

# SciPredict: Can LLMs Predict the Outcomes of Research Experiments in Natural Sciences?

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## Abstract

Accelerating scientific progress depends on developing and efficiently allocating resources towards the most promising research directions. In experimental sciences, this often means predicting which experiments will yield meaningful results before committing to costly physical validation. Although existing benchmarks evaluate AI systems on knowledge recall, simulated environments, or theoretical reasoning, assessing their ability to predict outcomes of practical experiments remains underexplored. We introduce SciPredict, a benchmark evaluating whether we can rely on current AI systems to predict experimental outcomes in three key domains: physics, biology, and chemistry. The benchmark comprises of 405 questions derived from recently published empirical studies (post-March 2025), which spans 33 subdomains, requiring models to reason about real experimental systems. Unlike most benchmarks that assess whether AI has reached human-level performance, experimental outcome prediction represents a domain where AI systems could substantially exceed human capabilities, integrating vast cross-domain knowledge, processing complex parameter interactions, and identifying non-obvious patterns that individual researchers cannot readily perceive. This raises two critical questions: *can models predict experimental outcomes with sufficient accuracy?* and *can we identify which predictions are trustworthy?* Our analysis reveals fundamental limitations on both fronts. Our evaluations on frontier models show that models accuracy ranges between 14% – 26% and accuracy of human domain experts is ≈ 20%. Although some frontier models exceed human performance model accuracy is still far below what would enable reliable experimental guidance. Second, even within this limited performance, models cannot distinguish reliable predictions from unreliable ones. Models only achieve ≈ 20% accuracy even when they self-report very high confidence in their answer and high feasibility in question (i.e., perceiving as it is highly feasible to predict the outcome without running the practical experiment). In contrast, human experts demonstrate strong calibration: the accuracy of human experts increases as they are get more confident in their answers and accuracy increases from ≈ 5% on questions they judge infeasible to ≈ 80% on questions they consider feasible to answer without experimentation. Our findings demonstrate that while frontier models are comparable to human experts in raw predictive accuracy, they fundamentally lack the calibration awareness required for reliable deployment in experimental planning. SciPredict establishes a rigorous evaluation framework for experimental outcome prediction and demonstrates that achieving superhuman performance in experimental science requires not just better predictions, but better awareness of prediction reliability.

## 1. Introduction

Reasoning deeply about the expected outcome of experiments before running them is a central part of scientific research and ensuring efficient progress. Researchers routinely make such predictions, deciding which hypothesis to test, which parameter regimes to explore, and which experiments to prioritize under time and resource constraints. In a wet lab, choosing the right conditions for a protein crystallization experiment can mean the difference between months of productive research and a dead end. In materials science, predicting which syn-

thesis parameters will yield a desired property helps avoid costly trial-and-error. Even in fundamental physics, identifying which parameter regimes merit experimental exploration shapes how we allocate beam time at particle accelerators and space on satellites. A system that could reliably anticipate experimental results would transform scientific practice, accelerating discovery by filtering suboptimal directions, identifying gaps in current theory, and suggesting where empirical investigation is most needed. As illustrated in Fig. 2 Large language models (LLMs) appear well-suited for this task. They encode vast scientific knowledge, can reason about com-

plex systems, and have demonstrated strong performance on scientific question-answering benchmarks.

In part due to the lack of comprehensive benchmarks, the progress toward improving the ability of LLMs to predict the outcomes of practical experiments has been slow. Among benchmarks that explore the use of LLMs to aid the scientific research process, most focus on areas such as literature review and paper writing [19, 20, 30], and reproducing simulated experiments [21, 27, 31, 35]. Benchmarks that address hypothesis or outcome prediction [7, 18, 34], are limited to AI research tasks and do not test LLMs’ understanding of how empirical experiments in the physical sciences behave.

We address this gap by introducing SciPredict, a benchmark designed to systematically evaluate the ability of LLMs to predict the outcomes of real practical experiments in physics, biology, and chemistry. Rather than assess performance on simulated or historical data, we ground our evaluation in recently published empirical studies, papers appeared after March 2025, beyond the training data cutoff dates of current frontier models. For each task, domain expert human annotators extract structured descriptions of experimental setups (the system under investigation, the conditions imposed, the measurements taken, and the interventions applied) and pair them with the reported empirical results. Additionally, annotators also provide any relevant background knowledge from prior literature that could aid in predicting experiment outcomes. We then query the models to predict the outcome considering the relevant experimental details. This design ensures we are testing genuine predictive reasoning rather than memorization or pattern-matching against training data.

The benchmark comprises 405 questions spanning 33 subdomains: 9 subdomains in physics, 10 subdomains in chemistry, and 14 subdomains in biology. Questions vary in format and we consider the following: multiple-choice, free-format, and numerical value to capture different aspects of experimental reasoning. Multiple-choice questions test whether models can discriminate among plausible alternative outcomes. Free-response questions assess whether models can articulate predictions in their own words, demonstrating understanding rather than recognition. Numerical value questions require models to predict a specific quantitative value or a range, the most stringent test of whether they have internalized the relevant relationships. For numerical value questions ground truth is given as a reasonable numerical value range and for free-format questions we provide 1-10 expert written rubrics for LLM based evaluations. We also experiment with providing background knowledge curated by domain experts which allows us to measure how much models benefit from explicit in-context information versus relying solely on their parametric knowledge.

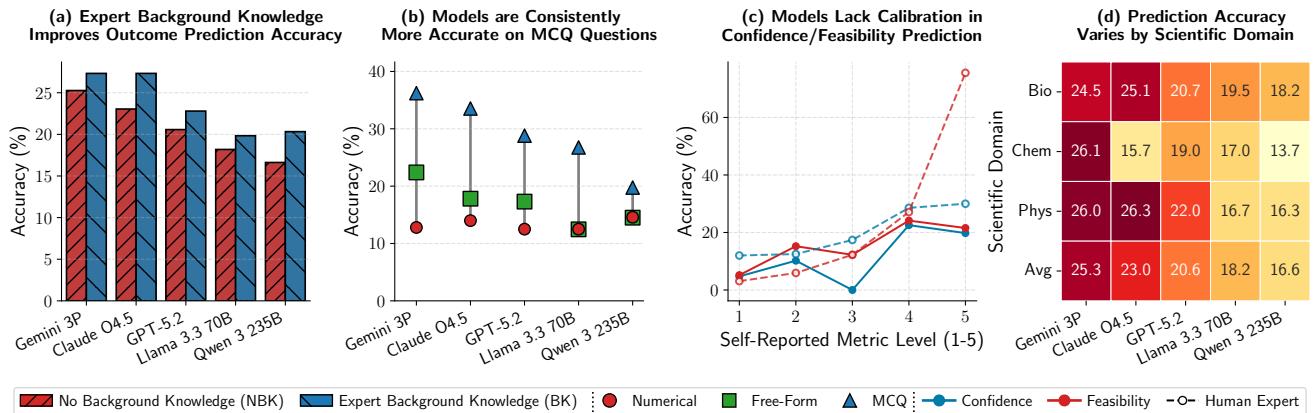
Our evaluations show that frontier LLMs achieve accuracy between 14% – 26% while human experts achieve  $\approx 20\%$ . Although some models exceed human performance, these accuracy levels remain insufficient for scientists to rely on model predictions when making resource-intensive experimental de-

cisions. More fundamentally, practical deployment requires not just higher accuracy, but the ability to identify which predictions are trustworthy. In practice, researchers want to invest in experiments whose outcomes are feasible to predict while remaining cautious on questions that are genuinely intractable without running the physical experiment. To evaluate this ability, we ask outcome predictors (models and human experts) to provide two self-assessments for each question: (i) feasibility, how feasible it is to predict the outcome from the provided experimental details (and background knowledge) without running the experiment, and (ii) confidence, how likely their specific answer is to be correct. We observe that models are not well calibrated. Model accuracy does not meaningfully improve with higher self-reported feasibility ratings or higher confidence. Human experts, in contrast, demonstrate strong calibration: their accuracy increases dramatically from  $\approx 5\%$  on questions they rate as infeasible (where physical experimentation is essential) to  $\approx 80\%$  on questions they judge feasible (where outcomes follow predictably from established principles and reasoning).

To understand what information models need to make accurate predictions, we systematically vary the availability of background knowledge. When provided with expert-curated background knowledge, models improve by an average of  $\approx 3\%$ , with gains ranging from 1.2% to 5.8% depending on the model.

When models attempt to generate their own background knowledge before answering, performance typically deteriorates. Even combining self-generated background with expert-curated knowledge yields inconsistent results, frequently performing worse than with expert knowledge alone. This pattern reveals a troubling limitation: models not only struggle to identify what background information would be helpful, but the context they generate often introduces misleading assumptions or irrelevant details that interfere with predictions. We investigate this further by filtering background knowledge per model, removing facts the model can already answer correctly when posed as standalone questions. Across nearly all models, accuracy drops when using this filtered background compared to the full expert-curated set, demonstrating that restating known information in the input context meaningfully aids prediction even when that information is already encoded in the model parameters.

To assess whether frontier models are truly ready for scientific deployment, we evaluate them not only on raw predictive accuracy but also on their calibration (the ability to accurately estimate their own confidence and the feasibility of an outcome prediction task), and their robustness across different tasks. Figure 1 summarizes some of our primary findings using a representative subset of state-of-the-art models. We observe that while models can approach human-level accuracy, more robust performance relies on expert background knowledge (BK) provided by human annotators rather than internal knowledge retrieval, a major bottleneck of the current state-of-the-art models according to our results. Additionally, multiple-choice questions (MCQs) are consistently easier for models compared



**Figure 1: Key findings of SciPredict.** Frontier models exhibit fundamental gaps in accuracy and calibration robustness in scientific experiment outcome prediction. We highlight four key failure modes using a representative subset of state-of-the-art models: Claude 04.5 (Claude Opus 4.5), OpenAI GPT-5.2, Gemini 3P (Gemini 3 Pro), Llama 3.3 (Meta Llama 3.3 70B), and Qwen 3 235B. (a) Providing expert-curated background knowledge (BK) as context for experiment outcome prediction consistently boosts performance over No Background Knowledge (NBK), suggesting models struggle to retrieve the required knowledge internally. (b) Accuracy generally degrades when moving from multiple-choice questions (MCQ) to questions requiring free-form answers (Free-Form) to Numerical value questions. (c) Unlike Human Experts (dashed lines), models show poor calibration in SciPredict tasks; the accuracy of the models’ answers to tasks do not correlate with their self-reported Confidence and perceived task prediction Feasibility. Both metrics are expected to have a *direct* correlation with accuracy. (d) SciPredict evaluates the accuracy of models predicting the outcome of scientific experiments in three domains of Biology, Chemistry, and Physics. Prediction accuracy is not uniform. The Avg field shown represents the weighted average of scores (weighted on the number of questions per domain), not the simple average of scores shown for the corresponding domains.

to free-form (and numerical) questions, which are also generally easier for models than Numerical-answer tasks (where models have to predict specific outcome numbers).

Our key contributions in this work are:

- We introduce SciPredict, comprising 405 expert-curated questions derived from empirical studies published after March 2025 across physics, biology, and chemistry. Each question includes structured experimental descriptions, expert-provided background knowledge, and ground-truth outcomes. The benchmark spans multiple question formats (multiple-choice, free-form, numerical value) and diverse subdomains, enabling systematic evaluation of models’ ability to predict real experimental results. For free-form questions we provide expert annotated rubrics and for numerical prediction questions we provide a reasonable range as the ground truth.
- We evaluate 15 frontier LLMs under multiple conditions, systematically varying background knowledge availability (expert-curated, self-generated, filtered, and combinations thereof), question format, and calibration dimensions. We establish human expert baselines through a separate cohort of domain specialists.
- We show that expert-curated background knowledge consistently improves performance. Self-generated background typically harms performance, even when combined with expert knowledge. We find that explicitly restating information

already encoded in model parameters improves accuracy, and filtering out facts the model can already answer correctly leads to worse performance. This reveals that models benefit from having relevant knowledge surfaced in the immediate context, regardless of whether that knowledge is accessible from their parameters.

- We show that while frontier LLMs match or exceed human experts in raw accuracy, however they cannot distinguish reliable predictions from unreliable ones. Model accuracy shows no meaningful correlation with self-reported confidence, perceived difficulty, or judged feasibility, whereas human experts are strongly calibrated to these signals.

## 2. Related Works

**Expert-level benchmarks in science and professional domains.** Recent studies suggest that LLMs can approach domain experts on selected tasks and in some cases surpass them, while still exhibiting notable gaps in reliability, safety, and grounded reasoning. In scientific computing, end-to-end computational fluid dynamics remains a stringent test of scientific reasoning, code generation, and numerical robustness, highlighting domain-specific weaknesses that general progress in NLP has not yet closed [26]. In healthcare, steady gains are reported for LLM in multi-turn evaluations, written by clinicians, but emphasize open challenges in robustness and safety-critical decision support [3]. Complementing these perspectives, recent biology evaluations find that frontier LLMs

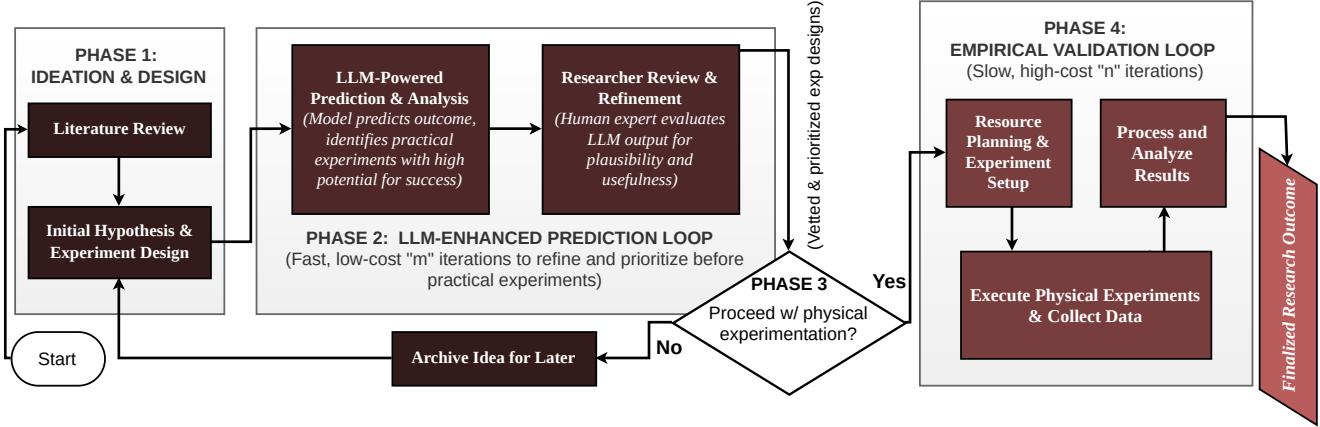


Figure 2: **LLM-enhanced efficient scientific research workflow.** The figure illustrates how LLM-powered experimental outcome prediction can be integrated into the scientific research process. Phase 1 involves ideation and experimental design through literature review and hypothesis formulation. Phase 2 represents a fast, low-cost “m” iterations to refine and prioritize before practical experiments. Based on this evaluation, researchers either proceed to Phase 3 (resource planning and experiment setup) and Phase 4 (empirical validation through physical experimentation), or archive the idea for later consideration. This workflow demonstrates how reliable LLM predictions could accelerate scientific discovery by filtering suboptimal experimental directions before committing to costly empirical validation.

can meet or exceed expert performance on several challenging benchmarks, while also cautioning that saturation effects and evaluation artifacts may inflate headline results [16]. Several other benchmarks focus on the evaluation of LLMs in questions from medicine [15, 23, 33], biomedical research [28], finance [8], and law [11]. [10] presents a benchmark of 100 PhD-level questions across a broad span of the aforementioned topics. Although these benchmarks require specialized knowledge, they have two primary shortcomings that our work addresses. First, most do not require the same degree of complex reasoning. Second, they are not situated in the empirical settings that define our benchmark, which is essential to assess real-world performance.

**AI/ML research benchmarks.** Recent benchmarks have begun evaluating LLMs on tasks that simulate the AI research cycle itself, extending beyond problem-solving or knowledge recall. [21, 27, 31, 35] evaluate LLMs for their ability to reproduce masked or full code repositories and experiment results given existing ML papers. [12] takes this a step further by evaluating how well LLMs can write experiment code for novel research ideas not seen during training. [6, 13, 14] evaluate agents on machine learning engineering tasks, assessing their ability to iteratively modify algorithms and improve performance across various datasets and tasks. [20] focuses on research methodology, requiring LLMs to predict masked out methodological details of AI research papers. [30] evaluates LLM agents’ ability to provide technical details, literature review, and open consulting to AI-related questions. [7, 18, 34] extend evaluation to the entire AI research cycle, asking LLM agents to propose novel ideas or hypotheses, design and execute experiments, and write papers or solutions

without a reference. While all of these benchmarks advance the evaluation of LLMs in research-oriented or engineering tasks, they primarily emphasize ideation, writing, or code execution. Our benchmark instead focuses on assessing LLMs’ ability to understand and predict empirical scientific outcomes, a skill particularly relevant for research in the physical sciences.

**Non-ML scientific research benchmarks.** LLMs have also been evaluated for their performance on scientific research tasks outside of AI. For example, [2] assesses LLMs on coding and problem-solving tasks in computational physics. [25] uses LLMs, leveraging their extensive domain knowledge and reliable program synthesis, to infer scientific equations directly from datasets; extending this, [29] turns LLMs into autonomous scientists that code, evaluate, and iteratively optimize the discovered equations. Similarly, [4] provides LLM agents with written biology papers and evaluates their ability to reproduce the methodology, code, and results. [19] tests LLMs on their ability to do literature review, protocol planning, and data analysis for biology research questions. While these benchmarks are valuable for evaluating LLMs’ abilities in problem-solving, coding, and scientific writing, they do not directly measure an LLM’s capacity to predict empirical scientific outcomes.

Work on outcome prediction has so far focused mainly on behavioral and social sciences. [9] and [24] evaluate LLMs on predicting experimental outcomes or reproducibility, but they operate in domains where measurements are often less precise and quantitative. In contrast, our benchmark targets the hard sciences, emphasizing quantitative prediction of empirical results. [22] provides qualitative analysis of how

well LLMs can answer theoretical physics questions using a physics knowledge toolbox, but unlike their position paper, we provide a standardized benchmark for quantitative evaluation.

