGGCCAGCAACTTCACAGGAGCCAAAAAGTGTCTAGTCAACTTAATTGAGAAGGTGGCAAGTTATGGTGTGAAGCCAAG
ATATGGTCTAGTGACATATGCCACATACCCAAAATTGGTCAAAGTGTCTGAAGCAGACAGCAGTAATGCAGACTGGG
TCACGAAGCAGCTCA</rna> What is the likely mRNA remaining percentage after siRNA treatment?
```

Response: The sequence leads to an mRNA remaining percentage of 28.00 after siRNA treatment.

siRNA Efficiency Prediction This task has 6688 test samples.

Example 1:

Prompt: You are a material scientist. Look at the chemical formula of the given crystalline material and predict its property. The output must be in a json format. For example: {property_name:predicted_property_value}.
Answer as precise as possible and in as few words as possible.
chemical formula: KPrMnNb06
property name: is_stable
Response: {is_stable : False}

MP_{classification} This task has 20575 test samples.

Example 1:

Prompt: You are a material scientist. Look at the chemical formula of the given crystalline material and predict its property. The output must be in a json format. For example: {property_name:predicted_property_value}.
Answer as precise as possible and in as few words as possible.
chemical formula: PbS
property name: SOC
Response: {SOC : True}

SNUMAT_{classification} This task has 4152 test samples.

Example 1:

Prompt: Please conduct a domain/motif search on the given protein sequence and provide your findings. The sequence is:
<protein>MGTTTHKFDRPLPPLPCPFSEVNPYVEQVDKETLEWLIDSEMLDDAETVERYRQAKYGWLSARTYP
YAEHHTLRLVSDWCWVLFAFDDAFCESDRRAEIRALPQLYAVLEDLDVGSEVDDVFAKSLLIEKGRIAAYGDDEQLD
RWRNVTKDYLFAQVWEAANREDEVVPSLEDYIFMRRRTGAMLTVFALIDVASGRSLSADEWRHPGMRAITESANDVVV
DNDLISYAKESNSGNRNNLVNLAEHRHYSRQEAMEEIGEMRNQAIADMVAVRPSLEALGSDAVLAYVRGLEFWISGSV
DYSLTSSRYTDARWTARQPSIR</protein>
Response: Based on computational analysis, the provided sequence potentially contains the following protein domains or motifs: DDXXXE motif domains

Domain/Motif This task has 1400 test samples.

Example 1:

Prompt: Analyze the following amino acid sequence, and determine the function of the resulting protein, its subcellular localization, and any biological processes it may be part of:

<protein>MANHKSTQKSIRQDQKRNLINKSRKSNVKTFLKRVTLAINAGDKVASEALSAHSKLAKAANKG
IYKLNTVSRKVSRLSRKIKQLEDKI</protein>

Response: The protein with the amino acid sequence is expected to exhibit rRNA binding, structural constituent of ribosome, contributing to the translation. It can be typically found in the ribonucleoprotein complex, ribosome of the cell.

Protein Function This task has 3494 test samples.

Example 1:

Prompt: <protein>MPLGLFSSGKAQVLCDEKIPGGKKKEPKQLSENCKGVTLKLDHTRVTIEKQIAE
GGFAIVYVASDRKNNKFALKRQFTKDNEKQLEACCREHSFLKCIGHKNIVEFVDSYTNCNGIWECMLTEYHQKNVL
QLMNERISQNQYLTNDEILSIFTDLCEAVSFIHNRQPPIIHRDLKVENVLISSHKPPHYVLCDFGSATTQILSVEKYGV
YVKSEVERNTTMCYRSPEMIDFYSGLEIGLKSDIWLGVLLYRLCCFCVPFEESPLAIQSVNYQFPSVPNIPDEIKVLIY
MLLDIDVNRRPSIYQTSLVLAFAEANHRKPSEEIQNKKCTDAVPSLKSCIQLMRDGNSPRNKRDSSPRNPEAPPIQSSSKM
ASLSQQVPSISNISMPSGSGTVETSVAPRLRPKATTVVNPVPSISPVPPVGLPHRLRPSKGSTDDETGSQVRKVPIDFHH
RQSFSGEEQLKPAAEADSAGPLSCPLIKPTDGLFTDLDKPALPRDRAQTDGKRRLPHESDIIIFQQQHRRNVSDTSQISRS
AFKPYSSQQTTSKTSSQVVRSEDMSQRQNGSGEWNPFLVAPFSNNNSISRKGQESAFMMDDSHFGMFDEIRRKEIPA
ELDSETSSIDSRDGPFGAAPFDQLTVSTSSAQPVSLPPGSVHLHTSIAPSPLRHVLTKAPPPVPRRTTSRGFQV</protein>

Response: The protein predicted from this sequence is not soluble.

Solubility This task has 2001 test samples.

Example 1:

Prompt: <protein>MGSSHHHHHHSQDLENLYFQGSMNIFEMLRIDEGLRLKIYKDTEGYYTIGIGHLL
TKPSLNAAKSELDKAIGRNTNGVITKDEAEKLFNQDVDAAVRGILRANKPVYDSLAVRRAALINMVFMGETGVAG
FTNSLRMLQKRWDEAAVNLAKSRWYNQTPNRTKRVITTFRTGTWDAYKNLRKLEQLYNRYKDPQDENKIGIDGIQQFC
DDLALDPASISVLIIAWKFRAATQCEFSKQEFDGMTELGCDSIEKLKAQIPKMEQELKEPGRFKDFYQFTFNFAKNPGQ
KGKLDLEMAIAWNLVLNGRFKFLDLWNKFLLEHHKRSIPKDTWNLLDFSTMIAADMSNYDEEGAWPVLIDDFVEFARPQ
IAAGTKSTTV</protein> [EC Number Prediction Multilabel Classification] What are the donor and acceptor molecules in this enzyme's reaction?

Response: Donor molecules utilized by enzymes are identified by their EC numbers. Donor molecules it utilizes are identified by EC number EC3.2.1.17, EC3.2.1.-.

Function-EC This task has 1919 test samples.

Example 1:

Prompt: Ab-Ag interaction detection: Any binding between

<protein>EVQLVESGANVVRPGGSLRLSCKASGFIFENFGFSWVRQAPGKGLQWAGLNWNGGDTRYADSVKGRFRMS

RDNSRNFVYLDMDKVGVDATFYYCARGTDYTIIDAGIHYQGSGTFWYFDLWGRGLTVSSXEIVLAQSPGTLSPGE RATLSCRASHNVHPKYFAWYQQKPGQSPRLIYGGSTRAAGIPGKFGSGSGTDFLTISRVDPEDFAVYYCQQYGGSPY TFGQGTKVEIKX</protein> and <protein>MRVMGIQKNYPPLWRGMIIIFWIMMICNAKQMWTQVYYGVPVWR DASTTLFCASDAKAYDPEAHNAWATHACVPTDPNPQEMQLKNVTENFMWKNMDVEQMHDVIISLWDQSLKPCVKLTPLC VTLNCTDVRNRTLNYYNNSTSNSLVSSDMEGEIKNCFSNMTTEL RDKNQKVYALFYRQDVIQNGNNNSYYRLINCNT SAMTQACPVSFNPIIHYCAPAGFAILKNDKEFNGTGPCKNVSTVQCTHGIKPVISTQLLNGSIAEEEIVIRSENIT NNAKTIIVQLNEPVEINCTRPNNTKSVRIGPGQTFYATGDIIGNIRQAHCNCNSRAKWNELHKVAEQLRTYFKNKTIIF TNHSGGDVELKTHMFNCGEFFYCNTTALFNSTWDNNSTREDNNSTGNDTITLQCRIKQIVRMWQRSGQAMYAPPIQGV IKCKSNITGLLTRDGGNNESTNETFRPGGGDMRDNRSELYKYKVVKIEPLGVAPTHAKRRVVQREKRAVGLGAVFFGF LGAAAGSTMGAASITLTQARQLLSGIVQQQSNLLKATEAQHQHLLKLTVWGIKQLQARVLAERYLGDDQQLGIWGCSGKL ICTTNVPWNSSWSNKTYGDIWDNMWLQWDKEISNYTNIIYALIEESQNQQEKENQDLLALDKWASLWNWFDISKWLWYIKIFIMIVGGLIGLIRIVFTIITIINRVRQGYSPLSFQTLHHQREPDRPERIEEEGGEQDKDRSIRLVGGFLALA WADDLRNLCLFIYHRLDFVLIAARAVSLLGHSSLKGLRLGWEALKYLWNLLAYWGKELKNSAVNLLDTVAIAVANWTDRVIEIGQR AGRAILNIPRRIRQGAERALV</protein>?