**LLM-driven scientific hypothesis generation** While some benchmarks ask LLMs to generate hypotheses for scientific experiment settings, these works differ from our work in important ways. [32] provides a benchmark where LLMs have to produce and rank novel hypotheses in chemistry when prompted with background information and a set of hand-picked inspiration facts. [17] proposes a multi-agent framework that combines language-model reasoning with a dual-mode evidence engine to generate and iteratively refine grounded, novel hypotheses in biomedicine. [1] examines the applicability of large language models for hypothesis generation, focusing their experiments on breast cancer therapy. [5] introduces an LLM-driven approach to automating experimental design that fuses relational learning-generated hypotheses with real-world lab constraints and is deployed on an automated cell and metabolomics platform. While our benchmark also asks LLMs to produce hypotheses in scientific settings, we crucially do not single out inspiration facts, which can heavily influence LLM performance on this task setting.

### 3. SciPredict Curation

SciPredict consists of 405 prediction tasks derived from empirical studies published after March 2025 across physics, biology, and chemistry. Each task presents models with the essential components of an experimental setup: the system under investigation, the conditions imposed, the measurements taken, and the interventions applied. Models must then predict outcome of the experiment.

The construction process balances several competing requirements. Questions must be challenging enough to distinguish model capabilities yet tractable enough that expert-curated background knowledge could plausibly aid prediction. Experimental setups must be described with sufficient precision for informed reasoning without simply revealing the answer. Ground truth outcomes must be objectively verifiable while accounting for the inherent variability in empirical measurements. We address these challenges through a multi-stage curation process involving domain experts at every step.

#### 3.1 Design Principles

**Domain selection.** We focus on three experimentally rich domains physics, biology, and chemistry, where empirical validations play a central role in knowledge creation. The domains were selected considering following criteria: 1) The domains involve high-stakes applications in engineering, medicine, and materials science where prediction errors carry real costs. 2) Experimental protocols in the domains are well-documented, enabling structured extraction of setup parameters and measured outcomes. 3) The domains provide sufficient diversity

to test whether models can generalize predictive reasoning across distinct scientific contexts.

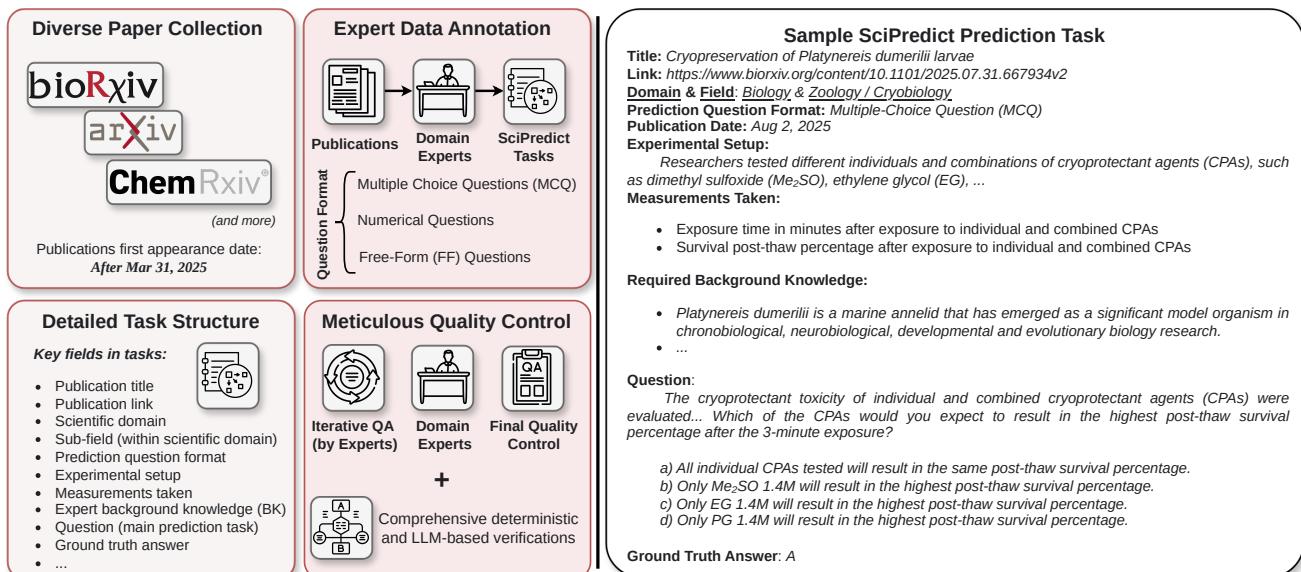
**Question formats.** To comprehensively evaluate scientific reasoning capabilities, we consider three types of question formats: multiple-choice (MCQ), free-form, and numerical value questions. MCQs allow programmatically gradable evaluations and make it easier for LLMs to isolate the correct outcome among plausible alternatives. Free-form questions evaluate whether the models can explain the expected results in their own words and whether this explanation is correct and close to how a scientist would describe and reason about an outcome. Numerical value tasks test models’ ability to capture quantitative effects rather than only qualitative measurements. For MCQs, ground truth specifies the correct option or options. For free-form questions, experts write detailed and comprehensive evaluation rubrics. For numerical value questions, experts define a reasonable range based on measurement precision and experimental variability, and we evaluate whether the model’s predicted value falls within this range.

#### 3.2 Data Collection

**Expert recruitment.** To construct our benchmark, we recruit a large cohort of experts in biology, physics, and chemistry. Among them, 54.5% hold a doctoral degree (PhD or equivalent), 34.3% hold a master’s degree, and 11.2% hold a bachelor’s degree. The experts represent a diverse set of countries, including the United States (14.3%), India (14.3%), United Kingdom (13.6%), Argentina (7.3%), and more. See Fig. 12 in Appendix A for more details.

**Task curation.** Each expert selects papers from their domain that first appeared online after March 31, 2025. This strict temporal cutoff ensures that experimental results do not appear in the pretraining data of current frontier models, guaranteeing we evaluate genuine prediction rather than memorization. Experts ensure selected papers are high quality and report practical experimental results, rather than computational simulations or purely theoretical work. Papers must document clear experimental protocols with sufficient methodological detail for informed reasoning about results.

From each selected paper, experts extract and construct the following components: 1) domain and specialized subdomain classification, 2) experimental setup details, 3) measurements taken from the experiment, 4) a prediction question about the experimental outcome, and 5) ground truth answer is directly extracted from the paper in a format specific to the question type. Experts also curate relevant background knowledge representing facts a well-informed scientist would consider when reasoning about the experiment: domain principles, prior findings, and theoretical frameworks. This background is drawn from source papers and expert knowledge. An example is provide in Fig. 3.



**Figure 3: Benchmark curation pipeline.** The benchmark construction process begins with paper collection from recent publications (post-March 31, 2025) across chemistry, biology, and physics domains from venues including ChemRxiv, arXiv, and bioRxiv. Domain experts extract experimental setups and outcomes from these papers through structured annotation, creating questions in three formats: multiple-choice (MCQ), numerical prediction, and free-form responses. Each question includes the experimental setup, measurements taken, and background knowledge useful for predicting outcomes.

**Human baseline recruitment.** In addition to the experts recruited to construct the benchmark, we recruit a separate group of experts to serve as human baseline subjects. Each human baseline subject is presented a question from our baseline and is asked to answer the question, provide reasoning for their answer, and rate their confidence in their answer. Similar to how we evaluate LLM baseline models, we also do another round of the questions, but this time revealing the required background information to the human baseline subject. For our human baseline subjects, 74.4% hold a doctoral degree, 17.9% hold a master’s degree, and 7.7% hold a bachelor’s degree. Regarding main area of expertise, 48.7% of them had main expertise in biology, 33.3% had main expertise in chemistry, and 17.9% had main expertise in physics. 33.3% of human baseline subjects were from the United States, 17.9% were from Argentina, 15.4% were from United Kingdom, 7.7% were from Mexico, and 5.1% were from Colombia. See Fig. 12 for more details. In order to ensure that human baseline subjects represent the expert level baseline we conduct a rigorous matching between the subdomain of their expertise and task subdomains. The expertise mapping is provided in Tab. 1.

### 3.3 Quality Control

All data undergoes a multi-stage review process to ensure scientific rigor. Initial screening filters questions where the first version of the paper appeared online on or before March 31, 2025, experiments are simulations or theoretical derivations,

answers are directly stated in experimental setup descriptions, phrasing is ambiguous, required predictions exceed available information, or ground truth conflicts with source papers. Questions passing initial screening goes through two layers of domain expert reviewers who verify: 1) experimental setup precision sufficiency for informed reasoning, 2) background knowledge necessity and sufficiency, 3) ground truth clarity and proper sourcing, and 4) appropriate difficulty level.

For MCQs, reviewers ensure distractors represent plausible alternatives arising from reasonable but incorrect assumptions rather than obviously wrong options. For free-form questions, reviewers confirm evaluation rubrics capture essential scientific reasoning without being overly prescriptive about phrasing. Also ensures that rubrics are mutually exclusive and collective exhaustive. Each rubric criteria is designed to be validated to a binary outcome (satisfied or not). For numerical value question, reviewers verify acceptable ranges are neither unrealistically narrow (demanding impossible precision) nor trivially broad (accepting nearly random guesses). Questions flagged during review undergo revision or removal if fundamental problems cannot be resolved.

### 3.4 Data Diversity

The benchmark spans 33 specialized subdomains across physics, biology, and chemistry, ensuring models encounter the full spectrum of experimental reasoning required in modern scientific practice. Within physics, questions draw from 9 subdomains such as experimental condensed matter physics,

quantum & atomic physics, and high energy particle physics. Biology questions cover 14 subdomains such as molecular biology, neuroscience, plant biology, and ecology. Chemistry spans 10 subdomains such as organic chemistry, catalysis, and polymer chemistry.

Question complexity varies systematically along multiple axes. Experimental systems range from controlled laboratory setups with few interacting components to complex biological systems with emergent properties. Some questions require single-step causal reasoning ("What happens when we increase temperature?"), while others demand multi-hop inference chains such as integrating thermodynamics, kinetics, and material properties. Background knowledge requirements also span a continuum from questions answerable via freshman-level principles to those requiring specialized domain expertise typically held only by active researchers in the relevant subdomain.

Domain distribution remains sufficiently balanced to prevent overfitting to particular experimental contexts: 25% questions come from physics, 50% from biology, and 25% from chemistry. Question format distribution is similarly controlled, with 40% multiple-choice, 32% free-form, and 28% numerical value questions. This distribution reflects the natural variety of prediction tasks scientists encounter sometimes we need binary yes/no answers, sometimes qualitative descriptions of mechanisms, and sometimes precise quantitative estimates.

Together, these diversity dimensions ensure the benchmark probes models' general capacity for experimental outcome prediction rather than narrow pattern-matching on particular experimental templates, question phrasings, or domain-specific conventions.

## 4. Evaluation Setup and Metrics

Our dataset  $\mathcal{D}$  comprises three subsets corresponding to different question formats: multiple-choice questions  $\mathcal{D}_{MCQ}$ , free-form responses  $\mathcal{D}_{FF}$ , and numerical value questions  $\mathcal{D}_{NUM}$ . We evaluate a collection of candidate LLMs indexed by  $m \in \mathcal{M}$ , where each model  $m$  produces a prediction  $\hat{y}_i^{(m)}$  for task  $i$ .

Beyond measuring prediction accuracy, we assess whether models can identify which predictions are reliable, a critical requirement for practical deployment in experimental planning. To this end, we collect three types of reliability assessments from both models and human experts: confidence scores  $\hat{c}_i^{(m)} \in \{1, 2, 3, 4, 5\}$  representing the level of model's confidence that its prediction is correct; difficulty ratings  $\hat{z}_i^{(m)} \in \{1, 2, 3, 4, 5\}$  capturing how challenging the model perceives the question to be; and feasibility judgments  $\hat{f}_i^{(m)} \in \{1, 2, 3, 4, 5\}$  indicating whether the outcome can be predicted without running the practical experiment.

### 4.1 Accuracy Metrics

We define accuracy separately for each question format to enable direct comparison across all three types while accounting

for their distinct evaluation requirements.

**Multiple-choice (MCQ).** Each question  $i \in \mathcal{D}_{MCQ}$  presents 3-4 options with ground truth answer  $g_i \in \{1, 2, 3, 4\}$  provided by domain expert annotators. Accuracy is the proportion of questions answered correctly:

$$\text{Acc}_{MCQ}^{(m)} = \frac{1}{|\mathcal{D}_{MCQ}|} \sum_{i \in \mathcal{D}_{MCQ}} \mathbb{1}[\hat{y}_i^{(m)} = g_i]. \quad (1)$$

This binary correctness criterion forms the basis for all subsequent analyses of confidence and feasibility calibration.

**Free-form (FF).** Each question  $i \in \mathcal{D}_{FF}$  has a reference answer  $y_i$  and an expert-written evaluation rubric. We employ an LLM judge  $J_\theta$  with a fixed prompt to assess whether the model's response  $\hat{y}_i^{(m)}$  demonstrates correct scientific reasoning:

$$s_i = J_\theta(\hat{y}_i^{(m)}, y_i) \in \{0, 1\}, \quad \text{Acc}_{FF}^{(m)} = \frac{1}{|\mathcal{D}_{FF}|} \sum_{i \in \mathcal{D}_{FF}} s_i. \quad (2)$$

This metric evaluates whether a careful grader would judge the answer correct regardless of stylistic differences from the reference, capturing understanding rather than surface-level pattern matching.

**Numerical value (NUM).** For each question  $i \in \mathcal{D}_{NUM}$ , domain experts specify an acceptable range  $[L_i, U_i]$  accounting for measurement precision and experimental variability. Accuracy reflects whether predictions fall within this scientifically reasonable interval:

$$\text{Acc}_{NUM}^{(m)} = \frac{1}{|\mathcal{D}_{NUM}|} \sum_{i \in \mathcal{D}_{NUM}} \mathbb{1}[L_i \leq \hat{y}_i^{(m)} \leq U_i]. \quad (3)$$

This captures practical utility, whether the model's quantitative prediction is sufficiently accurate for experimental planning, rather than demanding exact numerical matches.

### 4.2 Reliability Calibration

Reliable deployment in experimental science requires not only accurate predictions but also the ability to distinguish trustworthy predictions from unreliable ones. We assess reliability through three complementary measures that capture different aspects of epistemic self-calibration.

**Confidence.** For each prediction  $\hat{y}_i^{(m)}$ , we prompt the model to report its confidence level  $\hat{c}_i^{(m)} \in \{1, 2, 3, 4, 5\}$ , about the correctness of its prediction (1 = very low confidence, 5 = very high confidence). Well-calibrated confidence should stratify questions by actual performance: high-confidence predictions should prove correct more often than low-confidence ones. We analyze calibration by computing empirical accuracy within confidence bins and examining whether this relationship is sufficiently monotonic.

**Difficulty.** Models provide difficulty ratings  $\hat{z}_i^{(m)} \in \{1, 2, 3, 4, 5\}$  representing perceived question hardness from the model's perspective (1 = very easy to answer, 5 = very hard to answer). These ratings test whether models recognize their own

limitations: if well-calibrated, questions rated as easy should yield higher accuracy. Difficulty assessments also reveal whether different models identify similar questions as challenging, providing insight into which experimental scenarios pose fundamental reasoning difficulties versus model-specific weaknesses.

**Feasibility.** Perhaps most critical for experimental planning, feasibility judgments  $\hat{f}_i^{(m)} \in \{1, 2, 3, 4, 5\}$  indicate whether a question can be answered from first principles, domain knowledge and reasoning without physical experimentation (1 = impossible to answer without practical experiment, 5 = very feasible to answer without practical experiment). A researcher deciding whether to trust a model’s prediction would invest resources in experiments judged feasible to predict while remaining cautious about seemingly intractable problems. Well-calibrated feasibility would show high accuracy on questions the model rates as feasible and low accuracy on questions it rates as infeasible.

We compute calibration by stratifying questions according to each reliability measure and examining whether empirical accuracy varies as expected. For confidence and feasibility, we expect positive correlations with accuracy; for difficulty, we expect negative correlations. The strength and consistency of these relationships quantify how reliably models can identify their own trustworthy predictions.

### 4.3 Experimental Conditions

To understand what information models require for accurate predictions, we systematically vary the availability of background knowledge across four conditions:

**No Background Knowledge (NBK).** Models receive only the experimental setup, measurements, and question, testing whether parametric knowledge suffices for prediction.

**Background Knowledge (BK).** Models additionally receive expert-curated background knowledge representing facts a well-informed scientist would consider when reasoning about the experiment. This measures how much relevant context improves prediction when that context is explicitly surfaced.

**Self-generated Background (SBK).** Models first generate their own background knowledge before answering, assessing whether they can identify and articulate helpful context autonomously.

**Self-generated + Annotator Background (SABK).** Models receive both their self-generated context and expert-curated background, revealing whether combining sources yields additive benefits or introduces interference.

**Filtered Background Knowledge (FBK).** We also create a filtered background condition for each model by converting each background statement into a question, removing facts the model can already answer correctly, and measuring performance with this filtered set. This isolates whether stating known information in context improves prediction even when that information is theoretically accessible from parameters.

### 4.4 Models and Human Baseline

We evaluate 15 state-of-the-art LLMs in zero-shot settings: OpenAI o1-mini, o3, o3-mini, o4-mini, GPT-5.2; Anthropic Claude Sonnet 4.5, Opus 4.1, Opus 4.5; Google Gemini 2.5 Pro, 3 Flash, 3 Pro; Meta Llama 3.1 8B, Llama 3.3 70B; Alibaba Qwen 3 32B, Qwen 3 235B; and DeepSeek v3. All models receive identical task instructions and are evaluated using the accuracy metrics defined above.

For human baselines, each expert answers questions in their subdomain under both NBK and BK conditions, providing the same reliability assessments (confidence, difficulty, feasibility) that we collect from models. This parallel evaluation structure enables direct comparison of calibration between human experts and AI systems.

Our evaluation design allows us to assess: (i) task performance via accuracy across question formats and domains; (ii) confidence calibration via the relationship between self-reported probabilities and empirical correctness; (iii) difficulty calibration via correlation between perceived hardness and actual accuracy; and (iv) feasibility calibration via the gap between accuracy on questions judged answerable from theory versus those requiring empirical validation.