Response: Yes. Based on their primary structures, a physical interaction appears plausible.

Antibody-Antigen This task has 3301 test samples.

Example 1:

Prompt: I need to know if <rna>TGCTTCGTGCTTGCTGAAGTTAACCCGGCGGGGAACGA TTGTTCCCACGTGTTCCCACAGGAGAACCCCTGGAGACACTACCTTCCCACAGAATTCAAGGAGCTCAAAG GCCAGGAAATCTTTGAAAGGTACCATCTACCTGGAGGGCATCATCCTGAGTGAAGAGGACAAGCAAAAAGAGGAATGGA AGACTAGATAACACAGCTAAATGGAAGGAGAACCTCTGGCCTAAATGCAATAAGGAAATCTATGGCTACCGAGAGCAC AGGACACTCCTGACATTGTGTAACCCAAAGATAGAAACATGCAATTGTGCTACATGCCCTCCAGGCTCTGGAAAAACCA CAATGGCAAAGCAGCTAATGTTAGAATGGTCAGAGCGTAAGCAGGCCAGATTTCATGTGCCTTACATCAGCTGC AGGAAAGTAAATAACTAAACTTGCACTTTGCCCACCTCCTCCATGGACAATCC</rna> has any functional or structural interaction with <protein>HVLFEHAVGYALLALKEVEEISLLQPQVE ESVNLGKFHSIVRLVAFCPFASSQVALENANA VSEGVVHEDLRLLETHLPSKKKVVLLGVGDPKIGAAIQEELGYNQ TGIVAEILRGVRLHFHNLVKGLTDLACKAQLGLGHSYSRAKVFNVNRVDNMIIQSISSLQDKDINTFSMRVREWY GHFPELVKIINDNATYCRLAQFIGNRRELNEKDLEKLEELTMDGAKAKAILDASRSSGMMDISAIDLINIESFSSRVV SLEYRQSLHTYLRSKMSQVAPSL SALIGEAVGARLIAHAGSLTNLAKYPASTVQILGAEKALFRALKTRGNTPKYGLIFH STFIGRAAAKNGRISRYLANKCSIASRIDCFSEVPTSVFGEKLREQVEERLSFYETGEIPRKNLDMKEAMVQAEEAAA EITRKLEKQEKKRLKKKK</protein>.

Response: The interaction between the RNA and protein is predicted to be positive.

RNA-Protein This task has 4164 test samples.

Example 1:

Prompt: < dna > CAACGGTACCCAATGGTCCATCTCTAACATCGTTAGGGCCAATCGTGGCGGTATGCTA TTGTCACCTTCATCTCGTGTCTCCTCACTCAACTGAAAGTGGAGAACATTATTGTGCAATTGTGAAACCTCCAGC ATTGGAAAATCTGTGTTTAAGCTGGTGACCTGAAACCAAAAACAAGAAACATTGAAATGCAATGGCGGAGTGTAGTG AAGGAACAGCACCAACACAATAGGAGACATGTGAAATCCTTAGTGTCAAATGAGTACCCAAATGGCTATCTACTCTT ATCAAACCGGCAGCAAACCCCTCTGGGTAAATTAAACATGTTGGTGTCAATACCGTACAGATGAGTAAACCATGG GGAGGCCATTGGAACAAGCAGATGGTAAGGACCCCCCTATATTGTAAATCCTAGGGCAAAACTAAAGCATTAAAG TCCCCGGTGGTGGAGACGTATAAGTACAGCTGTTAAA</ dna > [Classification: epigenetic marks prediction] I need help with an Epigenetic Mark Prediction task. Here's

the sequence:

Response: EMP, or Epigenetic Marks Prediction, aims to identify epigenetic changes, successfully confirmed in yeast DNA sequences.

Epigenetic Marks Predictions This task has 28741 test samples.

Example 1:

Prompt: < dna > CTGCTGCTGCTGCTGGCTCTGGCTTTGTTGATGGTACATCATCATTAAAAAAA
 AACATATGCTGATCACTGTATGAAAGTTCAACAATGTTAGTG </ dna >: I need a detailed review of transcription factor binding sites in this DNA sequence.

Response: Upon examination, I can confirm that the mouse DNA sequence piece contains TF binding sites, which is crucial for gene expression.

TF-Mouse This task has 10005 test samples.

Example 1:

Prompt: < rna > AGCTACGGCCATATCACCTGAACATGCCTGATCTCGTCTGATCTCAGAAGCTAAC
 GGTAGGGCCTGGTTAGTAGTACTGGATGGAAGACCACCTGGGAATACCAGGTGCTGTAGGGG </ rna > How would you classify this sequence within non-coding RNA classes?

Response: The RNA sequence is categorized under the 5S_rRNA family based on its structural characteristics.

Non-coding RNA Function Classification This task has 2600 test samples.

Example 1:

Prompt: < rna > TAAAGCACTAACATAACATAACTTACTGTGGCTCAGAGTAAGCGCTTAGTAAAAATTGG
 AGTTATTTCAATAGATTCTATTCTATAATAAGGAGAAA </ rna > What does the sequence indicate about its potential RNA modifications? Please choose from the following options: ['Am', 'Cm', 'Gm', 'Um', 'm1A', 'm5C', 'm5U', 'm6A', 'm6Am', 'm7G', 'Psi', 'AtoI', 'none']

Response: AtoI. The RNA modifications predicted for the sequence are AtoI.

Modification Prediction This task has 1200 test samples.

Example 1:

Prompt: Analyze the interaction potential between < dna > CCTCCTGGGCTGTTACCAAGAG
 CCTTAACTAGGTGCGACCTGTTGATAGCTGGTAGTCCCAGGAACCAGGATTGGATGGAGGGTACAATGAGGCTCTGA
 GCTGCCTTCTCCCCTTCAGGGCTGGGGGCAGCAGCCATGCCTACCTGGGGGCCCGCGTCCCCAGATCGCTTGC
 CGGTGTCGCGAGGCTGAGAACAGGTTGGAAACAGCAGCCCCATGTGGAGCGCATCTCAGCGTGGGGGTGAGCGTC
 CTTCGAAGGACTGTCCGGACAACCCCCACATCTGGCTGCAGCTGGAGGGCCCAAGGAAAACGCCAGCAGGCCAGGT
 GAACGCCCTCTCCCCCATCCCTCCAGGCACCAAGGACCGCTTCCCCAGGGCGGAGGAGAGCAGGCCAGGAGAGCA

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GGGAAGAGGAGGGCCTGGGAGGATCTCCACTTCTGGTTCTCACTGGCAACCTCAGTGCCCCGTAGTTTGAG</d
na> and < dna > GGTCTGCAGGTAAAACATCCCAGCACCCTTCAGCAGGCCAAAGGAGCGGCCAGGGCCG
AGGGCACTGGACTGCAGCAGCCCCGACAAGGAGCCGTCTCCATGAATTAGTCACCAGAGCCGGCTTGGGATCTTGGT
CCCAGTTACCTTCTCGATAACCCCTCTAGGCGCAGCACGAATTCTGTTATCCAGACTTGCCTGGGATCTTGGT
GATATCGCCTCCTACACTCCAGGAGAGCTGGAGTCGCACCGGGCTGGGAAAATCCCTCCCTGCCATTCAAGGC
CCCAGAGCACAGTGGCTCCACCTTTGGCCAGATTGGCTGGGCAACCGGGCTACTCACGAGTTACGATCTTGA
CCGCCACATCGTAGCCCCACTTCTATGTTGCCAACACTGTGCCAACCCGCCCTTGGCAGCAGCTCCTGGTTC
TCCAGTTCTCGATGGACACCAAGGGGGCGGGG</ dna >.
```

Response: This DNA sequence suggests a high probability of promoter-enhancer interaction.

Enhancer-Promoter Interaction Prediction This task has 1762 test samples.

Example 1:

Prompt: < dna > AGAAACCTATGAATGCAGTCTTGTAGGAAAGCTTTTGAGAAGTCGGAGCTAATTAGACAT
CTGAGAACTCATACAGGAGAAAAACCTTATGAATGC </ dna >: Assist me in locating
transcription factor binding sites in this DNA sequence.

Response: My biological analysis indicates that TF binding sites are present
in the given DNA fragment.

TF-Human This task has 28741 test samples.

Example 1:

Prompt: < dna > TGTGCGCCCTCCGGCTGGCCACTCTGCCCTCCCTGCCAGCGCAGGTGAGCTGGCGCTT
GTCCTTAACCTTCTCAACGACGAGGCGGGACGGAGGCTCGGACGCCCTCCCCAGCCTCTGGCTGGCGCAAGTCGACTGC
GGTCGTCCTCAGTCCACGATGAAGTCATAGGGCTGTGGTCCGTGTGTGACGTCAGAAGATGGTCCTGGGATGT
CACTGCAGGCCGGGGGACCTGGCTACGGAAGGCCGGGGACCCGAGGGTAGAAAAAGGAAGTTGTC </ dna >:
Could you determine if this sequence contains a promoter?

Response: The DNA fragment includes identifiable promoter characteristics.

Promoter-300 This task has 5920 test samples.

Example 1:

Prompt: < dna > CTCTTGCCTTCCGGCCGGCGCCGATTCCGCCTCCGACCCAGCTGTGGCTGCCACGC
CAGCC </ dna > Does this sequence function as a core promoter?

Response: Yes, core promoter elements have been found in the given sequence.

Promoter-core This task has 5000 test samples.

Example 1:

Prompt: Based on their primary structures, is an interaction between <protein>MSGEENPASKPTPVQDVQGDGRVMSLHHRFVADSKDKEPEVVFIGDSLVQLMHQCEIWRELFSPHLALNF GIGGGDGTQHVWLWRLENGELEHIRPKIVVVVVVGTVNNHGHTAEQVTGGIKAIQVLVNERQPQARVVVLGLLPRGQHPNPLR EKNRQVNEVRAALAGHPRAHFLDADPGFVHSMDTISHHDMDYLHLSRLGYTPVCRALHSLLLRLAQQDQGQGAPLLE PAP</protein> and <protein>MWSPEREAEAPAGGDPAGLLPPEWEEDERMSFLSAFKRSREVNSTWDSDK MGFWAPLVLSHSRRQGVVRRLRLQEAQRKGSVPLGLATVLQDLLRRGELQRESDFMASVDSSWISWGVGVFLKPL KWTLSNMLGDNKVPAEEEVLAPELLKEKAEEVYRLYQNSPLSSHPPVALSELSTLCANSCPDERTFYLVLLQLQKEKRV TVLEQNGEKIVKFARGPRAVKSPVNDVDGVVYQLMQSEQQLSRKVESLSQEAERCKEEARRACRAGKKQLALRSL KAKQRTEKRIEALHAKLDLTVQGILDRIYASQTDQMVFNAQAGVGALKLSMKDTVEKAESLVDQIQELCDTQDEVSQT LAGGVTNGLDFDSEELEKELDILLQDFTTKEPLDLPDNPRNRHFTNSVPNPRISDAELEAEKLSLSEGGLVPSKSPK RQLEPTLKPL</protein> plausible in a human cell? Please answer 'Yes' if there is a stable physical association between two proteins and 'No' if not.

Response: It is likely that these proteins interact. The answer is Yes.

Human PPI This task has 237 test samples.

Example 1:

Prompt: Based on the primary amino acid chains, is there evidence for a stable physical association between yeast protein A (<protein>MSNYPLHQACMENEFFKVQELLHSKPSLLLQKDQDGRIPHLHWSVSFQAHEITSFLLSKMENVNLDDYPDD SGWTPFHIACSVGNLEVVKSLYDRPLKPDLNKITNQGVTCIHLAVGKKWFESQFLIENGASVRIKDFNQIPLHRAASV GSLKLIELLCGLGKSAVNWQDKQGWTPLFHALAEGHGDAAVLLVEKYGAEYDLDNKGAKAEDVALNEQVKKFFLNNV </protein>) and yeast protein B (<protein>METIDIQNRSFVVRWKCGRGDVINYQIKPLKKSIEVG IYKKLKSSVDDHASAVHIAPDTKTLTQDLYTTKSLHHKGSSSNIEEHRRSSQHSHSSNGSDNKRKERSYSSLSISGIQQQ SQEIPLRKLSASGFTLVKRVGNVSGNTMVQGDLEVKTDTDYYAFILDNSSSKNAKKKILFNASVINGDNQSMISTRSTP PARPTALSRTSTQQDMLFRVGQGRYLQGYLLKKRKRQLQGFKRFTLDFRYGTLSYYLNDHNQTCRGEIVISLSSVSAN KKDKIIIIDSGMEVWVLKATTKENWQSVDALQTCFDDQFEDKDTSTLEENPDILDDDKEVINKSSPQDHDLPTATTK SALSHRQHTQKDMDDIYVPLPSESYATFSMNRLIQQQRLEQCKKDSLSYKPTTLHQRSEGLNGTHSSSSVFTNNRVSSFN HSSSGMTSSDSLASEEVPSNKTIEHALYNQLADLELEVFSRFVTQGEVLFKDQHILCKKAKDTRVSLTSYLSSENDEFFDA EEEISRGVIIILPDTEDDINNIVEETPLLGKSDQNEFTKEVQLSGSEQIASSSVESYTTNDENHSRKHLKNRHKNRRGHP HHQKTKSAQSSTETFTSKDLFALSYPKSVTRNDIPEAAASPPSLLSFLRNKGDKLSSIAMPVTSNEPISILQLISETF EYAPLLTKATQRDPDITFVSAFAISFLSIYRDKTRTLRKPFPNPLLAETFELIREDMGFRILISEKVSHRPPVFAFFAEHLD WECSYTVTPSQFKWGSIELNNNEGILRLKFKTGELFEWTQPTTILKNLIAGERYMEPVNEFEVHSSKGDKSHILFDKAG MFSGRSEGFKVSIIPPPSSNRKKETLAGKWTQSLANETTHETIWEVGLVSNPKKKYGFTKFTANLNEITEIEKGNLPP DSRLRPDIRAYEEGNVDKAEEWKLKLEQLQRERRRNKGQDVEPKYFEVKSKNEWKYITGPKSYWERRKKHDWSDISQLW </protein>)? Please answer 'Yes' if there is a stable physical association between two proteins and 'No' if not.

Response: Interaction: Yes. The answer is Yes.

Yeast PPI This task has 394 test samples.

Example 1:

Prompt: : Return the EC number of the protein sequence.

<protein>MSILEWFVNILCGMAQYLTFSKNLTNDNLVNIYVKSNVGGTISVNLDPKSDIKNVKELVAPKLGLEPDDVK IIFAGKELLNSTVIEVLDFFSIDLHAVKVNKKIKNVIPDKPLCETLEELHQLNDQKNVESIEESNLKNEGKNKAHFFIYC ANPCKKINTGKLRVCCSECKHGAFTVDTDPQSWADVLKDNKITGVCNNVGCEGLYAKFYFKCASHPSQGENDTAVPLNLK KRNHKKIPCLACTDICDPVLVFSCDNRHVTCLECFKNYCGRSLKDRQFLSHPDFGTYLPCPAGCSNSFIEEVHHFRLTD

AQYEQYHRFATEEFILQAGGVLCPPGCGQQILIDQNCNRVQCSCGYVFCGKCLEGFHLGECLNPTDVFLSQNCDYPLD
 PEKLEKARWDEASSTVIKVLTCKPCPKCRTSTERAGGCMHMICTRANCFHWCVQCQGPWERDCMASHWFG</protein>
Response: : 2 . 3 . 2 . 31

Numerical EC (New-392) This task has 382 test samples.

Example 1:

Prompt: Return the EC number of the protein sequence. <protein>MAIPPYPDFRSAAF
 LRQHLRATMAFYDPVATDASGGQFHFLLDDGTVYNTHTRHLVSATRFVVTHAMLYRTTGEARYQVGMRHALEFLRTAFL
 DPATGGYAWLIDWQDGRATVQDTTRHCYGMAFVMLAYARAYEAGVPEARVWLAEAFDTAEQHFWQPAAGLYADEASPDW
 QLTSYRGQANMHACEAMISAFRATGERRYIERAEQLAQGICQRQAALSDRTHAPAAEGVVWEHFADWSVDWDYNRHD
 RSNIFRPWGYQVGHQTEWAKLLLQLDALLPADWHLPCAQRLFDTAVERGWDAEHGGLYYGMAPDGSICDDGKYHWVQA
 ESMAAAALVAVRTGDARYWQWYDRIWAYCWAHFVDHEHGAWFRLHRDNRTREKSAGKVDYHNMGACYDVLLWAL
 DAPGFSKESRSAALGRP</protein>

Response: 5 . 3 . 1 . 7

NumericalEC (Price-149) This task has 149 test samples.