### 4.5 Evaluation Protocol and Robustness

All free-form responses were evaluated using Gemini-3-Pro as the judge model, which assessed whether model predictions satisfied the expert-written rubrics. To verify robustness of our evaluation pipeline, we conducted several validation experiments. First, we replicated the evaluation using GPT-5.2 as an alternative judge model and observed no statistically significant differences in model rankings or aggregate accuracy scores. Second, we explored the sensitivity of model performance to inference hyperparameters, testing various decoding strategies (temperature settings from 0.0 to 1.0, top-p sampling with  $p \in \{0.9, 0.95, 1.0\}$ ). Across all tested configurations, performance variations remained within the error bars established through our three-trial experimental protocol. All reported accuracy metrics represent means computed across these three independent runs, with error bars indicating one standard deviation. This consistency across judge models and hyperparameter settings demonstrates that our findings reflect fundamental model capabilities rather than evaluation artifacts or sampling variance.

## 5. Main Results

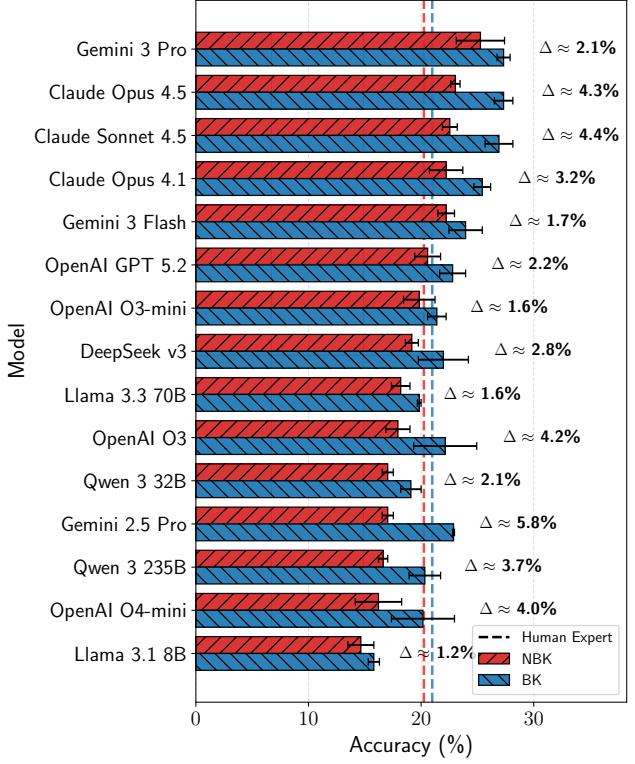
We evaluate whether frontier language models can predict experimental outcomes with sufficient accuracy and reliability for practical scientific deployment. Our analysis proceeds in two parts. First, we measure raw predictive performance: can models correctly anticipate what will happen when researchers execute the described experiments? Second, and more critically for real-world application, we assess whether models

possess the reliability awareness to identify which of their predictions merit trust, a capability we term *calibration*. A model that achieves 60% accuracy but cannot distinguish its correct predictions from incorrect ones offers little value for experimental planning, as researchers cannot determine which suggestions to pursue. Conversely, even modest accuracy becomes actionable when paired with reliable confidence estimates that guide resource allocation toward high-probability successes.

All experiments reported in this work were conducted with web search capabilities disabled for all evaluated models. This design choice is critical to ensure our benchmark measures genuine predictive reasoning rather than information retrieval. Since our evaluation draws from papers published after March 2025, beyond the training cutoff of current frontier models, enabling web search would allow models to potentially locate and access the original publications, thereby converting the prediction task into a lookup task. This would fundamentally undermine our goal of assessing whether models can reason about experimental outcomes from first principles and provided context. By disabling web search, we ensure that model predictions reflect only their parametric knowledge, reasoning capabilities, and ability to leverage the provided experimental details and background knowledge, rather than their capacity to search for and retrieve the ground truth answers.

We find that frontier models achieve accuracy between 14% and 26% on experimental outcome prediction, placing them roughly on par with domain expert performance of approximately 20%. While some models marginally exceed human baselines, these accuracy levels remain far below the threshold required for autonomous experimental guidance. More fundamentally, models exhibit severe calibration failures across all reliability metrics. Models  $m \in \mathcal{M}$  report high confidence  $\hat{c}_i^{(m)} \in \{4, 5\}$  even on questions where they achieve only 20% accuracy, judge questions as highly feasible to answer ( $\hat{f}_i^{(m)} = 5$ ) without experimentation yet perform no better on these items than on questions they rate as infeasible ( $\hat{f}_i^{(m)} = 1$ ), and show no systematic relationship between self-reported difficulty  $\hat{z}^{(m)}$  and actual performance  $\text{Acc}^{(m)}$ . Human experts, by contrast, demonstrate strong calibration: their accuracy ranges from approximately 5% on questions they judge infeasible (where physical experimentation is essential) to approximately 80% on questions they consider feasible (where outcomes follow predictably from established principles). This calibration gap proves more consequential than the accuracy gap, models not only lack the knowledge to predict reliably, but critically, they lack the self-awareness to recognize the boundaries of their predictive capabilities. Without this metacognitive foundation, even incremental accuracy improvements cannot translate into trustworthy scientific tools.

**Finding #1:** Providing curated background knowledge consistently improves the outcome prediction accuracy.



**Figure 4: Accuracy with and without background knowledge.** Accuracy (%) of each evaluated model under two input conditions: 1.) *w/o background knowledge*: the model receives only the experimental setup, measurements, and the question; 2.) *w/ background knowledge*: the same information as previous case with the addition of annotator-provided background knowledge collected during task generation.

A key factor in answering the questions correctly, for humans and presumably LLMs, is access to relevant background knowledge. We test this by running two conditions: (i) models answer without background knowledge (NBK) and (ii) models answer with curated background knowledge (BK). As shown in Fig. 4, removing the background knowledge substantially reduces the accuracy  $\text{Acc}^{(m)}$  across all models  $m \in \mathcal{M}$ , though the size of the drop varies by model (largest for GPT-5; smallest for Claude Sonnet 4.5). On average, BK improves accuracy by  $\sim 3\%$ . One interpretation is that curated background knowledge provides missing domain assumptions and narrows the space of plausible outcomes. It is also noted that confidence scores  $\hat{c}^{(m)}$  remain roughly the same across NBK and BK. This suggests that background information primarily benefits correctness rather than shifting self-reported confidence.

**Finding #2:** Human performance is close to the average model performance

We emphasize that human expert performance in our benchmark serves as a calibration reference point rather than an

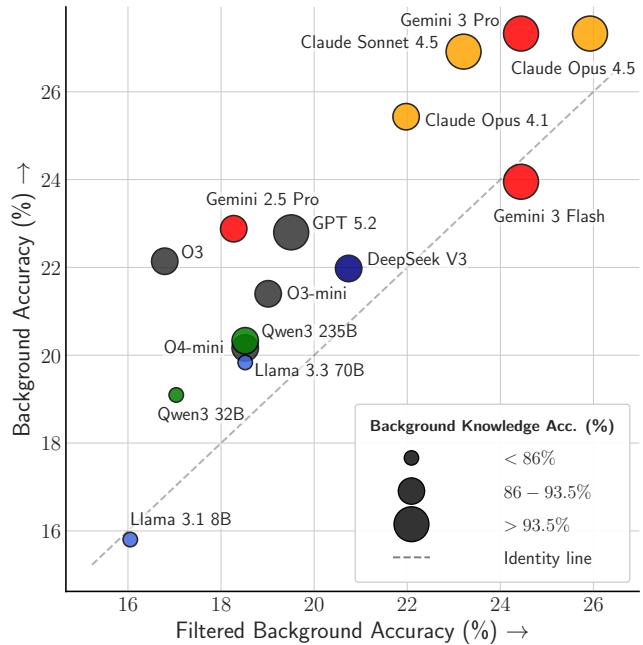
upper bound on achievable performance. Experimental outcome prediction represents a domain where AI systems could substantially exceed human capabilities by integrating vast cross-domain knowledge, processing complex multi-parameter interactions at scale, and identifying non-obvious patterns across millions of prior experiments capabilities that individual researchers cannot readily match. Our human baseline ( $\approx 20\%$  accuracy Fig. 4) reflects the inherent difficulty of predicting novel experimental outcomes without conducting the physical experiment, even for domain experts. Critically, human experts demonstrate strong calibration achieving 5% accuracy on questions they judge infeasible ( $\hat{f}_i^{(m)} = 1$ ) versus 80% on feasible questions ( $\hat{f}_i^{(m)} = 5$ ) indicating they possess reliable calibration awareness about prediction reliability that current models lack. To ensure high-quality expert baselines, 75% of our human evaluators hold doctoral degrees (PhD or equivalent), with the majority of remainder holding master’s degrees, all with demonstrated expertise in their respective domains. Furthermore, we assigned evaluation tasks to experts by matching our 33 fine-grained subdomains to individual expert specializations, ensuring that evaluators assessed questions within their area of active research expertise. This fine-grained matching maximizes the quality of human predictions while acknowledging that even domain experts face fundamental limitations when predicting complex experimental outcomes without empirical validation.

**Finding #3:** Across nearly all models, accuracy is higher with the full annotator background than with the filtered version, implying that including knowledge the model can already answer still boosts performance.

Fig. 5 shows that restating known facts in the input context enhances model performance, even when those facts are not strictly missing from the model’s parametric knowledge. By filtering the curated background per model-removing any background items for which the model can already answer the corresponding question correctly-the x-axis approximates performance when the context contains only “unknown” background. Yet most models fall in the upper triangle (above the  $y = x$  line), illustrating accuracy  $Acc^{(m)}$  is higher when the full curated background is provided, including facts the model demonstrably knows (BK). Repeating known information can foreground relevant priors, reduce ambiguity, align terminology and assumptions with the task, and provide a structured scaffold that helps models apply what they know to the specific prediction setting.

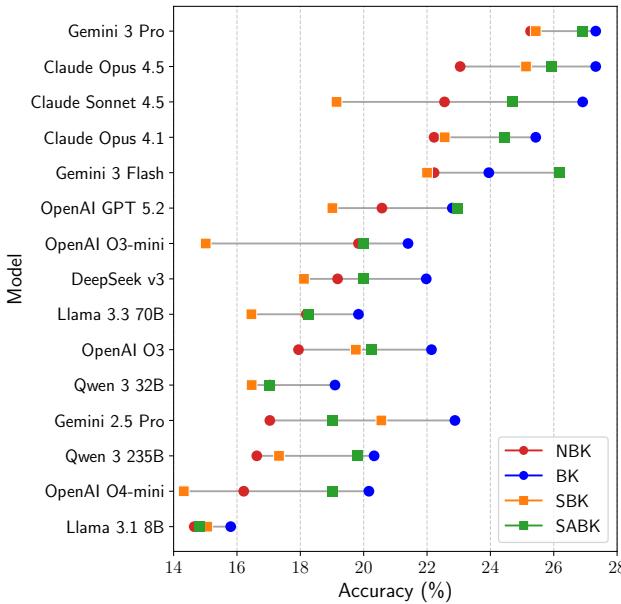
**Finding #4:** Models cannot reliably generate useful background knowledge: self-generated/synthetic background usually reduces accuracy, and even when combined with gold background it rarely improves performance.

To test whether models can supply their own helpful context, we evaluate settings where models self-generate background



**Figure 5: Restating known facts in context enhances model performance.** Scatter plot comparing each model’s benchmark accuracy when given the full annotator-curated background (y-axis; “w/ background (BK) accuracy (%)”) versus when given a filtered version of that background (x-axis; “w/ filtered background (FBK) accuracy (%”). Filtering is performed per model: each original background statement is converted into a question, the model answers these questions, and we remove the background statements whose corresponding questions the model answers correctly (i.e., we keep only background the model appears not to already know). Each point corresponds to one evaluated model, colored by model family; the dashed diagonal indicates equal performance under both context conditions ( $y = x$ ). Marker size encodes the percentage of background-related questions answered correctly by the model (larger circles = more background already known), as shown in the legend. Most points lie above the diagonal (upper triangle), indicating higher accuracy with the full background than with the filtered background. All models have a background knowledge accuracy  $> 70\%$ .

knowledge (SBK) and then answer, as well as a combined condition that appends this self-generated context to annotator-provided background (SABK). Fig. 6 shows that, in contrast to the clear gains from curated background knowledge, self-generated background is unreliable and often counterproductive: for most models, SBK lowers accuracy compared to providing no background at all, implying that the generated content is frequently irrelevant or misleading and can steer predictions away from the correct experimental outcome. Moreover, supplementing gold background with synthetic background (SABK) typically fails to yield consistent improvements, indicating that models struggle not only to generate helpful knowledge, but also to avoid introducing distracting or harmful information when additional context is available.



**Figure 6: Self-generated background knowledge is often harmful.** Accuracy (%) for each model under four context conditions: *NBK* (no background knowledge; models receive only the experimental setup, measurements, and question), *BK* (annotator-provided background knowledge), *SBK* (model self-generated/synthetic background knowledge), and *SABK* (self-generated background combined with annotator-provided background). Across most models, *BK* yields the highest accuracy, while *SBK* frequently degrades performance or provide no significant performance gain relative to *NBK*, indicating that models do not reliably identify or generate background knowledge that improves outcome prediction. Adding self-generated background on top of gold background (*SABK*) also rarely provides consistent gains, suggesting that extra synthetic context can introduce noise or misleading cues even when correct background is available.

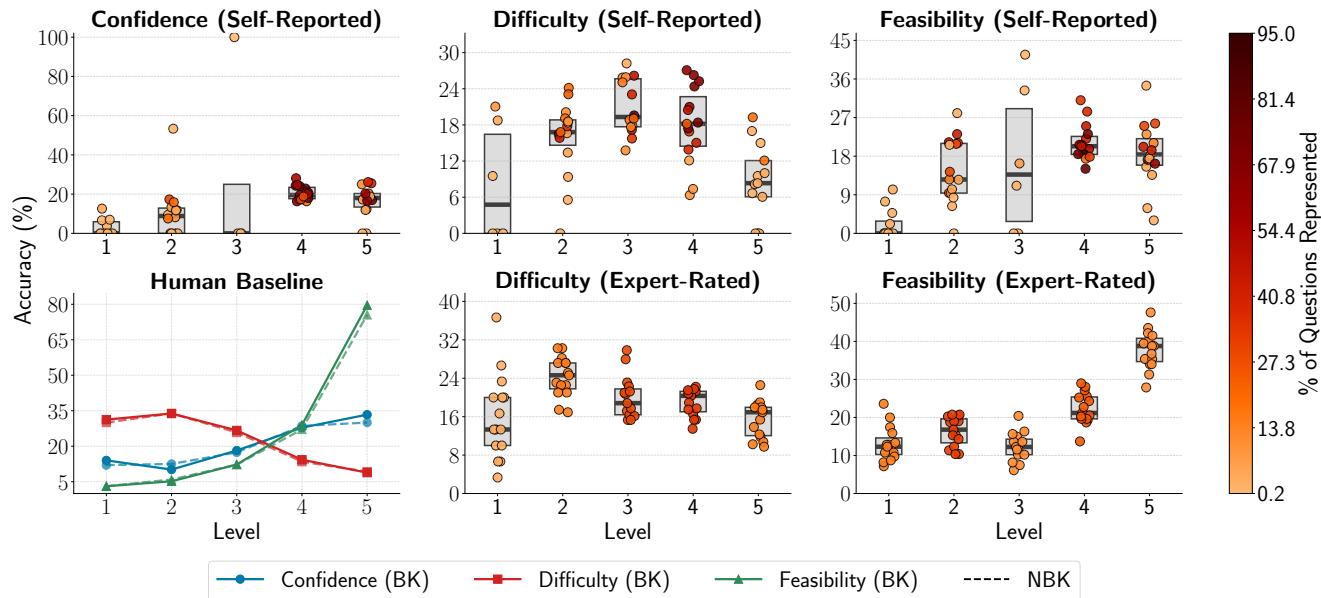
**Finding #5:** Self-assessed confidence/difficulty/feasibility by models are not aligned with performance, indicating calibration gaps. Human calibration shows confidence/difficulty/feasibility exhibit the expected correlation with accuracy

Fig. 7 shows whether forecasters  $m \in \mathcal{M}$  can anticipate their own errors by comparing empirical accuracy  $\text{Acc}^{(m)}$  to self-reported confidence  $\hat{c}^{(m)}$ , perceived difficulty  $\hat{z}^{(m)}$ , and perceived feasibility  $\hat{f}^{(m)}$  of answering without executing the underlying experiment. If these self-assessments were informative uncertainty estimates, accuracy would rise ( $\text{Acc}^{(m)} \uparrow$ ) monotonically with confidence ( $\hat{c}^{(m)} \uparrow$ ), fall with difficulty ( $\hat{z}^{(m)} \downarrow$ ), and rise with feasibility ( $\hat{f}^{(m)} \uparrow$ ). Instead, the top-row plots show weak, inconsistent, and often non-monotonic relationships: bins that models label as higher-confidence are not reliably more accurate, and increases in model-reported difficulty or decreases in model-reported feasibility do not

consistently correspond to lower accuracy. This lack of structure indicates substantial miscalibration in model self-reports, limiting their usefulness for prioritizing which predictions can be trusted or which cases warrant additional evidence collection. In contrast, the bottom-left subplot demonstrates that human confidence, difficulty, and feasibility judgments track correctness in the expected direction, and the same human-calibrated difficulty and feasibility scores impose a clear ordering over model performance in the bottom-middle and bottom-right subplots. Concretely, when evaluated against human calibration, models systematically achieve higher accuracy ( $\text{Acc}_i^{(m)} \uparrow$ ) on items judged more feasible ( $f_i^{(m)} \uparrow$ ) and less difficult ( $\hat{z}_i^{(m)} \downarrow$ ), implying that the benchmark’s variation in answerability is captured by human assessments even when models’ own self-evaluations fail to do so.

**Finding #6:** LLM-based error classification reveals that there are two error patterns that dominate across models: 1) factual extraction errors and logical reasoning flaws, with both factual contradiction and information fabrication affecting  $\approx 50\%$  of incorrect responses, 2) logical and reasoning flaws, with unsupported assumptions affecting  $\approx 80\%$  of incorrect responses.

To understand the nature of model failures in experimental outcome prediction, we employ an LLM judge to systematically classify errors across 16 specific error types grouped into five main categories. Results are provided in Fig. 8. The analysis reveals that failures concentrate in two primary areas: factual and extraction errors (affecting 80.09% of incorrect responses) and logical and reasoning flaws (affecting 87.42% across models). Within factual errors, factual contradiction 51.96% and information fabrication particularly 51.19% prevalent across models, indicating that models frequently fail to incorporate relevant experimental details when making predictions. Smaller models like Llama 3.1 8B show distinctly higher rates of disconnected reasoning 28.0% compared to frontier models ( $\leq 4\%$ ), suggesting that model scale correlates with reasoning sophistication. Deficiencies in scientific rigor, while considerably widespread ( $\approx 50\%$ ), primarily manifest as false certainty (43.61% across models), models expressing high confidence ( $\hat{c}_i^{(m)} \in \{4, 5\}$ ) in incorrect predictions ( $\hat{y}_i \neq g_i$ ), which directly explains our earlier finding that model confidence scores fail to stratify accuracy. Importantly, basic comprehension errors remain rare ( $< 10\%$  for most subtypes), confirming that models understand what is being asked but lack the reasoning capabilities to integrate experimental details, apply relevant domain principles, and assess prediction reliability. These error patterns indicate that improving experimental outcome prediction requires advances in factual grounding and logical reasoning rather than better instruction following or task comprehension. We conduct this analysis considering all the questions in the benchmark. We also conduct an additional analysis considering only the questions human experts marked as feasible to answer without running the practical experiment ( $\hat{f}_i^{(m)} = 5$ ). The results are provided in Fig. 13. We see similar



**Figure 7: Models are poorly calibrated in self-reported confidence, difficulty, and feasibility, whereas human calibration correlated with accuracy.** Top row: empirical accuracy (y-axis) plotted against model-provided 1) confidence in its answers, 2) perceived question difficulty, and 3) perceived feasibility of predicting the experimental outcome without running the experiment. Each circle corresponds to a single model at a particular confidence/difficulty/feasibility level, and circle color corresponds to the percentage of the number of questions assigned to that level by that model. Under well-calibrated assessments, accuracy should increase with confidence, decrease with difficulty, and increase with feasibility. The observed relationships are weak and often non-monotonic. Bottom row: calibration using human judgments. The left subplot reports the human baseline’s accuracy vs human confidence, difficulty, and feasibility, exhibiting the expected monotonic trends. The middle and right subplots report model accuracy as a function of human-calibrated difficulty and human-calibrated feasibility, respectively. Circle color corresponds to the percentage of the number of questions assigned to that level by humans. These plots also recover the expected trends, indicating that human calibration provides a substantially more reliable signal of question answerability than model self-reports.

error patterns in this case as well.

**Finding #7:** MCQs are substantially easier than free-form and numerical value tasks.

As shown in Fig. 9 we find that model accuracy is highly sensitive to answer format, with multiple-choice questions substantially easier than open-ended generation and especially numerical prediction. This gap is not merely a matter of “MCQs being easier because the correct option is visible,” but appears to reflect a broader dependence on recognition over generation: MCQs let models compare candidates and pick the closest match, while free-form and numerical formats require constructing a specific claim/value and committing to it. To isolate format from content, we convert MCQs into matched free-form prompts (MCQ→FF) and re-run evaluation. The resulting drop, visible across essentially all model families, shows that simply removing the provided options degrades accuracy even when the underlying experimental scenario is unchanged. This suggests that headline MCQ accuracy  $\text{Acc}_{\text{MCQ}}^{(m)}$  can overestimate how reliably a model would perform in realistic scientific workflows, where predictions are typically produced in open form  $\text{Acc}_{\text{FF}}^{(m)}$  (and often as quantities).

Finally, the steepness of the MCQ→free-form drop varies by model, implying meaningful differences in robustness to output constraints.

**Finding #8:** Performance varies by scientific domain, with Chemistry typically the most challenging.

Fig. 10 shows that Chemistry consistently have the lowest accuracy on average compared to Biology and Physics. This domain gap is particularly visible for the human baseline, where Chemistry accuracy is 8.82% compared to 23.15% (Biology) and 26.00% (Physics). Even the best-performing (frontier) models improve overall accuracy, but their gains are not uniform across domains, indicating that scaling or general instruction-following ability does not fully translate into robust empirical reasoning in Chemistry. This pattern suggests that our benchmark is sensitive to domain-specific experimental knowledge and intuitions.

**Finding #9:** Performance on this benchmark has a strong correlation with performance on HLE benchmark.

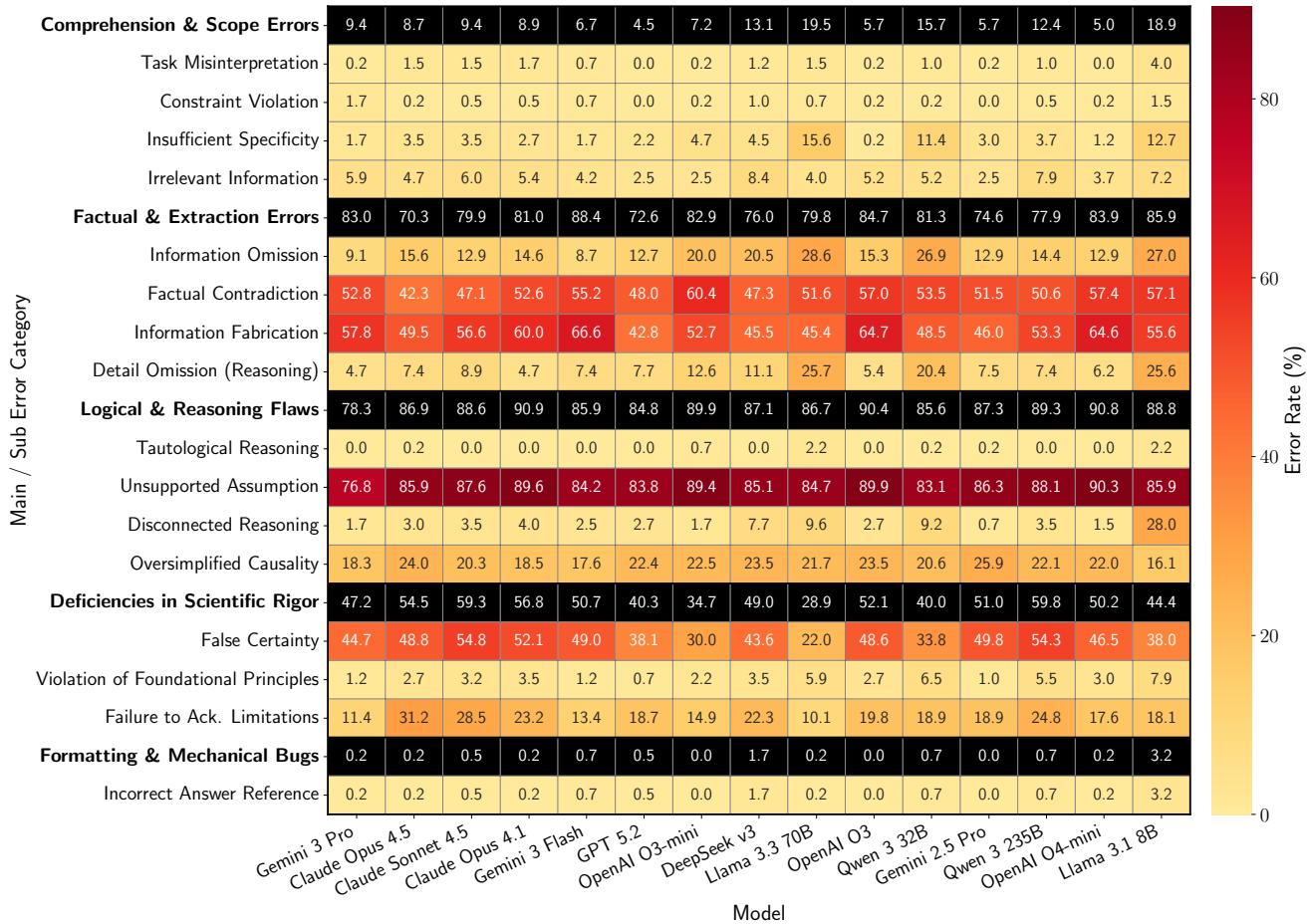


Figure 8: **Analysis of model errors.** We employ an LLM judge to systematically classify errors in model predictions according to a hierarchical taxonomy spanning five top-level (in black background) categories and 16 specific error types. The heatmap shows the percentage of incorrect responses containing each error type for each evaluated model. Error categories progress from surface-level issues (Comprehension & Scope) to deeper reasoning failures (Logical & Reasoning Flaws) to fundamental scientific deficiencies (Deficiencies in Scientific Rigor). Models can exhibit multiple error types simultaneously, so accumulative percentage scores within top-level categories may exceed 100%. SciPredict tasks contribute to top-level category percentages if flagged with at least one underlying error type.

Fig. 11 helps disentangle how much performance on SciPredict (NBK) reflects broad hard-reasoning capability versus a more task-specific ability to anticipate empirical outcomes from experimental descriptions. Although the overall association with HLE is positive, the dispersion around the trendline is substantial: models with similar HLE text-only accuracy can differ by several points on NBK accuracy. This residual structure is informative: some models overperform relative to what their HLE score would predict (e.g., DeepSeek v3 achieves comparatively strong NBK accuracy despite very low HLE, and Claude Sonnet 4.5 / Claude Opus 4.1 sit above the fitted line), while others underperform given their HLE level (e.g., Gemini 2.5 Pro, OpenAI O3, and GPT-5.2 fall below the line). These deviations suggest that, beyond general text-only reasoning, strong results on SciPredict also depend on scientific priors and experimental intuition: identifying which intervention details are causally relevant, mapping measurements to plausible mechanisms, and remaining robust when background context is withheld in the NBK setting.

## 6. Discussion and Conclusion

Our investigation reveals that while frontier LLMs achieve accuracy levels (14 – 26%) comparable to human experts ( $\approx 20\%$ ) in predicting experimental outcomes, this apparent parity masks a critical inadequacy: models fundamentally lack the calibration awareness required for trustworthy deployment in experimental planning. The most striking finding is the contrast in calibration robustness between models and humans. Human experts demonstrate strong calibration—their confidence correlates with correctness and their feasibility judgments stratify questions by actual answerability (from  $\approx 5\%$  accuracy on problems judged infeasible to  $\approx 80\%$  on those deemed feasible). Models, conversely, maintain roughly uniform performance ( $\approx 20\%$  accuracy) regardless of self-reported confidence, perceived difficulty, or feasibility assessments. This miscalibration is not merely a technical deficiency but represents a fundamental barrier to practical

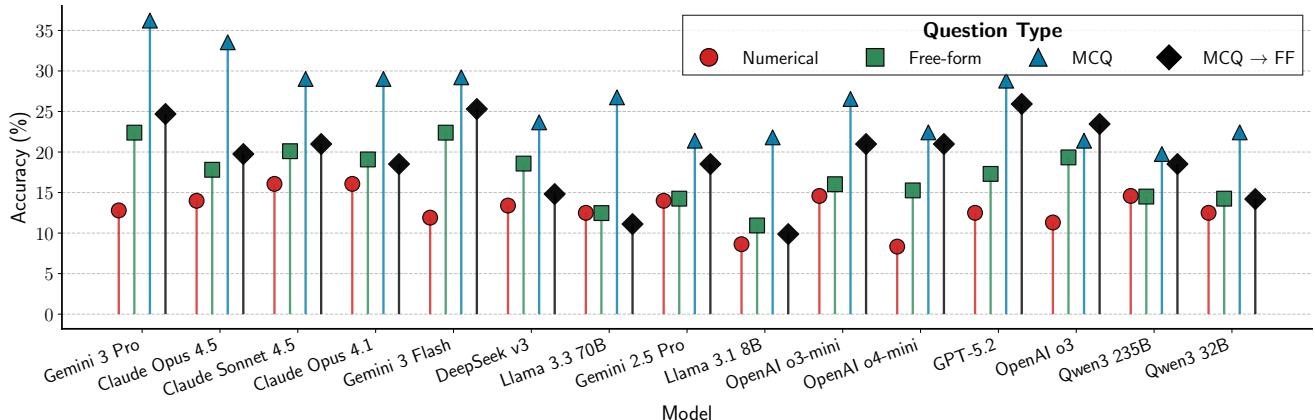


Figure 9: **Question format influence the accuracy. Accuracy decreases in the question type order of MCQ, free form and numerical value questions.** Answer format drives large swings in model accuracy under identical experimental content. We evaluate each model in the NBK setting across four response formats: MCQ, free-form, numerical value, and MCQ→FF (MCQs rewritten into matched free-form prompts and re-scored), which isolates the effect of removing provided answer options. Points denote per-model accuracy; error bars indicate uncertainty over the question set. Accuracy is consistently highest for MCQs, lowest for numerical prediction, and drops systematically when converting MCQs to free-form, showing that reported performance depends strongly on how predictions are elicited.

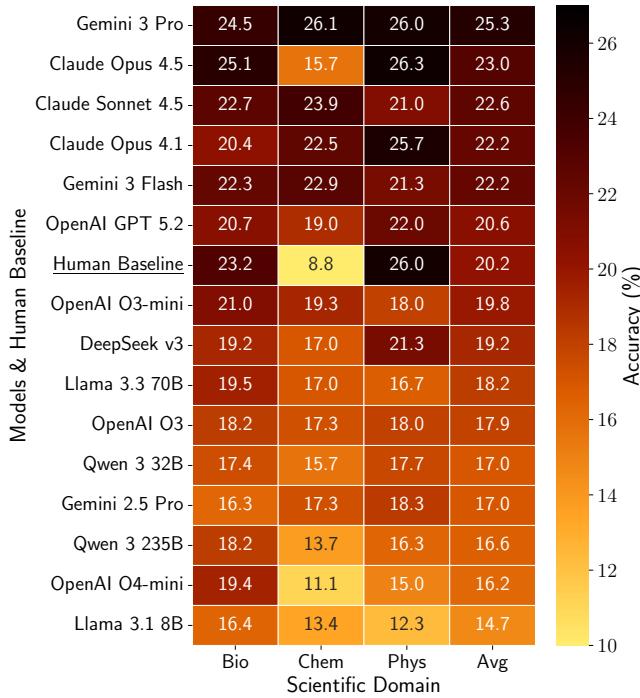
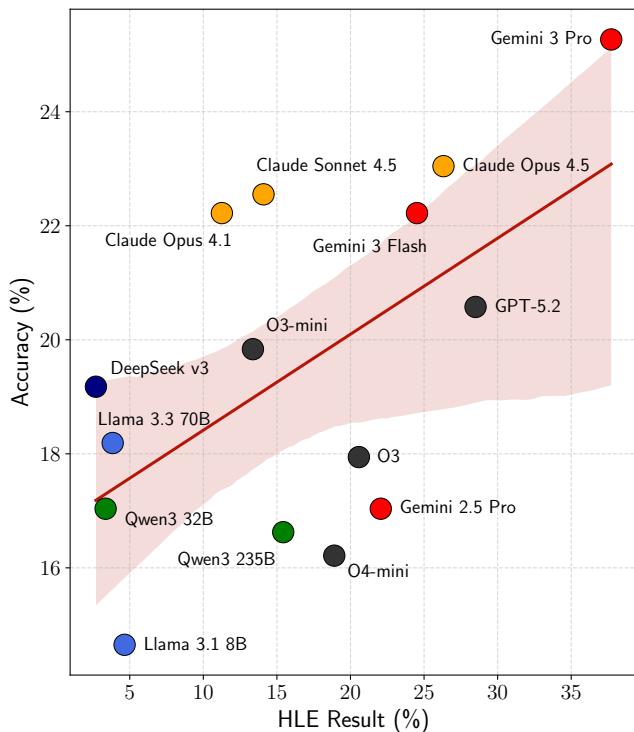


Figure 10: **Domain specific accuracy.** Heatmap of model accuracy (%) on benchmark questions, broken down by scientific domain (Biology, Physics, Chemistry). Results are provided for the evaluated models and human baseline. Overall, frontier models achieve the highest accuracies, but performance varies substantially by domain; Chemistry tends to be the most challenging subset, and several models (including the human baseline) exhibit performance degradation on Chemistry relative to Biology/Physics.

use. A scientist deciding whether to invest resources based on model predictions requires reliable uncertainty estimates, not just average accuracy. Our experiments with background knowledge reveal additional limitations: expert-curated context consistently improves performance by  $\approx 3\%$ , yet models cannot reliably identify or generate helpful background autonomously, self-generated background typically degrades predictions. Performance varies substantially across domains (chemistry proving most challenging) and formats (MCQ accuracy far exceeding free-form or numerical prediction), suggesting that scaling alone will not uniformly translate to better experimental prediction. The moderate correlation ( $r \approx 0.46$ ) between SciPredict and general reasoning benchmarks indicates that empirical prediction requires domain-specific intuitions and experimental familiarity that current training paradigms may not adequately develop.

These findings have important implications for scientific AI assistance. Current models can recognize plausible outcomes when presented with options but struggle to construct predictions independently or assess when experimental validation is truly necessary versus when outcomes follow predictably from established principles. Human experts develop these capabilities through laboratory experience, understanding the boundaries of theoretical predictability and recognizing which aspects of experimental setups are causally relevant. The calibration gap reflects a fundamental difference between pattern recognition in training data and genuine scientific reasoning about empirical systems. For AI to meaningfully accelerate discovery through experimental outcome prediction, achieving superhuman performance requires not merely better predictions but better awareness of prediction reliability, systems that can accurately assess their calibration robustness and identify



**Figure 11: Model accuracy on SciPredict correlates with performance on the HLE benchmark.** Benchmark performance correlates with general hard-reasoning performance. Scatter plot of each evaluated model’s accuracy on SciPredict in the no-background-knowledge (NBK) setting (y axis) versus its HLE text-only accuracy (x axis). The solid line shows a linear fit and the shaded region indicates the corresponding confidence bands. Overall, SciPredict NBK accuracy exhibits a moderate positive correlation with HLE performance (Pearson  $r \approx 0.46$ ), suggesting that broader reasoning capability explains some-but not all-variance in empirical outcome prediction.

when sufficient information exists to make reliable predictions versus when empirical validation is indispensable.

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## A. Additional Dataset Details

### A.1 Additional details about task contributors / human baseline participants

We provide additional visualizations of the degree, expertise, and country of origin diversity of the experts recruited for benchmark construction and human baseline. Overall, our experts have strong credentials in their respective fields. For the human baseline, we match experts with relevant expertise to task domains and subdomains; see Tab. 1 for more details.