Example 1:

Prompt: Through sequence analysis, forecast the protein's subcellular positioning in eukaryotic cells. <protein>AGFPEQEPEPKFWNDWAQKTLKDALKSLQTLNKNKAQN
 LILFLGDMGVPTVTAARILKGQLRGQPGEEGQLEMDKFPVALSKTYNTNAQVADSAGTATAYLCGVKANEVTGVSA
 AVRSQANTTQGNEVTSILRWAKDAGKSIGIVTTTRVNHATPSAAYAHCVDRDWYSDNEMPAADAVEAGCKDIARQLFENIP
 DIDVIMGGGRKYMYPKNTTDVEYPGQPKHSGTRKDGRNLVKEWVDRNTEKKGHYVWNKKDLLSLNPTKVDYLLGLFEPAD
 LPYDLERNKETDPSLSEMVEVAIKILRRNPNGFYLLVEGGRIDHGHHEGKDKQAIHEAVEMDRAIGRADLMTSTSITLV
 VTADHSHLFSGGGYTPRGNEIFGLAAFISDQPKFTAILYGNPGYKLVNGARENVSTVDYQDNSYLAQAAVPLSSETH
 GGEDAVFAKGPMAMLLHGTVHEQNYIPHAMAAYAACIGQNR</protein>

Response: membrane

Subcellular Localization This task has 2772 test samples.

Example 1:

Prompt: Analyze the provided protein sequence and predict the UniProtKB keywords associated with it. <protein>MAAADGGGPGGASVGTEEDGGVGHRTVYLFDRREKESELG
 DRPLQVGERSDYAGFRACVCQTLGISPEEKFVITTSRKEITCDNFDETVDGVTLYLLQSVNQLLLTATKERIDFLPHY
 DTLVKSGMYEYYASEGQNPLFALAELIDNSLSATSRSNIVRRRIQIKLLFDETQGKPAVAVIDNNGRGMTSKQLNWAVYR
 LSKFTRQGDFESDHSGYVRPVPVPRSLNSDISYFGVGGKQAVFFVGQSARMISKPADSQDVHELVLSKEDFEKKEKNKEA
 IYSGYIRNRKPSDSVHTNDDERFLHHIIIEEKDSFTAVVITGVQPEHIQYLKNYFHLWTRQLAHYHYYIHGPKGNE
 IRTSKEVEPFNNIDIEISMFEKGKVPKIVNLRIQDDMQTLYVNNTAADSFEFKAHVEGDDVVEGIIRYHPFLYDRETYPD
 DPCFPSKLKDEDDEDDCFIKAARGKRPIFECEFWNGRLIPYTSVEDFDWCTPPKKRGLAPIECYNRISGALFTNDKFQV
 STNKLTFMDLELKDKNTLFTRILNGQEQRMKIDREFALWLKDCKEYDKQIKFTLFKGIVTRPDLPSSKKQGPWATYAA
 IEWDGKIIYKAGQLVKTIKTLPLFYGSIVRFFLYGDHDGEVYATGGEVQIAQEPQALYDEVRTVPIAKLDRTVAEKAVKKY
 VEDEMARLPDRLSVTWPEGDELLPNEVRPAGTPIGALRIEILNKKGEAMQKLPGTSHGGSKKLLVELKVLHSSSGNKEI
 ISHISQHGGKWPYWFKKMENIQKLGNYTLKLQVVLNESADTYAGRPLPSKAIKFSVKEGKPEKFSFGLLDLPFRVGVPF
 NIPLEFQDEFGHTSQLVTDIQPVLEASGLSLHYEEITKGPNCVIRGVTAKGPVNCSQGKNYNLKVTLPGLKEDSQLKIR

LLPGHPRLKVKPDSEILVIENGTAFPFQVEVLDESDNITAQPKLIVHCKFSGAPNLPVYVVDCCSSSGTSILTGSAIQVQNIKKDQTLKARIEIPSCKDVAPVEKTIKLLPSSHARLQIFSVEGQKAIQIKHQDEVNWIAGDIMHNLIQMYDEGEREI NITSALAEKIKVNWTPEINKEHLLQGLLPDVQVPTSVKDMRYCQVSFQDDHVSLESAFTRVRLPDEPKHLKCEMKGGKTV QMGQELQGEVIIITDQYGNQIQAFSPSSLSSLSIAGVGLDSSNLKTTFQENTQSISVRGIKFIPGPPGNKDLCTWREF SDFIRVQLISGPPAKLLIDWPELKESIPVINGRDLQNPIIVQLCDQWDNPAPVQHVKISLTAKASNLKLMPSNQQHKTDE KGRANLGVFVFSVAFPRGEHTLQVKAIYNKSIIEGPIIKLMLPDEPKVRLNVKYDKDASFLAGGLFTDFMISVISEDDSI IKNINPARISMKMWKLSTSGNRPPANAETFSCNKIKDNDKEDGCFYFRDKVIPNKVGTYCIQFGFMMMDKTNILNSEQVIV EVLPNQPVKLVPKIKPPTPAVSNRVSASRTLVRDLHLSITDDYDNHTGIDLVTGTTIATIKGSNEEDTDTPLFIGKVRTL EFPFVNNGSAEIMSLVLAESSPGRDSTEYFIVFEPRPLLSRTLEPYIILPFMFYNDVKKQQMAALTKEKDQLSQSIVMYK SLFEASQQLLNEMKCQVEEARLKEAQLRNELKIHNIDIPTTQQVPHIEALLKRKLSEQEELKKKPRRSCLPNYTKGSD VLGKIAHLAQIEDDRAAMVISWHLASDMDCVVTLLTDAARRIYDETQGRQQVPLDSLTYKTLPDWKRSLPHFRNGKLYF KPIGDVFARDLLTFPDNVHCTVFGMLLGDTIILDNLDAANHYRKEVVKITHCPTLLTRDGDRIRSNKGFFGLQNKAP PMDKLRGMVFGAPVPKQCLILGEQIDLLQQYRSAVCKLDVNLDNSLEYLRTPDMRKKKQELDEHEKNLKLIEEKGTP IRKCNDSLRHSPKVENTDCPVPPKRMRREATQRNRIITKTDV</protein>

Response: 3D-structure ; Acetylation ; Alternative splicing ; Chromatin regulator ; Chromosome ; Direct protein sequencing ; Disease variant ; DNA damage ; DNA repair ; DNA-binding ; Hydrolase ; Hypogonadotropic hypogonadism ; Isopeptide bond ; Kallmann syndrome ; Microphthalmia ; Phosphoprotein ; Reference proteome ; Ubl conjugation

Keywords-CASPSimilarSeq This task has 184 test samples.

Example 1:

Prompt: Please list the UniProtKB keywords associated with the provided protein sequence. <protein>MTSVAKVYYQSQTQTESRPLMGPFIGRRRLVLTGDRSNVRMEHIADKRFYL KDLWTTFIDMQWRYKLLLFSATFAAGTWFLFGVVWYLVAVAHGDLLELDPPANHTPCVVQVHTLTGAFLFSLESQTTIGYGF RYIISEECPPLAIVLLIAQLVLTTILEIFITGTFLAKIARPKKRAETIRFSQHAVVASHNGKPCMIRVANMRKSLLIGCQ VTGKLLQTHQTKEGENIRLNQVNVTQVDTASDSPFLILPLTFYHVVDETSPLKDLPLRSCEGDFELVLILSGTVESTSATCQVRTSYLPEEILWGYEFTPAAISLASGKYIADFSLFDQVVKVASPGLRDSTVRYGDPEKLKLEESLRQAEGSAL SVRISNV</protein>

Response: ATP-binding ; Cell membrane ; Deafness ; Disease variant ; Epilepsy ; Intellectual disability ; Ion channel ; Ion transport ; Membrane ; Nucleotide-binding ; Potassium ; Potassium transport ; Reference proteome ; Transmembrane ; Transmembrane helix ; Transport ; Voltage-gated channel

Keywords-IDFilterSeq This task has 1112 test samples.