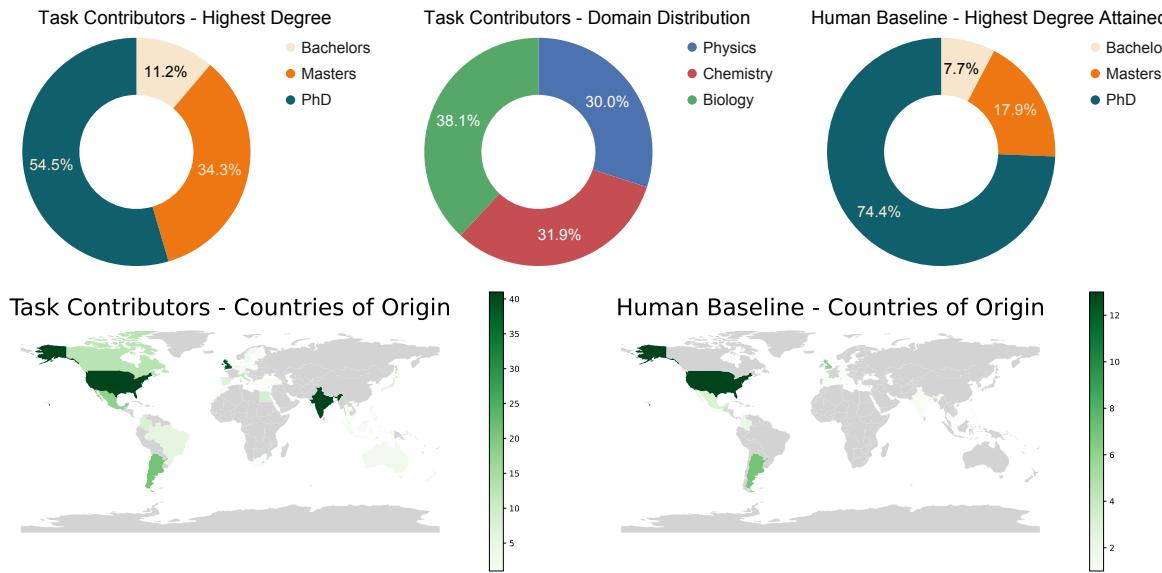


Figure 12: **Diversity of the experts recruited for benchmark construction and human baseline.** *Top left:* A plot of the highest degree distribution of experts recruited for benchmark construction. *Top center:* A plot of the domain expertise of experts recruited for benchmark construction. *Top right:* A plot of the highest degree distribution of experts recruited for human baseline. *Bottom left:* A heatmap of the countries of origin of experts recruited for benchmark construction. *Bottom right:* A heatmap of the countries of origin of experts recruited for human baseline.

### A.2 Human baseline expert - Task subdomain mapping

Table 1: Subfield expertise of human annotators, grouped by the task domains (Physics, Chemistry, Biology) and subdomains.

Task Domain	Subdomain	Human Baseline Subfields
Physics	All Physics	Advanced Chemical Engineering, Applied And Interdisciplinary Physics, Applied Physics And Interdisciplinary, Chemical Engineering, Classical And Mechanical Physics, Condensed Matter And Materials, Electromagnetism And Optics, Engineering Physics, High-energy And Nuclear Physics, Radiophysics & Electronics, Theoretical Physics, Zoology
	Condensed Matter & Materials Physics	Advanced Chemical Engineering, Applied Physics And Interdisciplinary, Chemical Engineering, Condensed Matter And Materials, Electromagnetism And Optics, Engineering Physics, Radiophysics & Electronics
	Materials Chemistry	Condensed Matter And Materials, Engineering Physics
	Optics, Photonics & Laser Physics	Applied Physics And Interdisciplinary, Condensed Matter And Materials, Electromagnetism And Optics, Engineering Physics, Radiophysics & Electronics, Zoology
	High-Energy / Nuclear / Particle Physics	Engineering Physics, High-energy And Nuclear Physics, Radiophysics & Electronics, Theoretical Physics, Zoology
	Applied & Instrumentation Physics	Applied And Interdisciplinary Physics, Applied Physics And Interdisciplinary, Classical And Mechanical Physics, Condensed Matter And Materials, Electromagnetism And Optics, Engineering Physics, High-energy And Nuclear Physics, Radiophysics & Electronics
	Quantum & Atomic Physics	Applied Physics And Interdisciplinary, Condensed Matter And Materials, Electromagnetism And Optics, Engineering Physics, Radiophysics & Electronics, Zoology

Task Domain	Subdomain	Human Baseline Subfields
Chemistry	Plasma & Nonlinear Physics	Applied Physics And Interdisciplinary, Classical And Mechanical Physics, Electromagnetism And Optics, Engineering Physics, Radiophysics & Electronics
	Biophysics	Advanced Chemical Engineering, Applied Physics And Interdisciplinary, Chemical Engineering, Condensed Matter And Materials, Electromagnetism And Optics, Radiophysics & Electronics
	Mechanical / Energy / Thermo / Fluid Physics	Classical And Mechanical Physics, Condensed Matter And Materials, Engineering Physics, Radiophysics & Electronics
	All Chemistry	Advanced Chemical Engineering, Analytical Chemistry, Antimicrobial Resistance, Bio-organic Chemistry, Biochemistry, Biochemistry And Molecular Biology, Catalysis And Environmental Chemistry, Chemical Biology, Chemical Engineering, Chemical Sciences, Digital Technologies Applied To Education, Electrochemistry, Engineering Physics, Green Chemistry, Materials And Inorganic Chemistry, Molecular And Cellular Biology, Molecular Biology And Genetics, Organic And Biological Chemistry, Principles Of Biochemistry, Pure Chemistry, Zoology
	Analytical Chemistry	Advanced Chemical Engineering, Analytical Chemistry, Antimicrobial Resistance, Bio-organic Chemistry, Biochemistry And Molecular Biology, Chemical Biology, Chemical Engineering, Chemical Sciences, Digital Technologies Applied To Education, Electrochemistry, Engineering Physics, Materials And Inorganic Chemistry, Molecular And Cellular Biology, Molecular Biology And Genetics, Organic And Biological Chemistry, Principles Of Biochemistry, Pure Chemistry
	Materials Chemistry	Analytical Chemistry, Bio-organic Chemistry, Biochemistry And Molecular Biology, Chemical Biology, Chemical Engineering, Digital Technologies Applied To Education, Electrochemistry, Materials And Inorganic Chemistry, Organic And Biological Chemistry
	Catalysis	Biochemistry, Biochemistry And Molecular Biology, Catalysis And Environmental Chemistry, Chemical Biology, Chemical Engineering, Chemical Sciences, Digital Technologies Applied To Education, Electrochemistry, Green Chemistry, Materials And Inorganic Chemistry, Principles Of Biochemistry, Pure Chemistry
	Physical Chemistry	Advanced Chemical Engineering, Analytical Chemistry, Chemical Engineering, Chemical Sciences, Digital Technologies Applied To Education, Materials And Inorganic Chemistry, Organic And Biological Chemistry, Principles Of Biochemistry, Pure Chemistry
	Organic Chemistry	Analytical Chemistry, Bio-organic Chemistry, Biochemistry And Molecular Biology, Catalysis And Environmental Chemistry, Chemical Biology, Chemical Engineering, Digital Technologies Applied To Education, Electrochemistry, Materials And Inorganic Chemistry, Organic And Biological Chemistry, Zoology
	Nanotechnology / Nanochemistry	Analytical Chemistry, Biochemistry, Biochemistry And Molecular Biology, Catalysis And Environmental Chemistry, Chemical Biology, Chemical Engineering, Digital Technologies Applied To Education, Electrochemistry, Green Chemistry, Materials And Inorganic Chemistry, Organic And Biological Chemistry, Principles Of Biochemistry, Pure Chemistry
Biology	Biochemistry	Antimicrobial Resistance, Biochemistry, Electrochemistry, Molecular And Cellular Biology, Molecular Biology And Genetics, Organic And Biological Chemistry, Principles Of Biochemistry, Pure Chemistry
	Inorganic Chemistry	Analytical Chemistry, Catalysis And Environmental Chemistry, Materials And Inorganic Chemistry
	Environmental Chemistry	Advanced Chemical Engineering, Analytical Chemistry, Chemical Engineering, Materials And Inorganic Chemistry, Zoology
	Polymer Chemistry	Chemical Engineering, Digital Technologies Applied To Education, Materials And Inorganic Chemistry, Organic And Biological Chemistry
	All Biology	Antimicrobial Resistance, Bio-organic Chemistry, Biochemistry, Biochemistry And Molecular Biology, Biological Engineering, Biological Sciences, Biomedical Engineering, Biomedical Sciences, Biotechnology, Cell Biology, Chemical Biology, Chemical Engineering, Clinical Drug Development, Developmental Biology, Ecology, Genetics, Green Chemistry, Immunology, Microbiology, Microbiology And Cell Science, Molecular And Cellular Biology, Molecular Biology, Molecular Biology And Genetics, Neurobiology And Behavior, Observational Oceanography, Physiology, Plant Sciences, Research And Data Analysis, Software Engineering, Systems And Synthetic Biology, Taxonomy And Biodiversity, Zoology
	Microbiology	Antimicrobial Resistance, Biochemistry, Biological Engineering, Biological Sciences, Biomedical Engineering, Biomedical Sciences, Cell Biology, Chemical Engineering, Ecology, Microbiology, Microbiology And Cell Science, Molecular And Cellular Biology, Molecular Biology And Genetics, Neurobiology And Behavior, Software Engineering, Systems And Synthetic Biology, Taxonomy And Biodiversity
	Cancer Biology / Oncology	Antimicrobial Resistance, Biochemistry, Biological Engineering, Biological Sciences, Biomedical Engineering, Biomedical Sciences, Cell Biology, Chemical Engineering, Clinical Drug Development, Developmental Biology, Genetics, Immunology, Microbiology And Cell Science, Molecular And Cellular Biology, Molecular Biology, Molecular Biology And Genetics, Research And Data Analysis, Software Engineering, Taxonomy And Biodiversity
Ecology	Neuroscience / Neurobiology	Antimicrobial Resistance, Biochemistry, Biological Engineering, Biomedical Engineering, Cell Biology, Chemical Engineering, Clinical Drug Development, Developmental Biology, Genetics, Immunology, Molecular And Cellular Biology, Molecular Biology, Molecular Biology And Genetics, Neurobiology And Behavior, Physiology, Systems And Synthetic Biology
	Ecology	Biochemistry, Biological Engineering, Biological Sciences, Biomedical Engineering, Biomedical Sciences, Cell Biology, Chemical Engineering, Ecology, Genetics, Microbiology, Microbiology And Cell Science, Observational Oceanography, Plant Sciences, Research And Data Analysis, Systems And Synthetic Biology, Taxonomy And Biodiversity
	Immunology	Bio-organic Chemistry, Biochemistry, Biological Engineering, Biomedical Engineering, Biomedical Sciences, Chemical Engineering, Immunology, Microbiology And Cell Science, Software Engineering, Systems And Synthetic Biology, Zoology

Task Domain	Subdomain	Human Baseline Subfields
	Molecular Biology	Antimicrobial Resistance, Bio-organic Chemistry, Biochemistry, Biological Engineering, Biological Sciences, Biomedical Engineering, Biomedical Sciences, Cell Biology, Chemical Engineering, Genetics, Microbiology And Cell Science, Molecular And Cellular Biology, Molecular Biology, Molecular Biology And Genetics, Research And Data Analysis, Software Engineering, Taxonomy And Biodiversity
	Pharmacology / Toxicology	Biochemistry, Biological Sciences, Biomedical Sciences, Cell Biology, Clinical Drug Development, Genetics, Immunology, Microbiology And Cell Science, Observational Oceanography, Physiology, Research And Data Analysis, Software Engineering
	Plant Biology	Biochemistry, Biological Sciences, Developmental Biology, Ecology, Genetics, Observational Oceanography, Plant Sciences, Research And Data Analysis, Systems And Synthetic Biology, Taxonomy And Biodiversity
	Animal Behavior	Biochemistry, Biological Sciences, Cell Biology, Clinical Drug Development, Developmental Biology, Genetics, Microbiology, Molecular Biology, Observational Oceanography, Physiology, Systems And Synthetic Biology, Taxonomy And Biodiversity, Zoology
	Cell Biology	Antimicrobial Resistance, Bio-organic Chemistry, Biochemistry, Biological Engineering, Biological Sciences, Biomedical Engineering, Biomedical Sciences, Cell Biology, Chemical Engineering, Clinical Drug Development, Developmental Biology, Genetics, Immunology, Microbiology And Cell Science, Molecular And Cellular Biology, Molecular Biology, Molecular Biology And Genetics, Neurobiology And Behavior, Physiology, Research And Data Analysis, Software Engineering, Taxonomy And Biodiversity
	Physiology	Biochemistry, Biological Engineering, Biological Sciences, Biomedical Engineering, Biotechnology, Cell Biology, Chemical Engineering, Clinical Drug Development, Genetics, Microbiology, Molecular And Cellular Biology, Molecular Biology, Neurobiology And Behavior, Observational Oceanography, Physiology, Plant Sciences, Systems And Synthetic Biology, Taxonomy And Biodiversity
	Biochemistry	Biochemistry, Biochemistry And Molecular Biology, Biological Engineering, Biomedical Engineering, Cell Biology, Chemical Biology, Chemical Engineering, Clinical Drug Development, Genetics, Molecular Biology, Physiology, Software Engineering, Zoology
	Genetics	Biochemistry, Biological Sciences, Biomedical Sciences, Cell Biology, Clinical Drug Development, Genetics, Microbiology, Microbiology And Cell Science, Molecular Biology, Observational Oceanography, Plant Sciences, Systems And Synthetic Biology, Taxonomy And Biodiversity
	Bioengineering / Biomaterials	Antimicrobial Resistance, Biochemistry, Biological Sciences, Biomedical Sciences, Cell Biology, Green Chemistry, Microbiology And Cell Science, Molecular And Cellular Biology, Molecular Biology, Molecular Biology And Genetics, Observational Oceanography, Physiology, Systems And Synthetic Biology

Table 2: Task distribution by scientific subfield: number of tasks per Biology, Physics, and Chemistry subdomain.

Field	Subfield	Count
Physics	Condensed Matter & Materials Physics	33
	Materials Chemistry	17
	Optics, Photonics & Laser Physics	16
	High-Energy / Nuclear / Particle Physics	15
	Applied & Instrumentation Physics	13
	Quantum & Atomic Physics	10
	Plasma & Nonlinear Physics	5
	Biophysics	3
	Mechanical / Energy / Thermo / Fluid Physics	2
Chemistry	Analytical Chemistry	18
	Materials Chemistry	17
	Catalysis	16
	Physical Chemistry	14
	Organic Chemistry	13
	Nanotechnology / Nanochemistry	10
	Biochemistry	8
	Inorganic Chemistry	6
	Environmental Chemistry	4
	Polymer Chemistry	3
Biology	Microbiology	36
	Cancer Biology / Oncology	28
	Neuroscience / Neurobiology	19
	Ecology	17
	Immunology	16
	Molecular Biology	14
	Pharmacology / Toxicology	13
	Plant Biology	13
	Animal Behavior	13
	Cell Biology	10
	Physiology	9
	Biochemistry	8
	Genetics	8
	Bioengineering / Biomaterials	3

## B. Example Data

### B.1 Task examples

#### Physics: Free-Form Question

**Paper Title:** Compact Continuous Cold Atomic Beam from a Single Cell with 3D Cooling and Ultra-low Light Shift

**Link to The Paper:** <https://arxiv.org/abs/2510.13126>

**Experimental Setup:** Researchers investigated a compact single-cell source of a continuous cold-atom beam ( $^{87}\text{Rb}$ ) that achieves simultaneous 3D cooling by integrating a two-dimensional magneto-optical trap (2D MOT) with an off-axis moving optical molasses (OM). A vapor-cell apparatus (overall length  $\approx 170$  mm) provided transverse MOT cooling with circularly polarized beams detuned by  $\Delta\text{MOT} = -4\Gamma$  from the  $F = 2 \rightarrow F' = 3$   $D_2$  transition and a cylindrical quadrupole field ( $\approx 10$  G cm $^{-1}$ ), where  $\Gamma$  is the natural linewidth. Longitudinal cooling and velocity control were realized with two pairs of lin $\perp$ lin OM beams oriented  $20^\circ$  to the extraction axis, detuned by  $\Delta\text{OM} = -5\Gamma$  and symmetrically shifted by  $\pm\delta\text{OM}$  to set the mean atomic speed ( $\approx 5$ – $20$  m s $^{-1}$ ) over an OM interaction length  $\text{IOM} \approx 50$  mm. Custom in-vacuum mirrors formed the off-axis geometry and incorporated a 0.8 mm output aperture to collimate the beam (cooling length  $\text{lc} \approx 50$  mm) while suppressing near-resonant stray light. The setup included permanent-magnet field generation, state-preparation “plug” lasers 40 mm downstream for sharp time-of-flight (TOF) edges, and fluorescence detection at 294 mm with a calibrated photomultiplier tube (PMT) to extract longitudinal temperature, velocity, and flux. For coherence diagnostics, two  $\pi/2$  Raman beams separated by  $L = 100$  mm in a magnetically shielded region produced spatial-domain Raman–Ramsey fringes, enabling quantification of decoherence and ultra-low light shift (typ. -0.51 Hz) under operating MOT power.

**Measurements Taken:**

- Time-of-flight (TOF) time series and distribution obtained from the emitted fluorescence from the atoms in  $F=2$  state, collected with imaging optics and recorded by a calibrated PMT at a primary detection distance of 294 mm.

**Outcome Prediction Question:** Researchers investigated the longitudinal temperature and atomic flux of a continuous cold  $^{87}\text{Rb}$  beam using a time-of-flight (TOF) method. The temperature was extracted from the FWHM of the TOF distribution, while the flux was obtained from the integrated spectral density. Based on measurements for a saturation intensity of 1.67 mW/cm $^2$ , what outcome would researchers expect for the change in longitudinal temperature and atomic flux when the MOT power is increased?

**Ground Truth Answer:** Increasing MOT power raises the flux but affects the temperature only weakly.

**Background Knowledge:**

- Combining a 2D MOT with an off-axis moving OM yields a high-flux beam with significantly reduced longitudinal temperature compared to conventional MOT-based sources.
- Continuous operation of cold-atom beam sources eliminates the dead time inherent to pulsed sources and thus suppresses aliasing noise from undersampling.

**Rubrics:**

- Response states that increasing the magneto-optical trap power increases atomic flux.
- Response states that increasing the magneto-optical trap power has a little influence on temperature.