Example 1:

Prompt: Analyze the given protein sequence and generate the relevant UniProtKB keywords. <protein>MWLKLFFLLYFLVLFVLRARFFEAIVWYETGIFATQLVDPVALSFKKLKTILECRGLGYSGLPEKKDVRELVEKGSDLMEGELYSALKEEEASESVSNTNFSGEMHFYELVEDTKDGIVLWQVIANDRSP LVGKIHWEKMVKKVSRCGIRTGTFNCSSDPRYCRRRGWVRSTLIMSVPTSTSKGKVMLKEYSGRKIEVEHIFKWITAH AASRIKTIYNAEHLKEEWNKSDQYWLKIKYLFANLDQPPAFFSALSIKFTGRVEFIFVNVENWDNKSYMTDIGIYNMPsyIL RTPEGIYRYGNHTGEFISLQAMDSFLRSLQPEVNDLFVLSLVLVNLMAWMDLFITQGATIKRFVVLISTLGTYNNSLLIIS WLPVLGFLQLPILDSFYEYSLKLLRYSNTTLLASWVRADWMFYSSHPALFLSTYLGHGLLIDYFEKKRRNNNNDEVNAN NLEWLSSLWDWYTSYLFHPIASFQNFPVESDWDEDPLFLERLAFFDLWLHPLIPTDYIKNLPWRFKCLGVQSEEEMSE GSQDTENDSESENTDTLSSKEVFEDKQSVLHNSPGTASHCDAEACSCANYCQTCERKGRSYGSYNTNEDMEPDWLT WPADMHCTECVVCLENFENGCLLMLGPCGHVFHQNCIVMWLAGGRHCCPVCRWPSYKKQPYAQHQPLSNDVPS</protein>

tein>

Response: Endoplasmic reticulum ; Membrane ; Metal-binding ; Reference proteome ; Transferase ; Transmembrane ; Transmembrane helix ; Ubl conjugation pathway ; Zinc ; Zinc-finger

Keywords-UniProtSeq This task has 4562 test samples.

Example 1:

Prompt: Please predict the folding type of the protein sequence, the prediction range is from 0 to 1194. <protein>MLTAEEKAAVTGFWGKVDVVGQAQALGRLLVVY PWTQRFFQHFGNLSSAGAVMNNPKVKAHGKRVLDAFTQGLKHLDLKGAFAQLSGLHCNKLHVNPQNFRLLGNVLALVV ARNFGGQFTPNVQALFQKVAGVANALAHKYH</protein>

Response: 0

Fold Type This task has 3243 test samples.

Example 1:

Prompt: Predict the GO term based on the protein sequence.

<protein>MAAADGGGPGGASVGTEEDGGVGHRTVYLFDRREKESELGDRPLQVGERSDYAGFRACVCQTLGISPEEK FVITTSRKEITCDNFDETVDKGVTLYLLQSVNQLLTATKERIDFLPHYDTLVKSGMYEYYASEGQNPLPFALAEIDLNS SLSATSRNIGVRRIQIKLLFDETQGKPAVAVIDNGRGMTSKQLNNWAVYRLSKFRQGDFESDHSGYVRPVPVPRSLNSD ISYFGVGGKQAVFFVGGQSARMISKPADSQDVHELVLSKEDFEKKENKEAIYSGYIRNRKPSDSVHITNDDERFLHHLII EEEKEKDSFTAVENTGVQPEHIQYLKNYFHLWTRQLAHYIHYIHGPKGNEIRTSKEVEPFNNIDIEISMFEKGKVPKIVN LREIQDDMQTLYVNTAADSFEFKAHVEGDGVVEGIIRYHPFLYDRETYPDDPCFPSKLKDEDDEDCFILEKAARGKRPI FECFWNGRLIPYTSVEDFDWCTPPKKRGLAPIECYNRISGALFTNDKFQVSTNKLTMDLELKLKDNTLFTRILNGQEQQ RMKIDREFALWLKDCKEYDKQIKFTLFKGVIIRPDLPSSKKQGPWATYAAIEWDGKIYKAGQLVKTIKTLPLFYGSIVRF FLYGHDGEVYATGGEVQIAAMEPQALYDEVRTVPIAKLDRVAEKAVKKYVEDEMARLPDRLSVWPEGDELLPNEVRPA GTPIGALRIEILNKKGEAMQKLPGTSHGGSKLLVELKVILHSSSGNKEIISHISQHGGKWPWFKKMENIQKLGNYTLK LQVVLNESNADTYAGRPLPSKAIKFsvilleKFSVKEGKPEKFSGLLDLPFRVGVPF... (We hide the remaining sequences for readability)</protein>

Response: Barr body ; site of double-strand break ; ATP binding ; ATP hydrolysis activity ; DNA binding ; protein homodimerization activity ; chromosome organization ; dosage compensation by inactivation of X chromosome ; double-strand break repair ; inactivation of X chromosome by heterochromatin formation ; negative regulation of double-strand break repair via homologous recombination ; nose development ; positive regulation of DNA repair ; positive regulation of double-strand break repair via nonhomologous end joining

GO-CASPSimilarSeq This task has 184 test samples.

Example 1:

Prompt: Given a protein sequence, predict the corresponding Gene Ontology term that describes its molecular function, biological process, and cellular component. <protein>MTSVAKVYYSQTTQTESRPLMGPGIIRRRLVTKDGRSNVRMEHIADKFLYLKDLWTTF

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IDMQWRYKLLLFSATFAGTWFLFGVVWYLVAVAHGDLLLEDPPANHTPCVVQVHTLTGAFLFSLESQTTIGYGFRISEECPLAIVLLIAQLVLTTILEIFITGTFIPLAKIARPKKRAETIRFSQHAVVASHNGKPCMIRVANMRKSLLIGCQVTGKLLQTHQTKEGENIRLNQVNVTFQVDTASDSPFLILPLTFYHVVDETSPLKDLPLRSCEGDFELVLILSGTVESTSATCQVRTSYLPEEILWGYEFTPAISLSASGKYIADFSLFDDQVVKVASPSGLRDSTVRYGDPEKLIKLEESLRQAEGSALSVRISNV</protein>
```

Response: astrocyte projection ; basolateral plasma membrane ; cell body ; ciliary base ; plasma membrane ; presynapse ; ATP binding ; ATP-activated inward rectifier potassium channel activity ; inward rectifier potassium channel activity ; adult walking behavior ; cellular response to potassium ion ; central nervous system myelination ; glutamate reuptake ; non-motile cilium assembly ; potassium ion homeostasis ; potassium ion import across plasma membrane ; potassium ion transport ; regulation of long-term neuronal synaptic plasticity ; regulation of monoatomic ion transmembrane transport ; regulation of resting membrane potential ; visual perception

GO-IDFilterSeq This task has 1112 test samples.

Example 1:

Prompt: For a given protein sequence, identify the appropriate Gene Ontology term that corresponds to its molecular function, biological process, and cellular component. <protein>MWLKLFLLYFLVLFVLAFFEAIVWYETGIFATQLVDPVALSFKKLKTILECRGLGYSGLPEKKDVRELVEKGDLMEGELEYSLAKEEEASESVSNTNSGEMHFYELVEDTKDGIVLVQVIANDRSPLVGKIHWEMVKVSVSRFGIRTGTFNCSSDPRYCRRRGWRSTLIMSVPQTSTSKGKVMLKEYSGRKIEVEHIFKWITAHASRIKTIYNAEHLKEEWNKSDQYWLIKLYNLDQPPAFFSALSIKFTGRVEFIFVNVENWDNKSYMTDIGIYNMPSYILRTPEGIYRYGNHTGEFISLQAMDSFLRSLQPEVNDLFVLSLVLVNLMAWMDLFITQGATIKRFVVLISTLGTYNSSLISWLPVLGFLQLPYLDSFYEYSLKLLRYSNTTTLASWVRADWMFYSSHPLALSTYLGHGLLIDYFEKKRRNNNNDEVNANNLEWLSSLWDWYTSLYFPIASFQNFPVESDWDEDPLFLERLAFFPDWLHPLIPTDYIKNLPWRFKCLGVQSEEEMSEGSQDTENDSESENTDTLSSEKEVFEDKQSVLHNSPGTASHCDAEACSCANKYCQTSPCERKGRSYGSYNTNEDMEPDWLTWPADMNHCTECVVCLENFENGCLLMGLPCGHVFHQNCIVMWLAGGRHCCPVCRWPSYKKQPYAQHQPLSNDVPS</protein>

Response: endoplasmic reticulum ; endoplasmic reticulum membrane ; endoplasmic reticulum quality control compartment ; metal ion binding ; ubiquitin protein ligase activity ; ubiquitin-protein transferase activity ; central nervous system development ; endoplasmic reticulum mannose trimming ; protein ubiquitination ; ubiquitin-dependent ERAD pathway

GO-UniProtSeq This task has 4562 test samples.

Example 1:

Prompt: According to the relevant data reported in the scientific literature, the Gene symbol of a given protein can be used to predict which tissues the protein is expressed in. TMEM198

Response: adrenal gland , appendix , breast , bronchus , cerebral cortex , colon , fallopian tube , gallbladder , kidney , nasopharynx , prostate , rectum , salivary gland , seminal vesicle , skeletal muscle , small intestine , stomach , urinary bladder

gSymbol2Tissue This task has 2181 test samples.

Example 1:

Prompt: Get the cancer name that is associated with the given gene symbol.

MLLT1

Response: AL

gSymbol2Cancer This task has 148 test samples.

Example 1:

Prompt: Return the cancer name associated with the given gene name.

myeloid/lymphoid or mixed-lineage leukemia (trithorax homolog, Drosophila); translocated to, 1 (ENL)

Response: AL

gName2Cancer This task has 148 test samples.

Example 1:

Prompt: Translate the given SMILES formula of a molecule <SMILES>

CCC(C)C1CNCCCNC1 </SMILES> into its IUPAC name.

Response: <IUPAC> 3-butan-2-yl-1,5-diazocane </IUPAC>

S2I This task has 2993 test samples.

Example 1:

Prompt: Could you provide the SMILES for <IUPAC> 4-ethyl-4-methyloxolan-2-one </IUPAC> ?

Response: Of course. It's <SMILES> CCC1(C)COCC1 </SMILES> .

I2S This task has 2993 test samples.

Example 1:

Prompt: Given the SMILES representation <SMILES> S=P1(N(CC1=CC=C1)C(=O)N(C)C1=CC=C1)N(C)C1=CC=C1 </SMILES>, what would be its molecular formula?

Response: It is C₇H₁₅C₁₂N₂O₅PS .

S2F This task has 2993 test samples.

Example 1:

Prompt: What is the molecular formula of the compound with this IUPAC name <IUPAC> 2,5-diphenyl-1,3-oxazole </IUPAC> ?

Response: C₁₅H₁₁NO

I2F This task has 2993 test samples.

Example 1:

Prompt: Could you provide a description of this molecule? <SMILES>
C/C=C/C1=CC2=C(C=C1)OC(=C2C)C3=CC=C(C=C3)OC4=C(C=CC(=C4)C5=C(C6=C(O5)C=CC(=C6)/C=C/C)O </SMILES>

Response: The molecule is a natural product found in *Piper aequale* with data available.

Molecular Description This task has 1000 test samples.

Example 1:

Prompt: Describe this molecule: <SMILES> CCOC(=O)C1=CN=CN1[C@H](C)C1=CC=CC=C1 </SMILES>

Response: The molecule is an imidazole derivative with short-acting sedative, hypnotic, and general anesthetic properties. Etomidate appears to have gamma-aminobutyric acid (GABA) like effects, mediated through GABA-A receptor. The action enhances the inhibitory effect of GABA on the central nervous system by causing chloride channel opening events which leads to membrane hyperpolarization.

Molecule Captioning This task has 2538 test samples.

Example 1:

Prompt: Examine the given protein sequence and share a brief overview of its attributes: <protein>MKIVLASNNQGKLAELKAMLAPLGVLQQLRQAELGIPEAAEPFRTFVENALAKARHA SALSGLPALADDAGLCVEFGGLPGVDTAFYAVQFGYAKGDANNVKALLAQMAGITDRRAALVSTLVAVRSA EDPEPLIACGRVAGEVALEPMGSNGFGDFPVMFIPFEGQTFAQLPVEVKNANSHRGKATRQMMLMRER WIT </protein>

Response: A concise description of the protein with the specified amino acid sequence includes: Pyrophosphatase that catalyzes the hydrolysis of nucleoside triphosphates to their monophosphate derivatives, with a high preference for the non-canonical purine nucleotides XTP (xanthosine triphosphate), dITP (deoxyinosine triphosphate) and ITP. Seems to function as a house-cleaning enzyme that removes non-canonical purine nucleotides from the nucleotide pool, thus preventing their incorporation into DNA/RNA and avoiding chromosomal lesions.

Protein Functional Translation-Molins This task has 2633 test samples.

Example 1:

Prompt: Predict the general functional description of the protein sequence.
<protein>MAAADGGGPGGASVGTEEDGGGVGHRTVYLFDRREKESELGDRPLQVGERSDYAGFRACVCQTLGISPEEK FVITTSRKIEITCDNFDETVDGVTLYLLQSVNQLLTATKERIDFLPHYDTLVKGSMYELYASEGQNPLPFALAEIDLNS SLSATSRNIGVRRIQIKLLFDETQGKPAVAVIDNGRGMTSKQLNNWAVYRLSKFTRQGDFESDHSGYVRPVVPVRSLSND ISYFGVGGKQAVFFVGQSARMISKPADSQDVHELVLSKEDFEKKEKNKEAIYSGYIRNRKPSDSVHITNDDERFLHHLII EEEKEKDSFTAVVITGVQPEHIQYLKNFHLWTRQLAHYHYYIHGPKGNEIRTSKEVEPFNNIDIEISMFEKGKVPKIVN </protein>