## Physics: Multiple-Choice Question

**Paper Title:** Ionization and temperature measurements in warm dense copper using x-ray absorption spectroscopy

**Link to The Paper:** <https://arxiv.org/abs/2509.13272>

**Experimental Setup:** Researchers investigated the ionization and temperature of warm dense copper (Cu) using X-ray absorption spectroscopy (XAS) at the OMEGA Laser Facility to characterize plasmas at several times solid density. The experimental configuration consists of a planar target and a separate backlighter positioned 3 mm away. A series of 60 laser beams, delivering 3.4–5.4 kJ per side of 351 nm light, and the achieved laser intensity is 161 - 770 TW/cm<sup>2</sup> over the three pulse length configurations, was symmetrically focused onto a planar buried-layer target composed of 125  $\mu$ m CH ablatars enclosing a 10  $\mu$ m-thick Cu foil (8.96 g/cm<sup>3</sup> solid density) with a 500  $\mu$ m diameter, surrounded by an Au washer. The laser spot ( $\approx$  880  $\mu$ m diameter) was smoothed with distributed phase plates and spectral dispersion to generate uniform counter-propagating shocks. A 6  $\mu$ m Ge backlighter foil, coated on graphite and irradiated with six additional beams ( $\approx$ 1.2 kJ, 500 ps pulse), is produced at a spot diameter of 140  $\mu$ m. The transmitted x-rays were recorded using the EFX flat-crystal spectrometer (Si 111) over the 6.3–11.4 keV range on an image plate with Mn, Fe, and W filters serving as fiducial markers. Shock timing and planarity, as well as shock break-in and break-out of the Cu layer, were verified through a line-imaging VISAR system and a streaked optical pyrometer (SOP) on one-sided targets, ensuring symmetric compression and precise backlighter synchronization. 3 VISAR measurement is done with 1 ns, 2 ns, or 3 ns square pulses using 14 beams per side, respectively. Each measurement has two VISAR channels with different sensitivities; one leg was set with 33.66  $\mu$ m/ns/fringe, and the second with 13.538  $\mu$ m/ns/fringe.

**Measurements Taken:**

- Shock breakout times (in ns) and planarity were measured with the VISAR system.
- Shock velocity time history as a function of position across the target measured with the VISAR system.

**Outcome Prediction Question:** An investigation into shock breakout times and shock velocity time histories as a function of position across the target of warm dense copper (Cu) plasma is conducted using a VISAR system. The experimental configuration consists of a planar target and a separate backlighter positioned 3 mm away. A series of 60 laser beams was symmetrically focused onto a planar buried-layer target surrounded by an Au washer. The laser spot was smoothed with distributed phase plates and spectral dispersion to generate uniform counter-propagating shocks, compressing the Cu layer. A Ge backlighter foil, coated on graphite and irradiated with six additional beams, is produced. The transmitted X-rays were also recorded using the EFX flat-crystal spectrometer. Which behavior is most likely observed?

- A. Shocks were non-planar over the target region, and warm dense copper shows Ionization Potential Depression (IPD).
- B. Shocks were highly planar over the target region, and the absorption spectra of warm dense copper features blue shift of both the K-edge and the bound-bound resonance 1s $\rightarrow$ 3p absorption relative to the cold edge.
- C. Shocks were highly planar over the target region, and the absorption spectra of warm dense copper features red shift of both the K-edge and the bound-bound resonance 1s $\rightarrow$ 3p absorption relative to the cold edge.
- D. Shocks were highly planar over the target region, and the absorption spectra of warm dense copper features blue shift of the K-edge relative to the cold edge, but no shift for the bound-bound resonance 1s $\rightarrow$ 3p absorption.

**Ground Truth Answer:** B

**Background Knowledge:**

- Generating warm dense matter in the laboratory often involves significant temporal and spatial gradients that complicate the analysis of experimental observables. Incorporating gradients in the analysis of experimental data, while possible, increases the uncertainties in the inferred plasma conditions.
- At these high-density conditions, the measured Cu K-edge exhibits sensitivity to the electron temperature, allowing for a direct inference of the temperature from the slope of the Cu K-edge.
- Temperature sensitivity of the K-edge can still be the dominant edge effect, in general, as the temperature nears the Fermi energy, the K-edge shape of the non-degenerate material becomes unsuitable as a temperature inference.

## Physics: Numerical Value Question

**Paper Title:** A sub-volt near-IR lithium tantalate electro-optic modulator

**Link to The Paper:** <https://arxiv.org/abs/2505.00906>

**Experimental Setup:** Researchers fabricated a TFLT MZM operating at a near-IR wavelength of 737 nm. The fabricated unbalanced MZM consists of a directional coupler as an input beamsplitter and a  $L = 5$  mm long electrode in the ground-signal-ground configuration, followed by another directional coupler at the output. Grating couplers are used to couple light on and off the chip to near-IR single-mode fibers. The optical layer of the device is defined using 150 keV electron-beam lithography with 500 nm-thick ma-N2405 resist on top of a 200 nm-thick x-cut TFLT-on-SiO<sub>2</sub> layer. The waveguide width is designed to be 600 nm. The SiO<sub>2</sub> layer is 2  $\mu$ m-thick and is on a Si substrate. The TFLT is etched by 100 nm using an Ar+-based inductively coupled plasma reactive ion etching. Etch-induced re-deposition is removed using a high-pH solution. The devices are then annealed in an O<sub>2</sub> atmosphere at 520°C for 2 h to mitigate etch-induced imperfections. For the MZMs, an 800 nm-thick SiO<sub>2</sub> cladding layer is then deposited by plasma-enhanced chemical vapor deposition. The DC bias stability of two electro-optic Mach-Zehnder modulators is compared. The first modulator is fabricated using thin-film lithium tantalate (TFLT), and the second, serving as a counterpart, is fabricated with a similar process using thin-film lithium niobate (TFLN). For the test, each modulator is subjected to a constant on-chip optical power of 4.3 dBm at a wavelength of 737 nm. A DC step voltage is applied to each device to set its operating point at quadrature bias. The output optical power from the modulator is then monitored over 16 minutes in ambient conditions to measure any drift from this bias point. To measure the DC bias stability of MZM over long timescales. First, it applied a 0.1 Hz-frequency square wave to the modulator using an on-chip optical power, and measured the modulator response with a photodetector.

**Measurements Taken:**

- The output optical power as a function of time over 16 minutes for the TFLT modulator.
- The output optical power as a function of time over 16 minutes for the TFLN modulator.
- The total DC bias drift, in decibels (dB), for the TFLT modulator.
- The total DC bias drift, in decibels (dB), for the TFLN modulator.

**Outcome Prediction Question:** An experiment compares the long-term stability of two Mach-Zehnder modulators, one made from thin-film lithium tantalate (TFLT) and a counterpart from thin-film lithium niobate (TFLN). Both are operated with 4.3 dBm of on-chip optical power at 737 nm and biased at quadrature. The output power is monitored for 16 minutes to quantify the DC bias drift. To measure the DC bias stability of MZM over long timescales. First, it applied a 0.1 Hz-frequency square wave to the modulator using an on-chip optical power, and measured the modulator response with a photodetector. Based on the experimental results, what is the total measured DC bias drift, in decibels (dB), for the thin-film lithium niobate (TFLN) modulator?

**Ground Truth Answer:**  $\Delta$ DC bias drift = [7.2–8.8] dB at 16 min for the TFLN modulator operated at 4.3 dBm optical power (737 nm). No CI/SE/SD reported → fallback  $\pm 0.8$  dB applied.

**Background Knowledge:**

- In particular, the relaxation rate will increase with more applied optical power and can be exacerbated with applied DC or RF field. This effect reduces the DC stability of electro-optic circuits, such as Mach-Zehnder modulators (MZMs), and has been one of the main challenges faced by TFLN photonics

## Biology: Free-Form Question

**Paper Title:** Dopamine induces fear extinction by activating the reward-responding amygdala neurons

**Link to The Paper:** <https://PMC12067255>

**Experimental Setup:** Researchers tested whether ventral tegmental area (VTA) dopamine signaling in the basolateral amygdala (BLA) drives fear extinction by acting on reward-responding posterior BLA (pBLA) neurons versus fear-coding anterior BLA (aBLA) neurons, using adult mice (DAT-IRES-Cre; EYFP controls; subtype mapping with Rspo2-Cre for aBLA and Ppp1r1b/Cartpt-Cre for pBLA). DAT-Cre mice received bilateral VTA injections of Cre-dependent ChR2-EYFP (activation) or eNpHR3.0-EYFP (inhibition); controls received EYFP; optic fibers were implanted over pBLA or aBLA to manipulate VTA→BLA terminals. Training: Day 1 contextual fear conditioning (baseline ~3 min, then 3 footshocks, 0.60 mA, 2 s); Day 2 45-min extinction (no shocks); Day 3 10-min retrieval. Intervention (extinction only): starting 5 min into extinction, deliver 8 cycles of 3-min light separated by 2-min no-light (activation: blue 450–470 nm, 8–12 mW, 20 Hz pulses; inhibition: green 520–550 nm, 8–12 mW, continuous) with fibers targeted to pBLA or aBLA. Behavior videos were recorded with VideoFreeze software and freezing level was scored manually by experimenters who were blinded to conditions or automatically with DeepLabCut behavior analysis toolbox and custom Python code (68). Freezing was quantified in 5-min bins across extinction and again during retrieval.

**Measurements Taken:**

- Extinction learning: Percent freezing per 5-min bin across the 45-min Day 2 session (9 bins). Scored manually by experimenters who were blinded to conditions or automatically with DeepLabCut behavior analysis toolbox and custom Python code (68).
- Extinction memory: Percent freezing during the Day 3 retrieval test (10 min). Scored manually by experimenters who were blinded to conditions or automatically with DeepLabCut behavior analysis toolbox and custom Python code (68).

**Outcome Prediction Question:** Mice underwent contextual fear conditioning (Day 1: context + three 0.60 mA, 2 s shocks), 45-min extinction (Day 2, no shocks), and 10-min retrieval (Day 3). During extinction, VTA dopamine terminals in pBLA (Ppp1r1b<sup>+</sup>) or aBLA (Rspo2<sup>+</sup>) were optogenetically manipulated beginning 5 min into the session using 8 cycles of 3 min light separated by 2 min: activation (blue 450–470 nm, 8–12 mW, 20 Hz) or inhibition (green 520–550 nm, 8–12 mW, constant). Freezing was binned in 5-min windows across extinction and measured again at retrieval. How do these projection-specific manipulations (activation and inhibition of VTA dopamine terminals in the pBLA and in aBLA) affect fear extinction and retrieval compared with EYFP controls?

**Ground Truth Answer:** Activation of VTA dopamine terminals in the pBLA promotes faster extinction and improved retrieval, indicating an enhancement of extinction learning. In contrast, inhibition of pBLA dopamine input impairs both extinction and retrieval. Activation of VTA terminals in the aBLA leads to increased freezing later in extinction and poorer retrieval performance, suggesting interference with extinction memory formation, while inhibition of aBLA terminals produces no reliable behavioral change.

**Background Knowledge:**

- Fear extinction is a form of new learning that allows for the adaptive control of fear behaviors and is commonly studied using Pavlovian conditioning tasks.
- aBLA Rspo<sup>+</sup> neurons encode negative valence and drive aversive behaviors whereas pBLA Ppp1r1b<sup>+</sup> neurons encode positive valence and drive appetitive behaviors.
- VTA dopamine as a teaching signal: DA activity to shock omission can initiate extinction learning and is required for extinction.
- Terminal activation (ChR2, blue, pulsed) vs inhibition (eNpHR3.0, green, constant) at BLA terminals tests sufficiency/necessity of VTA→BLA pathways.
- Freezing is the behavioral measure; decreases across 5-minute bins and at retrieval indicate successful extinction.

**Rubrics:**

- The response should state that activation of ventral tegmental area dopamine terminals in the posterior basolateral amygdala of adult mice promotes faster extinction compared to control. Use of acronyms such as VTA or pBLA are acceptable.
- The response should state that activation of ventral tegmental area dopamine terminals in the posterior basolateral amygdala of adult mice improves retrieval compared to control. Use of acronyms such as VTA or pBLA are acceptable.
- The response should state that inhibition of ventral tegmental area dopamine terminals in the posterior basolateral amygdala of adult mice impairs extinction compared to control. Use of acronyms such as VTA or pBLA are acceptable.
- The response should state that inhibition of ventral tegmental area dopamine terminals in the posterior basolateral amygdala of adult mice impairs retrieval compared to control. Use of acronyms such as VTA or pBLA are acceptable.
- The response should state that activation of ventral tegmental area terminals in the anterior basolateral amygdala of adult mice leads to increased freezing later in extinction compared to control. Use of acronyms such as VTA or aBLA are acceptable.
- The response should state that activation of ventral tegmental area terminals in the anterior basolateral amygdala of adult mice leads to poorer retrieval performance compared to control. Use of acronyms such as VTA or aBLA are acceptable.
- The response should state that inhibition of ventral tegmental area terminals in the anterior basolateral amygdala of adult mice produces no reliable behavioral change compared to control. Use of acronyms such as VTA or aBLA are acceptable.

## Biology: Multiple-Choice Question

**Paper Title:** Social Tolerance and Innovation in Capuchins: socially more tolerant brown capuchins are better problem-solvers than less tolerant white-faced capuchins

**Link to The Paper:** <https://www.biorxiv.org/content/10.1101/2025.09.05.674457v1.full>

**Experimental Setup:** Researchers tested three groups of white-faced capuchins (*Cebus capucinus*) (n = 23 individuals in total) and three groups of brown capuchins (*Sapajus apella*) (n = 20 individuals in total) to explore and compare the relationship between social tolerance and problem-solving propensities. To measure social tolerance, they prepared an area of 1 m<sup>2</sup> per five animals in the group, in which they distributed apple pieces and measured the proportion of individuals within the co-feeding area at each scan sample. To measure problem-solving propensities, they designed three versions of novel extractive foraging devices requiring one to three steps to acquire the food reward. For the first puzzle, animals had to rotate a door to either the left or right to access a hidden reward (1/24 of an apple) by reaching into a box. For the second puzzle, animals had to pull on a chain reaching out of a box, which moved a blockade out of the way so that they could push in a door and reach into the box. For the third puzzle, animals had to pull a metal rod blocking a slider that had to be pulled upwards and held in position to reach into the box and then pull on a chain to access the hidden reward. Researchers analyzed the approaching, exploring, and solving behaviour separately.

**Measurements Taken:**

- Proportion of individuals within the co-feeding area at each scan sample (social tolerance)
- Proportion of individuals within the puzzle area at each scan sample (social tolerance)
- Number of approaches to a food puzzle area
- Approaching a food puzzle area duration
- Approaches to a food puzzle area latency
- Number of exploration events (touch, sniff, interact) during the approaches to a food puzzle area
- Number of times the capuchins successfully solved the puzzles
- Exploration of food puzzle events latency
- Time to solve a puzzle

**Outcome Prediction Question:** Researchers tested three groups of white-faced capuchins (*Cebus capucinus*) and three groups of brown capuchins (*Sapajus apella*) to explore and compare the relationship between social tolerance and problem-solving propensities. To measure social tolerance, they prepared an area of 1 m<sup>2</sup> per five animals in the group, in which they distributed apple pieces and measured the proportion of individuals within the co-feeding area at each scan sample. To measure problem-solving propensities, they designed three versions of novel extractive foraging devices requiring one to three steps to acquire the food reward. Which of the following outcomes is most likely?

- A. Both species should show the same levels of social tolerance and problem-solving propensities.
- B. White-faced capuchins should show the highest level of social tolerance and problem-solving propensities.
- C. White-faced capuchins should show the lowest level of social tolerance and problem-solving propensities.
- D. White-faced capuchins should show the highest level of social tolerance and the lowest level of problem-solving propensities.

**Ground Truth Answer:** C

**Background Knowledge:**

- Social tolerance has increasingly been linked to the facilitation of social learning across a variety of species, including chimpanzees, orangutans, macaques, capuchin monkeys, lemurs, and birds.
- White-faced capuchins (*Cebus capucinus*) and brown capuchins (*Sapajus apella*) exhibit a diverse array of traditions.
- White-faced capuchins (*Cebus capucinus*) are less known for using tools (but see Barrett et al., 2018), but they regularly engage in object use (Boinski, 1988).
- Robust capuchins (*Sapajus spp.*) have fewer documented social traditions but exhibit a wide range of foraging traditions, including tool-use, and show notable social tolerance in these contexts, tolerating close proximity of conspecifics.

## Biology: Numerical Value Question

**Paper Title:** GsMTx4-loaded GelMA promotes tendon regeneration and suppresses heterotopic ossification via the Apelin signaling pathway

**Link to The Paper:** <https://www.sciencedirect.com/science/article/pii/S0142961225004260?via%3Dihub>

**Experimental Setup:** Researchers employed Male Sprague Dawley (SD) rats (10–12 weeks old, weighing 250–300 g) as animal model for studying tendon repair and regeneration. A central defect (1 mm in width and 5 mm in length) was created in the Achilles tendon using two parallel No.15 surgical blades. Subsequently, the skin was sutured using 4-0 Vicryl sutures. The rats received temgesic (0.3 mg/kg of body weight) for three consecutive days following the surgery to manage pain. The rats were randomly assigned to one of four groups: Achilles tendon defect (ATD) (no treatment), GelMA, GelMA + 50 µg GsMTx4, GelMA + 100 µg GsMTx4. At the time of injury, a mixture of GelMA and LAP (Lithium Phenyl-2,4,6-Trimethylbenzoylphosphinate) (20 µl), loaded with 50 or 100 µg GsMTx4 where appropriate, was placed within the ATD of treated animals and transformed into the gel state with a blue light source (3 W, 405 nm) for 30 s at a distance of 2 cm from the defect. These animals were euthanized at 2, 4, and 8 weeks post-treatment, with six rats per group per time point. The harvested Achilles tendons were fixed in 4% paraformaldehyde at room temperature for 24 h. Following fixation, the samples were rinsed with running water and dehydrated with an ethanol gradient, and embedded in paraffin. The blocks were sectioned at 5 µm thickness using a microtome and stained with Hematoxylin and Eosin (H&E). Semi-quantitative analysis of H&E staining results was conducted according to the modified Bonar score.

**Measurements Taken:**

- Histologic Bonar Score (ATD, GelMA, GelMA + 50 µg GsMTx4, GelMA + 100 µg GsMTx4): 2 weeks; 4 weeks; 8 weeks.

**Outcome Prediction Question:** Researchers employed Male Sprague Dawley (SD) rats (10–12 weeks old, weighing 250–300 g) as animal model for studying tendon repair and regeneration. A central defect (1 mm in width and 5 mm in length) was created in the Achilles tendon using two parallel No.15 surgical blades. The rats were randomly assigned to one of four groups: Achilles tendon defect (ATD) (no treatment), GelMA, GelMA + 50 µg GsMTx4, GelMA + 100 µg GsMTx4. At the time of injury, a mixture of GelMA and LAP (Lithium Phenyl-2,4,6-Trimethylbenzoylphosphinate) (20 µl), loaded with 50 or 100 µg GsMTx4 where appropriate, was placed within the ATD of treated animals and transformed into the gel state with a blue light source. The animals were euthanized at 2, 4, and 8 weeks post-treatment. The harvested Achilles tendons were embedded in paraffin, sectioned using a microtome, and stained with Hematoxylin and Eosin (H&E). Semi-quantitative analysis of H&E staining results was conducted according to the modified Bonar score (BS). Based on the reported values of the BS for Achilles tendon repair and regeneration, what is the predicted difference of the BS (in points) between the GelMA and the GelMA + 100 µg GsMTx4 groups 8-weeks post treatment?

**Ground Truth Answer:**  $\Delta$  BS (GelMA - GelMA + 100 µg GsMTx4) 8-weeks post treatment = 4 - 6 points; derived from BS GelMA 8-weeks post treatment = ~9 points, BS GelMA + 100 µg GsMTx4 8-weeks post treatment = ~4 points. Note: No CI/SE/SD reported -> fallback  $\pm$  10% units (rounded) applied.

**Background Knowledge:**

- Tendon regeneration is highly relied on the surrounding mechanical environment.
- Studies have demonstrated the importance of Piezo1 in modulating cellular behaviors to mechanical cues, such as cell migration, differentiation, proliferation, and extracellular matrix synthesis.
- GelMA hydrogel demonstrates excellent biocompatibility and sustained release properties.
- The mechanosensitive ion channel Piezo1 is inhibited by the peptide GsMTx4

## Chemistry: Free-Form Question

**Paper Title:** An investigation of the physical and chemical changes of Pd nanoparticles on carbon supports in response to the release of hydrogen from aqueous formate solutions

**Link to The Paper:** <https://chemrxiv.org/engage/chemrxiv/article-details/68d16d29f2aff16770fa93bd>

**Experimental Setup:** Researchers prepared and analyzed Pd nanoparticles supported on carbon materials to examine their structural and chemical evolution during hydrogen release from aqueous sodium formate. Three supports were used: carbon black (Vulcan XC-72), nitrogen-doped carbon (NC), and graphitic carbon nitride ( $\text{g-C}_3\text{N}_4$ ). Nitrogen-doped carbon was obtained by heating a melamine–carbon black mixture at 700 °C under nitrogen, while  $\text{g-C}_3\text{N}_4$  was synthesized by heating urea at 500 °C in air. Pd catalysts were produced by reducing  $\text{H}_2\text{PdCl}_4$  with  $\text{NaBH}_4$  in trisodium citrate solution at 25 °C, yielding a 1 wt% Pd loading. The product was filtered, washed, and dried at 85 °C for 24 h, and selected samples were calcined at 250 °C for 3 h in air. Structural and compositional analyses included inductively coupled plasma–optical emission spectrometry (PerkinElmer 7300 DV) to determine Pd content, X-ray diffraction (Rigaku SmartLab SE,  $\text{Cu K}\alpha$ ,  $2\Theta = 2\text{--}100^\circ$ ) to assess crystallinity, and nitrogen physisorption (Micromeritics ASAP 2020) using BET and BJH models to measure surface area and pore volume. Pd dispersion was quantified by CO chemisorption (Micromeritics ASAP 2020C, 30 °C, pre-reduced at 100 °C for 0.5 h), and nanoparticle morphology was examined by aberration-corrected scanning transmission electron microscopy (Thermo Fisher Themis Z, 300 kV). Catalytic performance was tested in a 50 mL batch reactor containing 250 mg of catalyst and 10 mL of 1 M sodium formate at 65 °C under  $\text{N}_2$  with stirring at 500 rpm for 2 h, where gas evolution was monitored by pressure change and analyzed using a micro-gas chromatograph. In-situ X-ray absorption spectroscopy was performed at the Stanford Synchrotron Radiation Lightsource beamline 4-1 to monitor Pd oxidation states during reaction using Pd K-edge XANES and EXAFS scans (24126–25238 eV, 0.5 × 4 mm beam). Catalyst reuse tests were carried out by recovering the solid after reaction, washing with deionized water, drying at 80 °C, and re-calcining at 180 or 250 °C for 3 h when required. All synthesis, characterization, and catalytic experiments were conducted under controlled temperature and atmospheric conditions to ensure reproducibility.

**Measurements Taken:**

- Pd oxidation state and local atomic structure characterized by in-situ X-ray Absorption Spectroscopy (XAS, SSRL beamline 4-1) with Pd K-edge XANES and EXAFS scans (24126–25238 eV, beam size 0.5 × 4 mm) under reaction conditions.
- Palladium loading (wt%) measured using Inductively Coupled Plasma–Optical Emission Spectroscopy (ICP-OES, PerkinElmer 7300 DV) to quantify Pd content on carbon supports.

**Outcome Prediction Question:** Palladium nanoparticles supported on carbon materials were assessed as catalysts for hydrogen release from aqueous sodium formate. Three supports- carbon black (Vulcan XC-72), nitrogen-doped carbon (NC), and graphitic carbon nitride ( $\text{g-C}_3\text{N}_4$ )- were employed, with NC synthesized by heating a melamine–carbon black mixture at 700 °C under  $\text{N}_2$  and  $\text{g-C}_3\text{N}_4$  prepared by urea pyrolysis at 500 °C in air. Pd catalysts (1 wt%) were obtained by reducing  $\text{H}_2\text{PdCl}_4$  with  $\text{NaBH}_4$  in trisodium citrate at 25 °C, followed by drying and optional calcination at 250 °C. Structural and chemical characterization included ICP–OES for Pd content, XRD for crystallinity,  $\text{N}_2$  physisorption for surface area, CO chemisorption for Pd dispersion, and STEM for nanoparticle morphology. Catalytic performance was evaluated in a batch reactor (65 °C, 1 M sodium formate) by monitoring gas evolution and composition via micro-GC. In-situ XANES/EXAFS at the Pd K-edge tracked oxidation-state changes during reaction, and reuse tests examined catalyst stability following washing and re-calcination. What will in-situ XANES analysis reveal about the role of palladium oxide (PdO) as an active catalyst for formate dehydrogenation?

**Ground Truth Answer:** In-situ XANES experiments unambiguously demonstrate that PdO is rapidly reduced to metallic Pd and then forms Pd hydride upon exposure to a formate solution, showing that PdO does not play a direct role in the mechanism of  $\text{H}_2$  formation.

**Background Knowledge:**

- Palladium nanoparticles on carbon supports (Pd/C) are effective for catalyzing hydrogen release from aqueous formate solutions but typically suffer from a gradual decrease of activity.
- Nitrogen doping of carbon supports is observed to enhance the rates of hydrogen release from aqueous formate solutions

**Rubrics:** The response must state that palladium oxide (PdO) does not play a direct role as the active catalyst in the mechanism of  $\text{H}_2$  formation.

## Chemistry: Multiple-Choice Question

**Paper Title:** Lab-Scale Thermal Decomposition of Hydrogen Peroxide as Green Propellant over Low-Cost Catalysts Based on Copper Deposited on Different Supports

**Link to The Paper:** <https://www.mdpi.com/2226-4310/12/5/440>

**Experimental Setup:** Researchers investigate the thermal degradation of the  $\text{H}_2\text{O}_2$  green monopropellant. Three distinct catalysts—copper supported on  $\gamma$ -alumina, graphite, and MNC clay—were used. Conversely, a LABSYS evo-gasorption apparatus (Category: DTA/TG/DSC, Model: Setaram Instrumentation) was used to perform differential thermal analysis– thermogravimetry (DTA–TG) measurements in order to investigate the thermal breakdown of  $\text{H}_2\text{O}_2$  at constant atmospheric pressure ( $p = 1 \text{ atm}$ ). A syringe was used to inject a 30% (w/w)  $\text{H}_2\text{O}_2$  microdroplet into the metallic sample cell. It was investigated how the three different catalysts affected the  $\text{H}_2\text{O}_2$  thermogram. A microdroplet of liquid  $\text{H}_2\text{O}_2$  was combined with a modest amount (a few micrograms) of powdered catalyst in the aluminum sample cell for each thermal study. Before each run, the following experimental conditions were maintained:

- (i) Carrier gas: argon, with a flow rate of  $50 \text{ mL}\cdot\text{min}^{-1}$ ;
- (ii) Heating rate:  $10 \text{ }^{\circ}\text{C}\cdot\text{min}^{-1}$ , from room temperature up to  $250 \text{ }^{\circ}\text{C}$ ;
- (iii) The  $\text{H}_2\text{O}_2$  droplet was added directly to the catalyst particles already placed in the aluminum cell. After sealing the apparatus, a stabilization period of approximately 2 min was allowed for the system (carrier gas and sample) to equilibrate. The thermal run was then initiated to record the DTA–TG thermograms.

Experiments were run at two constant temperatures:  $0 \text{ }^{\circ}\text{C}$  and  $36 \text{ }^{\circ}\text{C}$

**Measurements Taken:**

- Differential pressure ( $\Delta P$ , in kPa) vs time (minutes) was recorded.
- $\Delta P$  for each catalyst ( $\text{Cu}/\gamma$ -alumina,  $\text{Cu}/\text{graphite}$ ,  $\text{Cu}/\text{clay}$ ) compared to the uncatalyzed control.
- $\Delta P$  at  $0 \text{ }^{\circ}\text{C}$  and  $36 \text{ }^{\circ}\text{C}$  to assess temperature effects on decomposition rate.

**Outcome Prediction Question:** Which of the following statements best describes the observed catalytic activity (as measured by differential pressure,  $\Delta P$ , vs time) for the decomposition of 30 %  $\text{H}_2\text{O}_2$  over the three copper-supported catalysts ( $\text{Cu}/\gamma$ -alumina,  $\text{Cu}/\text{graphite}$ ,  $\text{Cu}/\text{clay}$ ) compared to the uncatalyzed decomposition, at  $36 \text{ }^{\circ}\text{C}$  and  $0 \text{ }^{\circ}\text{C}$ ?

- A. At both temperatures all three catalysts produce rates almost identical to each other; the rates follow a similar trend, with  $0 \text{ }^{\circ}\text{C}$  just being slower than  $36 \text{ }^{\circ}\text{C}$ , each gives a large increase over the uncatalyzed reaction at both temperatures.
- B. At  $0 \text{ }^{\circ}\text{C}$  all three catalysts give a similar rate, none of them is clearly faster than another, but at  $36 \text{ }^{\circ}\text{C}$   $\text{Cu}/\gamma$ -alumina gives the highest rate (largest  $\Delta P$  increase), followed by  $\text{Cu}/\text{graphite}$ , then  $\text{Cu}/\text{clay}$ , each significantly faster than uncatalyzed at both temperatures.
- C. At  $0 \text{ }^{\circ}\text{C}$ ,  $\text{Cu}/\text{clay}$  a rate that is slower than the uncatalyzed reaction at the beginning, then becomes faster than the uncatalyzed reaction, while  $\text{Cu}/\text{graphite}$ , and  $\text{Cu}/\gamma$ -alumina have a similar rate and are higher than the uncatalyzed reaction. At  $36 \text{ }^{\circ}\text{C}$  all three are faster than uncatalyzed reaction,  $\text{Cu}/\gamma$ -alumina is the fastest, closely followed by  $\text{Cu}/\text{graphite}$ , then  $\text{Cu}/\text{clay}$ .
- D. At  $0 \text{ }^{\circ}\text{C}$  all three catalysts begin slightly faster than the uncatalyzed reaction then all three become much faster, the variability being larger than the difference between the catalysts. At  $36 \text{ }^{\circ}\text{C}$  the reaction with all three catalysts is much faster than the uncatalyzed reaction, with  $\text{Cu}/\gamma$ -alumina being much faster than  $\text{Cu}/\text{graphite}$ , then  $\text{Cu}/\text{clay}$  lags because the copper particles came off the support particles.

**Ground Truth Answer:** C

**Background Knowledge:**

- As the world increasingly focuses on sustainable and environmentally friendly solutions, there is a growing interest in exploring greener alternative propellants that offer comparable performance while mitigating the drawbacks associated with hydrazine and its derivatives.
- The thermal decomposition of hydrogen peroxide ( $\text{H}_2\text{O}_2$ ) as a promising green propellant was performed over free-noble metallic-based catalysts deposited on abundant supports.
- Green monopropellants have the potential for long-term cost savings due to reduced safety measures, disposal costs, and regulatory compliance requirements associated with hazardous materials such as hydrazine.

## Chemistry: Numerical Value Question

**Paper Title:** Time-resolved photo-electrochemical measurements to study band bending of BiVO<sub>4</sub> photoanodes

**Link to The Paper:** <https://chemrxiv.org/engage/chemrxiv/article-details/68b1a2e2728bf9025e19a17e?>

**Experimental Setup:** Thin-film BiVO<sub>4</sub> photoanodes were investigated in a three-electrode photo-electrochemical RRDE cell under chopped AM 1.5G illumination. Light switch-ON/OFF transients were recorded over 0–2.5 V vs RHE, and the disk photocurrent during switch-ON was fit with exponentials to isolate the fast space-charge reorganization time constant ( $\tau_{\text{fast}}$ ) (along with slower components).

**Measurements Taken:**

- Disk photocurrent transients\*\* at light switch-ON/OFF (current vs time) across 0–2.5 V vs RHE.
- Exponential fits of transients to extract characteristic time constants (including  $\tau_{\text{fast}}$ ) in seconds; report the average  $\tau_{\text{fast}}$  (switch-ON) over the potential window.
- Steady-state J–E curves\*\* under illumination.
- RRDE ring current\*\* (Pt ring) vs time/potential for O<sub>2</sub> detection/validation.
- Assignment of  $\tau_{\text{fast}}$  to space-charge reorganization based on transient behavior.

**Outcome Prediction Question:** Thin-film BiVO<sub>4</sub> photoanodes were tested in a three-electrode photo-electrochemical RRDE cell under chopped AM 1.5G illumination. During light “switch-ON” steps over 0–2.5 V vs RHE, the disk photocurrent transients were fit with exponentials to isolate the fast space-charge reorganization process ( $\tau_{\text{fast}}$ ). At these conditions, what is the average value of  $\tau_{\text{fast}}$  in seconds (s) for the switch-ON process?

**Ground Truth Answer:** 0.0022±0.002 s.

**Background Knowledge:**

- BiVO<sub>4</sub> is a semiconductor photoanode used for oxygen evolution under illumination; its behavior is probed in a three-electrode photoelectrochemical cell.
- Band bending at the semiconductor/electrolyte interface creates a space-charge region that governs carrier separation and the early transient response.
- Time-resolved photoelectrochemistry with chopped AM 1.5G illumination measures photocurrent transients at light on/off to extract characteristic time constants.
- A rotating ring–disk electrode (RRDE) uses a Pt ring to detect dissolved O<sub>2</sub> produced at the disk, distinguishing disk photocurrent from ring current.
- The flat-band potential is the potential where band bending vanishes and is estimated from cyclic-voltammetry features; potentials are reported vs RHE.
- Exponential fitting of transients yields  $\tau_{\text{fast}}$  and slower components that reflect interfacial charge reorganization and reaction kinetics.

## B.2 Example human responses

Physics: Numerical Value Question

**Paper Title:** Recent Highlights from the STAR Experiment

**Link to The Paper:** <https://arxiv.org/abs/2508.08444>

**Experimental Setup:** Researchers investigated the Beam Energy Scan-II (BES-II) program at the STAR experiment, which was used to measure net-proton cumulant ratios in Gold-on-Gold (Au+Au) collisions at various center-of-mass energies (from 7.7 to 27 GeV) in the Fixed-Target mode. BES-II employed a new centrality definition, RefMult3X, corresponding to pseudorapidity acceptances fulfilling  $|\eta| < 1.6$ . The Time-Projection Chamber (TPC) for low transverse momentum ( $0.4 < pT < 0.8$  GeV/c) and the Time-Of-Flight (TOF) detector for greater transverse momentum ( $0.8 < pT < 2.0$  GeV/c) were used to identify protons and anti-protons. Only particles falling within the speed window of  $|y| < 0.5$  were included in the analysis. The most central collisions (0-5% centrality class) were the focus of the measurements, which were methodically adjusted for experimental variables such detector efficiency, event pile-up, and centrality bin width.

**Measurements Taken:**

- Net-proton cumulants (C1, C2, C3, C4) as a function of collision centrality and collision energy.
- The relative dynamical correlation of transverse momentum as a function of collision energy.

**Outcome Prediction Question:** In the STAR experiment's Beam Energy Scan-II (BES-II), what was the measured value of the net-proton cumulant ratio C4/C2 at the collision energy of 19.6 GeV for the 0-5% centrality class?

**Ground Truth Answer:** [0.25-0.40]

Note: The range is informed graphically in Figure 3. The range was estimated by the pixel coordinates of the error bars and axis ticks.

**Background Knowledge:**

- The upgrades done to STAR for BES-II enabled a new centrality definition, RefMult3X, which achieves better centrality resolution due to larger multiplicity within the acceptance.
- Experimentally measured proton multiplicity distributions are described by the central moments, which depend on the cumulants. In particular, the second cumulant C2 is the variance  $\sigma^2$ , and the ratio between the fourth and second cumulant, C4/C2, is  $\kappa\sigma^2$ , where  $\kappa$  is the kurtosis.
- When there are no intrinsic correlations among the measured particles, all ratios of the cumulants are unity, so Poisson statistics is a trivial baseline for experimentally measured cumulant ratios.

## Human Responses

**Answer (NBK):** The measured value of the net-proton cumulant ratio  $C_4/C_2$  at the collision energy of 19.6 GeV for the 0-5% centrality class is 0.4.

**Reasoning (NBK):** Theoretically, the ratio of the fourth- to the second-order net-proton cumulant ( $C_4/C_2$ ) is often called the moment product  $\kappa\sigma^2$ . Here,  $\kappa$  is the kurtosis and  $\sigma^2$  is the variance. The theoretical Poisson baseline for net-proton cumulant ratios is unity or 1. Hence, the measured value must be  $\leq 1$ .