LREIQDDMQTLYVNNTAADSFEFKAHVEGDGVVEGIIRYHPFLYDRETYPDDPCFPSKLKDEDDEDCFILEKAARGKRPI
 FECFWNGRLIPYTSVEDFDWCTPPKKRGLAPIECYNRISGALFTNDKFQVSTNKLTFMDLELKLKDKNLTLFTRILNGQEQR
 RMKIDREFALWLKDCHEKYDKIJKFTLFKGVITRPDLPSKKQGPWATYAAIEWDGKIYKAGQLVKTIKTLPLFYGSIVRF
 FLYGDHDGEVYATGGEVQIAAMEPQALYDEVRTVPIAKLDRTVAEKAVKKYVEDEMARLPDRLSVTWPEGDELLPNEVRPA
 GTPIGALRIEILNKKGEAMQKLPGTSHGGSKLLVELKVILHSSSGNKEIISHISQHGGKWPWFKKMENIQKLGNYTLK
 LQVVLNESNADTYAGRPLPSKAIFSVKEGKPEKFSFGLLDLPFRVGVPNFNIPLEFQDEFGHTSQLVTDIQPVLEASGLS
 LHYYEITKGPNCVIRGVTAKGPVNCSQGKYNLNKVTLPGLKEDSQILKIRLLPGHPRRLKVKPDSEILVIENGTAFPQV
 EVLDESDNITAQPKLIVHCKFSGAPNLPVYVVDCCSSGTSILTGSAIQVQNIKKDQTLKARIEIPSCCKDVAPVEKTICKL
 PSSHVARLQIFSVEGQKAIQIKHQDEVNWIAGDIMHNLIQMYDEGEREINITSALAEEKVNWTPEINKHELLQGLLPD
 VQVPTSVKDMRYCQVSFQDDHVSLESAFTRPLPDEPKHLKCEMKGGKTVQMGQELQGEVIIITDQYGNQIQAFSPSSL
 SSSLSIAGVGLDSSNLKTTFQENTQSISVRGIKFIPGPPGNKDLCTWREFSDFIRVQLISGPPAKLLLIDWPELKESIPV
 INGRDLQNPIIIVQLCDQWDNPAPVQHVVKISLTKASNLKLMPSNQHQHTDEKGRANLGVFVFAPRGEHTLQVKAIYNKSI
 IEGPIIJKLMILPDEPKPVRLNVKYDKDASFLAGLFTDFMISVISEDDSIIKNINPARISMKMWKLSLSTSGNRPPANAETF
 SCNKIKDNDKEDGCFYFRDKVIPNKVGTYCQIFGFMMMDKTNILNSEQVIVEVLPNQPVKLVPKIKPPTPAVSNVRVASR
 TLVRDLHLSITDDYDNHTGIDLVTGIIATIKGSNEEDTDTPLFIGKVRTLEFPFVNGSAEIMSLVLAESSPGRDSTEYFI
 VFEPRLPLLSRTLEPYILPFMFYNDVKKQQMAALTKEKDQLSQSIVMYKSLFEASQQLLNEMKCQVVEEARLKEAQLRNE
 LKIHNDIPTTQQVPHIEALLKRLKSEQEELKKKPRRSCTLPTYKSGDVLGKIAHLAQIEDDRAAMVISWHLASDMDC
 VVTLLTDAAARRIYDETQGRQQVLPQLDSIYKKTLPDWKRSLPHFRNGKLYFKPIGDPVFARDLLTFPDNVEHCETVFGMLL
 GDTIILDNLDAANHYRKEVVKITHCPTELRDGDRIRSNGKFGGLQNKAPPMDKLRGMVFGAPVPKQCLILGEQIDLLQQ
 YRSAVCKLDNSVNVKDLNSQLEYLRTPDMRKKKQELDEHEKNLKLIEEKGMTPIRKCNDSLHRSPKVETTDCPVPPKRMRR
 EATRQNRIITKTDV</protein>

Response: Non-canonical member of the structural maintenance of chromosomes (SMC) protein family that plays a key role in epigenetic silencing by regulating chromatin architecture (By similarity). Promotes heterochromatin formation in both autosomes and chromosome X, probably by mediating the merge of chromatin compartments (By similarity). Plays a key role in chromosome X inactivation in females by promoting the spreading of heterochromatin . Recruited to inactivated chromosome X by Xist RNA and acts by mediating the merge of chromatin compartments: promotes random chromatin interactions that span the boundaries of existing structures, leading to create a compartment-less architecture typical of inactivated chromosome X (By similarity). Required to facilitate Xist RNA spreading (By similarity). Also required for silencing of a subset of clustered autosomal loci in somatic cells, such as the DUX4 locus . Has ATPase activity; may participate in structural manipulation of chromatin in an ATP-dependent manner as part of its role in gene expression regulation . Also plays a role in DNA repair: localizes to sites of DNA double-strand breaks in response to DNA damage to promote the repair of DNA double-strand breaks . Acts by promoting non-homologous end joining (NHEJ) and inhibiting homologous recombination (HR) repair .

Protein Functional Translation-CASPSimilarSeq This task has 184 test samples.

Example 1:

Prompt: Predict the functional description of the protein sequence below.
 <protein>MTSVAKVVYSQTTQTESRPLMGPGLRRRVLTKDRSNVRMEHIADKRFYLKDLWTTFIDMQWRYKLLLLF
 SATFAGTWFLFGVVWYLVAVAHDLLLEDPPANHTPCVVQVHTLTGAFLSLESQTTIGYFRYISEECPLAIVLLIAQL
 VLTTILEIFITGTFLAKIARPKKRAETIRFSQHAVVASHNGKPCLMIRVANMRKSLLIGCQVTGKLLQTHQTKEGENIRL
 NQVNVTFQVDTASDSPFLILPLTFYHVVDETSPLKDLPLRSGEGLDFELVLILSGTVESTSATCQVRTSYLPEEILWGYEF
 TPAISLSASGKYIADFSLFQVVKVASPSGLRDSTVRYGDPEKLKLEESLREQAEKEGSALSVRISNV</protein>
Response: May be responsible for potassium buffering action of glial cells in

the brain. Inward rectifier potassium channels are characterized by a greater tendency to allow potassium to flow into the cell rather than out of it. Their voltage dependence is regulated by the concentration of extracellular potassium; as external potassium is raised, the voltage range of the channel opening shifts to more positive voltages. The inward rectification is mainly due to the blockage of outward current by internal magnesium. Can be blocked by extracellular barium and cesium (By similarity). In the kidney, together with KCNJ16, mediates basolateral K(+) recycling in distal tubules; this process is critical for Na(+) reabsorption at the tubules.

Protein Functional Translation-IDFilterSeq This task has 1112 test samples.

Example 1:

Prompt: Predict the general functional description of the protein sequence.
<protein>MWLKLFFLLYFLVLFVLARFFAIVWYETGIFATQLVDPVALSFKKLKTIERCRLGYSGLPEKKDVREL
 VEKSGDLMEGELYSALKEEEASESVSSTNFSGEMHFYELVEDTKDGIVLQVVIANDRSPLVGKIHWEKMKVKVSRCFGIRT
 GTFNCSSDPRYCRRRGWVRSTLIMSPQTSTSKGKVMLKEYSGRKIEVEHIFKWITAHAAASRIKTIYNAEHLKEEWNKSD
 QYWLIKYLFAFLDQPPAFFSALSIKFTGRVEFIFVNVENWDNKSYMTDIGIYNMPSYILRTPEGIYRYGNHTGEFISLQA
 MDSFLRSLQPEVNDLFVLSLVLVNLMAWMDLFITQGATIKRFVVLISTLGTYNNSLLIISWLPVLGFLQLPYLDSFYEYSL
 KLLRYSNTTLASWVRADWMFYSSHAPALFLSTYLGHLIDYFEKKRRNNNNDEVNANNLEWLSSLWDWYTSLFHPIA
 SFQNFPVESDWDEDPDLFLERLAFLPDLWLHPLIPTDYIKNLPWRFKCLGVQSEEMSEGSQDTENDSESENTTLSSEK
 EVFEDKQSVLHNSPGTASHCDAEACSCANKYCQTSPCERKGRSYGSYNTNEDMEPDWLTWPADMLHCTECVVCLENFENG
 CLLMGLPCGHVFHQNCIVMWLAGGRHCCPVCRWPSYKKQPYAQHQPLSNDVPS</protein>

Response: Acts as an E2-dependent E3 ubiquitin-protein ligase, probably involved in the ER-associated protein degradation pathway.

Protein Functional Translation-UniProtSeq This task has 4562 test samples.

Example 1:

Prompt: Generate a molecule with <SMILES>
Response: <SMILES> CCCOC1=CC=C(C=C1)C(=O)OCCN(CC)CC </SMILES>

Unconditional Molecular Generation This task has 800 test samples.

Example 1:

Prompt: Generate a protein sequence with <protein> </protein>.
Response: <protein>MASSNVSSLNNNTFLGKAARILKQEGERIPATAVTAYAMAVFYTLVDIPERDTDMLI
 SNGVLNVVPTIISKVARKSATIRLDVQARKEPTLPTKRASANYEPEE</protein>

Unconditional Protein Generation This task has 1000 test samples.

Example 1:

Prompt: Synthesize a protein sequence with the appropriate folding and stability properties for the desired function. 1. The protein should be able to modulate glycine decarboxylation via glycine cleavage system in a way that leads to a desirable outcome.

Response: The designed protein's amino acid sequence is as follows:

<protein>MNIIKTGIKQSLVSGIYSKGIRAFCTHYSAELEWVKLSDDNKVATVGLSSFGAQRLGKINYVELP
KEHRKCRREEKFGVLESSNATAFGLYAPVSGEVLEVNEKLKKSPSLLNEDPANNWMVKFKVSKPDEFKKLMDSNK
YKKFVQWYR</protein>

Protein Design This task has 1176 test samples.

Example 1:

Prompt: With the provided reactants and reagents, propose a potential product.

<SMILES> CCI.O=C(O)C1=CC=CC=C1Br.CN(C)C=O.O.O=C([0-1])O.[Na+1] </SMILES>

Response: <SMILES> CCOC(=O)C1=CC=CC=C1Br </SMILES>

Forward Reaction Prediction This task has 1000 test samples.

Example 1:

Prompt: Based on the given chemical reaction, can you propose some likely reagents that might have been utilized? <SMILES>

CCCBBr.CCOCCN1C(CN2CCNCC2)=NC3=CC=CC=C31 </SMILES>

Response: <SMILES> CCO.O=C([0-1])[0-1].[K+1].[K+1] </SMILES>

Reagent Prediction This task has 1000 test samples.

Example 1:

Prompt: Please suggest potential reactants for the given product. <SMILES>

COC1=C(N)C=CC2=C1CCCC(N3CCOCC3)C2 </SMILES>

Response: <SMILES> COC1=C([N+1](=O)[0-1])C=CC2=C1CCCC(N3CCOCC3)C2 </SMILES>

Example 2:

Prompt: With the provided product, recommend some probable reactants that were likely used in its production.<SMILES>

[CH3:1][C:2]([CH3:3])([CH3:4])[0:5][C:6](=[0:7])[n:15]1[c:14]2[cH:13][cH:12][c:11]([C:9]([CH3:8])=[0:10])[cH:19][c:18]2[cH:17][cH:16]1 </SMILES>

Response: <SMILES> CC(C)(C)OC(=O)O[C:6]([0:5][C:2]([CH3:1])([CH3:3])[CH3:4])=[0:7].[CH3:8][c:9]1[cH:10][cH:11][c:12]([S:13](=[0:14])(=[0:15])[0:16][C@H:17]2[CH2:18][NH:19][C@H:20]3[C@H:21]2[0:22][CH2:23][C@H:24]3[OH:25])[cH:26][cH:27]1 </SMILES>

Example 3:

Prompt: Identify possible reactants that could have been used to create the specified product. <SMILES> CC1=CC=C(N)N=C1N </SMILES>

Response: <SMILES> CC(C#N)CCC#N.N </SMILES>

Retrosynthesis Prediction This task has 4156 test samples.

Example 1:

Prompt: <SMILES> NC1=CC=C2OCOC2=C1.O=CO </SMILES> Based on the reactants and reagents given above, suggest a possible product.

Response: A possible product can be <SMILES> O=CNC1=CC=C2OCOC2=C1 </SMILES> .

Forward Synthesis This task has 4062 test samples.

Example 1:

Prompt: Give me a molecule that satisfies the conditions outlined in the description: The molecule is a member of the class of tripyrroles that is a red-coloured pigment with antibiotic properties produced by *Serratia marcescens*. It has a role as an antimicrobial agent, a biological pigment, a bacterial metabolite, an apoptosis inducer and an antineoplastic agent. It is a tripyrrole, an aromatic ether and a ring assembly.

Response: Here is a potential molecule: <SMILES> CCCCCCC1=C(C)NC(/C=C2=C(C3=CC=CN3)C=C2O)=C1 </SMILES>

Molecule Generation This task has 2493 test samples.

Example 1:

Prompt: You are provided with a set of clinical trial summaries. Extract the chemical-disease relations from the summaries and present your findings in the format of (Subject, Object). Eating disorders and the associated behavioural problems and drug abuse are uncommon in pregnancy. When they do occur they are often unrecognized because of denial but when significant may pose a risk to both the mother and her fetus. This case illustrates a number of problems that may be encountered in women with eating disorders in pregnancy, including prolonged and recurrent metabolic disturbances and diuretic abuse. In particular it illustrates the derangements of thyroid function seen in pregnant women with eating disorders and reminds us that when a cause for thyrotoxicosis remains obscure, thyroxine abuse should be considered and explored.

Response: (thyroxine, thyrotoxicosis)

Chemical Disease Interaction Extraction This task has 50 test samples.

Example 1:

Prompt: Identify the chemical entities mentioned in the given text. Hence , to elucidate the cellular mechanisms that can address these divergent reports , we studied intestinal absorption of the dual substrate loperamide in portal vein - cannulated P - gp - competent and P - gp - deficient mice .

Response: loperamide

Chemical Entity Recognition This task has 100 test samples.

Example 1:

Prompt: Your task is to extract the subject and object entities from the provided text and establish the corresponding relation triples. Please format your answers as (Subject, Relation, Object). ORF 17583, a histamine H₂-receptor antagonist, inhibited gastric acid secretion in pylorus-ligated rats (ED₅₀ = 4.9 mg/kg intraduodenal; 3.4 mg/kg p.o.; and 0.21 mg/kg i.p.) and in total gastric fistula or Heidenhain pouch dogs stimulated by betazole (ED₅₀ = 0.12 mg/kg p.o. and 0.08 mg/kg i.v.), histamine, tetragastrin, bethanechol, 2-deoxy-D-glucose or a meal (ED₅₀ values ranged from 0.11-0.26 mg/kg p.o.). The nonspecific inhibition of gastric acid by ORF 17583 supports the existence of interdependence between histamine and the gastrin and cholinergic receptors on the parietal cell surface. Antisecretory potency of ORF 17583 after intraduodenal administration in pylorus-ligated rats was 6.4 times greater than cimetidine, 1.8 times greater than ranitidine, equal to that of omeprazole and 8 times less than that of famotidine. Oral antisecretory potency of ORF 17583 in gastric fistula dogs was 31 times greater than cimetidine, 3.7 times greater than ranitidine and equal to that of omeprazole and famotidine. Studies using equieffective antisecretory doses of ORF 17583 and ranitidine in dogs suggested that ORF 17583 has a short duration of antisecretory activity similar to that of ranitidine.

Response: (ORF 17583, antagonist, histamine H₂-receptor), (ORF 17583, antagonist, histamine H₂-receptor)

Chemical Protein Interaction Extraction This task has 70 test samples.

Example 1:

Prompt: The following is a marker of acute hepatitis B infection What of the following is the right choice?

- (A) DNA polymerase (B) Hepatitis core antigen (C) Anti HBs (D) IgG to core antigen

Response: The final answer is (A).

General Multiple Choice Question This task has 1001 test samples.

Example 1:

Prompt: 'C' wave in JVP is due to

Response: Tricuspid valve bulging into right atrium

Open-Ended Question This task has 1004 test samples.

Example 1:

Prompt: Is routine intraoperative frozen-section examination of sentinel lymph nodes in breast cancer worthwhile?

Response: Maybe, in breast cancer patients having SLN biopsy, the failure of routine intraoperative FS is largely the failure to detect micrometastatic disease. The benefit of routine intraoperative FS increases with tumor size. Routine FS may not be indicated in patients with the smallest invasive cancers.

True/False Question This task has 100 test samples.

TMscore for Conditional Protein Generation

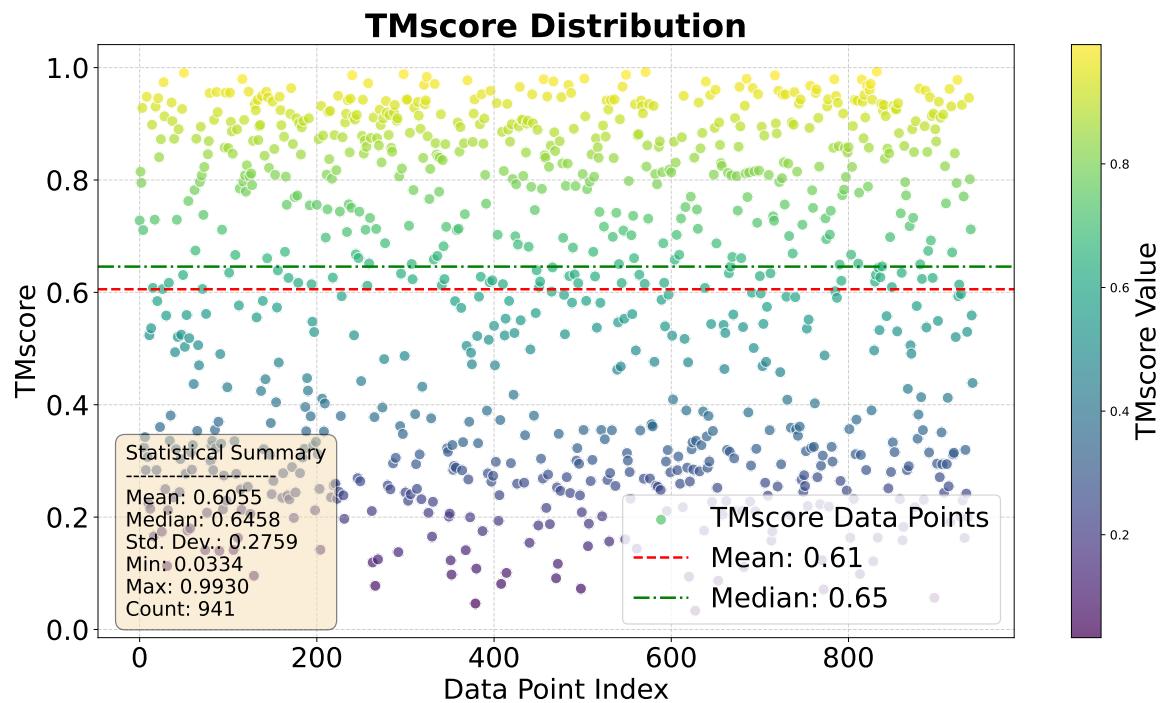


Figure 23 | TMscore for last 1000 samples