Additionally, various previous experiments support the fact that the  $C_4/C_2$  value is close to unity for all collision energies for the smallest rapidity acceptance, and for higher collision energies. For example, according to Adam et al. (2021), during the BES-I experiment of the STAR detector at RHIC, the mean  $C_4/C_2$  ratio in the 0-5% bin is  $\sim 0.4$ . This result is also supported by Bleicher et. al. (1999) during the Ultra-Relativistic Quantum Molecular Dynamics (UrQMD) experiment.

**Confidence (NBK):** Somewhat confident in your answer

**Difficulty (NBK):** Easy to answer

**Answer (BK):** The measured value of the net-proton cumulant ratio  $C_4/C_2$  at the collision energy of 19.6 GeV for the 0-5% centrality class is 0.4.

**Reasoning (BK):** Theoretically, the ratio of the fourth- to the second-order net-proton cumulant ( $C_4/C_2$ ) is often called the moment product  $\kappa\sigma^2$ . Here,  $\kappa$  is the kurtosis and  $\sigma^2$  is the variance. The theoretical Poisson baseline for net-proton cumulant ratios is unity or 1. Hence, the measured value must be  $\leq 1$ .

Additionally, various previous experiments support the fact that the  $C_4/C_2$  value is close to unity for all collision energies for the smallest rapidity acceptance, and for higher collision energies. For example, according to Adam et al. (2021), during the BES-I experiment of the STAR detector at RHIC, the mean  $C_4/C_2$  ratio in the 0-5% bin is  $\sim 0.4$  [Figure 8]. This result is also supported by Bleicher et. al. (1999) during the Ultra-Relativistic Quantum Molecular Dynamics (UrQMD) experiment [Figures 6 and 30].

**Confidence (BK):** Somewhat confident in your answer

**Difficulty (BK):** Easy to answer

**Feasibility:** Very feasible to answer without running the experiment

**Feasibility Reasoning:** Theoretically, the ratio of the fourth- to the second-order net-proton cumulant ( $C_4/C_2$ ) is often called the moment product  $\kappa\sigma^2$ . Here,  $\kappa$  is the kurtosis and  $\sigma^2$  is the variance. The theoretical Poisson baseline for net-proton cumulant ratios is unity or 1. Hence, the measured value must be  $\leq 1$ , which can be directly concluded from the known theory on this topic.

Additionally, various previous experiments support the fact that the  $C_4/C_2$  value is close to unity for all collision energies for the smallest rapidity acceptance, and for higher collision energies. For example, according to Adam et al. (2021), during the BES-I experiment of the STAR detector at RHIC, the mean  $C_4/C_2$  ratio in the 0-5% bin is  $\sim 0.4$  [Figure 8]. This result is also supported by Bleicher et. al. (1999) during the Ultra-Relativistic Quantum Molecular Dynamics (UrQMD) experiment [Figures 6 and 30].

Hence, using the existing literature on previously performed experiments, the measured value of  $C_4/C_2$  can be logically estimated for the BES-II experiment of the STAR detector at RHIC.

## C. Additional Results

Table 3: Different versions of Gemini, OpenAI, Claude Sonnet, Llama, Qwen, and Deepseek evaluated on Chemistry, Biology, Physics, and all domains. Best values within each family are highlighted. **Conf.** := Confidence Score; **Diff.** := Difficulty Level; **Feas.** := Feasibility Score.

Model	Experimental Setup	Chemistry			Biology			Physics			All Domains						
		Calibration (1-5)			Calibration (1-5)			Calibration (1-5)			Calibration (1-5)						
		Accuracy (%)	Conf.	Diff.	Feas.	Accuracy (%)	Conf.	Diff.	Feas.	Accuracy (%)	Conf.	Diff.	Feas.	Accuracy (%)	Conf.	Diff.	Feas.
Gemini 3-pro	NBK	26.14 ± 5.40	4.37 ± 0.01	3.56 ± 0.03	3.55 ± 0.04	24.47 ± 1.24	4.38 ± 0.02	3.44 ± 0.01	3.55 ± 0.09	26.00 ± 0.00	4.56 ± 0.02	3.39 ± 0.01	3.71 ± 0.10	25.27 ± 1.92	4.42 ± 0.01	3.46 ± 0.01	3.59 ± 0.06
	BK	28.43 ± 0.98	4.39 ± 0.03	3.52 ± 0.02	3.50 ± 0.07	27.26 ± 0.75	4.39 ± 0.02	3.40 ± 0.07	3.59 ± 0.03	26.33 ± 2.08	4.56 ± 0.01	3.25 ± 0.00	3.89 ± 0.06	27.33 ± 0.79	4.43 ± 0.01	3.40 ± 0.04	3.64 ± 0.02
	SBK	28.43 ± 0.00	4.43 ± 0.00	3.45 ± 0.00	3.71 ± 0.00	26.11 ± 0.00	4.45 ± 0.00	3.19 ± 0.00	3.89 ± 0.00	21.00 ± 0.00	4.63 ± 0.00	3.24 ± 0.00	4.00 ± 0.00	25.43 ± 0.00	4.49 ± 0.00	3.27 ± 0.00	3.87 ± 0.00
	SABK	30.39 ± 0.00	4.48 ± 0.00	3.42 ± 0.00	3.79 ± 0.00	25.12 ± 0.00	4.44 ± 0.00	3.20 ± 0.00	3.78 ± 0.00	27.00 ± 0.00	4.68 ± 0.00	3.14 ± 0.00	4.01 ± 0.00	26.91 ± 0.00	4.51 ± 0.00	3.24 ± 0.00	3.84 ± 0.00
Claude Opus 4.5	FBK	25.49 ± 0.00	4.35 ± 0.00	3.53 ± 0.00	3.47 ± 0.00	24.63 ± 0.00	4.32 ± 0.00	3.49 ± 0.00	3.35 ± 0.00	23.00 ± 0.00	4.63 ± 0.00	3.32 ± 0.00	3.75 ± 0.00	24.44 ± 0.00	4.40 ± 0.00	3.40 ± 0.00	3.48 ± 0.00
	NBK	15.69 ± 0.98	3.19 ± 0.08	4.04 ± 0.03	2.78 ± 0.08	25.12 ± 0.49	3.30 ± 0.00	3.98 ± 0.02	2.92 ± 0.04	26.33 ± 2.08	3.48 ± 0.03	4.01 ± 0.02	3.17 ± 0.06	23.05 ± 0.51	3.32 ± 0.04	4.00 ± 0.02	2.95 ± 0.01
	BK	22.88 ± 1.50	3.20 ± 0.01	4.03 ± 0.01	2.85 ± 0.06	27.09 ± 0.85	3.38 ± 0.02	3.92 ± 0.05	3.00 ± 0.01	32.33 ± 2.08	3.51 ± 0.04	3.93 ± 0.00	3.14 ± 0.03	27.33 ± 0.75	3.37 ± 0.02	3.95 ± 0.03	3.00 ± 0.01
	SBK	17.65 ± 0.00	3.27 ± 0.00	4.01 ± 0.00	2.86 ± 0.00	27.00 ± 0.00	3.46 ± 0.00	3.81 ± 0.00	3.12 ± 0.00	29.00 ± 0.00	3.51 ± 0.00	3.90 ± 0.00	3.23 ± 0.00	25.14 ± 0.00	3.43 ± 0.00	3.88 ± 0.00	3.08 ± 0.00
Claude Sonnet 4.5	SABK	18.63 ± 0.00	3.40 ± 0.00	3.91 ± 0.00	3.01 ± 0.00	26.60 ± 0.00	3.48 ± 0.00	3.83 ± 0.00	3.17 ± 0.00	32.00 ± 0.00	3.64 ± 0.00	3.77 ± 0.00	3.41 ± 0.00	25.93 ± 0.00	3.50 ± 0.00	3.83 ± 0.00	3.19 ± 0.00
	FBK	23.53 ± 0.00	3.19 ± 0.00	4.02 ± 0.00	2.89 ± 0.00	26.60 ± 0.00	3.28 ± 0.00	3.97 ± 0.00	2.95 ± 0.00	32.00 ± 0.00	3.39 ± 0.00	3.97 ± 0.00	3.12 ± 0.00	25.93 ± 0.00	3.28 ± 0.00	3.98 ± 0.00	2.95 ± 0.00
	NBK	23.86 ± 1.50	3.98 ± 0.02	3.77 ± 0.01	3.24 ± 0.05	22.66 ± 0.85	4.04 ± 0.02	3.63 ± 0.02	3.47 ± 0.03	21.00 ± 2.00	4.14 ± 0.04	3.74 ± 0.02	3.39 ± 0.03	22.55 ± 0.75	4.05 ± 0.01	3.69 ± 0.01	3.40 ± 0.01
	BK	26.80 ± 1.50	4.05 ± 0.03	3.75 ± 0.03	3.31 ± 0.02	28.08 ± 2.15	4.06 ± 0.02	3.57 ± 0.03	3.54 ± 0.03	24.67 ± 1.53	4.10 ± 0.03	3.67 ± 0.02	3.47 ± 0.06	26.91 ± 1.23	4.07 ± 0.02	3.64 ± 0.02	3.47 ± 0.02
Claude Opus 4.1	SBK	16.67 ± 0.00	4.10 ± 0.00	3.73 ± 0.00	3.53 ± 0.00	20.00 ± 0.00	4.11 ± 0.00	3.53 ± 0.00	3.64 ± 0.00	20.00 ± 0.00	4.11 ± 0.00	3.79 ± 0.00	3.52 ± 0.00	19.16 ± 0.00	4.11 ± 0.00	3.64 ± 0.00	3.58 ± 0.00
	SABK	19.61 ± 0.00	4.11 ± 0.00	3.75 ± 0.00	3.42 ± 0.00	25.12 ± 0.00	4.11 ± 0.00	3.52 ± 0.00	3.66 ± 0.00	29.00 ± 0.00	4.06 ± 0.00	3.82 ± 0.00	3.47 ± 0.00	24.69 ± 0.00	4.10 ± 0.00	3.65 ± 0.00	3.55 ± 0.00
	FBK	23.53 ± 0.00	3.99 ± 0.00	3.80 ± 0.00	3.16 ± 0.00	23.65 ± 0.00	3.94 ± 0.00	3.67 ± 0.00	3.40 ± 0.00	22.00 ± 0.00	3.95 ± 0.00	3.85 ± 0.00	3.33 ± 0.00	23.21 ± 0.00	3.96 ± 0.00	3.75 ± 0.00	3.32 ± 0.00
	NBK	22.55 ± 2.59	4.00 ± 0.06	3.76 ± 0.03	2.99 ± 0.06	20.36 ± 0.28	4.01 ± 0.01	3.61 ± 0.01	3.20 ± 0.00	25.67 ± 4.16	4.09 ± 0.03	3.77 ± 0.00	3.29 ± 0.02	22.22 ± 1.48	4.03 ± 0.01	3.69 ± 0.01	3.17 ± 0.01
Gemini 3-Flash	BK	22.55 ± 0.00	4.02 ± 0.03	3.74 ± 0.02	3.10 ± 0.07	26.11 ± 1.71	4.05 ± 0.01	3.54 ± 0.02	3.28 ± 0.04	27.00 ± 1.00	4.11 ± 0.01	3.66 ± 0.00	3.37 ± 0.00	25.43 ± 0.65	4.05 ± 0.01	3.62 ± 0.02	3.26 ± 0.02
	SBK	24.51 ± 0.00	4.10 ± 0.00	3.69 ± 0.00	3.29 ± 0.00	28.01 ± 0.00	4.15 ± 0.00	3.48 ± 0.00	3.50 ± 0.00	24.00 ± 0.00	4.16 ± 0.00	3.67 ± 0.00	3.57 ± 0.00	25.53 ± 0.00	4.14 ± 0.00	3.58 ± 0.00	3.46 ± 0.00
	SABK	28.43 ± 0.00	4.09 ± 0.00	3.74 ± 0.00	3.27 ± 0.00	22.17 ± 0.00	4.13 ± 0.00	3.47 ± 0.00	3.45 ± 0.00	25.00 ± 0.00	4.13 ± 0.00	3.65 ± 0.00	3.64 ± 0.00	24.44 ± 0.00	4.12 ± 0.00	3.58 ± 0.00	3.50 ± 0.00
	FBK	20.59 ± 0.00	3.97 ± 0.00	3.76 ± 0.00	2.96 ± 0.00	22.17 ± 0.00	3.97 ± 0.00	3.67 ± 0.00	3.15 ± 0.00	23.00 ± 0.00	3.98 ± 0.00	3.78 ± 0.00	3.39 ± 0.00	19.98 ± 0.00	3.97 ± 0.00	3.72 ± 0.00	3.16 ± 0.00
OpenAI GPT-5.2	NBK	22.88 ± 1.50	4.43 ± 0.03	3.58 ± 0.01	4.23 ± 0.01	22.33 ± 2.48	4.37 ± 0.01	3.32 ± 0.04	4.32 ± 0.02	21.33 ± 2.31	4.47 ± 0.03	3.45 ± 0.03	4.34 ± 0.01	22.22 ± 1.08	4.41 ± 0.02	3.42 ± 0.02	4.30 ± 0.01
	BK	24.84 ± 4.08	4.42 ± 0.03	3.56 ± 0.04	4.24 ± 0.01	23.97 ± 1.24	4.41 ± 0.01	3.25 ± 0.02	4.35 ± 0.02	23.00 ± 1.00	4.52 ± 0.04	3.39 ± 0.08	4.37 ± 0.05	23.95 ± 1.62	4.44 ± 0.01	3.36 ± 0.02	4.33 ± 0.01
	SBK	23.53 ± 0.00	4.50 ± 0.00	3.48 ± 0.00	4.26 ± 0.00	21.78 ± 0.00	4.47 ± 0.00	3.19 ± 0.00	4.41 ± 0.00	20.83 ± 0.00	4.51 ± 0.00	3.38 ± 0.00	4.36 ± 0.00	21.99 ± 0.00	4.49 ± 0.00	3.31 ± 0.00	4.36 ± 0.00
	SABK	28.43 ± 0.00	4.48 ± 0.00	3.49 ± 0.00	4.28 ± 0.00	24.14 ± 0.00	4.50 ± 0.00	3.13 ± 0.00	4.43 ± 0.00	28.00 ± 0.00	4.55 ± 0.00	3.40 ± 0.00	4.41 ± 0.00	26.17 ± 0.00	4.51 ± 0.00	3.29 ± 0.00	4.39 ± 0.00
Human Baseline	FBK	29.41 ± 0.00	4.40 ± 0.00	3.58 ± 0.00	4.21 ± 0.00	23.65 ± 0.00	4.34 ± 0.00	3.27 ± 0.00	3.48 ± 0.00	21.00 ± 0.00	4.44 ± 0.00	3.51 ± 0.00	4.29 ± 0.00	24.44 ± 0.00	4.38 ± 0.00	3.46 ± 0.00	4.26 ± 0.00
	NBK	18.95 ± 2.04	3.53 ± 0.04	3.49 ± 0.01	3.61 ± 0.05	20.69 ± 1.48	3.59 ± 0.02	3.37 ± 0.03	3.60 ± 0.02	22.00 ± 1.73	3.61 ± 0.02	3.37 ± 0.00	3.67 ± 0.05	20.58 ± 1.03	3.58 ± 0.02	3.40 ± 0.03	3.62 ± 0.00
	BK	19.93 ± 0.57	3.59 ± 0.06	3.43 ± 0.01	3.69 ± 0.01	25.78 ± 2.80	3.73 ± 0.02	3.27 ± 0.01	3.74 ± 0.02	19.67 ± 1.53	3.63 ± 0.07	3.27 ± 0.00	3.70 ± 0.03	22.80 ± 1.79	3.67 ± 0.02	3.31 ± 0.01	3.72 ± 0.01
	SBK	17.65 ± 0.00	3.60 ± 0.00	3.36 ± 0.00	3.70 ± 0.00	18.72 ± 0.00	3.70 ± 0.00	3.20 ± 0.00	3.79 ± 0.00	21.00 ± 0.00	3.60 ± 0.00	3.32 ± 0.00	3.71 ± 0.00	19.01 ± 0.00	3.65 ± 0.00	3.27 ± 0.00	3.76 ± 0.00
OpenAI O3-mini	SABK	18.63 ± 0.00	3.62 ± 0.00	3.34 ± 0.00	3.70 ± 0.00	24.63 ± 0.00	3.79 ± 0.00	3.17 ± 0.00	3.86 ± 0.00	24.00 ± 0.00	3.55 ± 0.00	3.28 ± 0.00	3.72 ± 0.00	22.96 ± 0.00	3.69 ± 0.00	3.24 ± 0.00	3.80 ± 0.00
	FBK	20.59 ± 0.00	3.49 ± 0.00	3.50 ± 0.00	3.55 ± 0.00	20.30 ± 0.00	3.60 ± 0.00	3.37 ± 0.00	3.56 ± 0.00	18.00 ± 0.00	3.64 ± 0.00	3.42 ± 0.00	3.68 ± 0.00	19.51 ± 0.00	3.58 ± 0.00	3.41 ± 0.00	3.60 ± 0.00
	NBK	8.82	2.59	3.78	2.52	23.15	3.13	3.39	2.92	26.00	3.07	3.26	3.05	20.25	2.98	3.46	2.85
	BK	9.80	2.65	3.78	2.52	23.65	3.22	3.32	2.92	27.00	3.30	3.24	3.05	20.99	3.10	3.42	2.85
DeepSeek v3	NBK	19.28 ± 5.91	4.34 ± 0.02	3.25 ± 0.06	4.41 ± 0.01	21.02 ± 1.50	4.38 ± 0.02	3.08 ± 0.04	4.46 ± 0.03	18.00 ± 2.00	4.42 ± 0.05	3.16 ± 0.00	4.46 ± 0.01	19.84 ± 1.49	4.38 ± 0.01	3.14 ± 0.03	4.44 ± 0.02
	BK	21.24 ± 2.26	4.42 ± 0.03	3.16 ± 0.05	4.48 ± 0.05	22.00 ± 1.03	4.48 ± 0.01	3.94 ± 0.02	4.56 ± 0.00	20.33 ± 0.58	4.51 ± 0.03	3.07 ± 0.00	4.53 ± 0.05	21.40 ± 0.87	4.47 ± 0.01	3.02 ± 0.03	4.53 ± 0.02
	SBK	11.70 ± 0.00	4.45 ± 0.00	3.11 ± 0.00	4.45 ± 0.00	16.08 ± 0.00	4.46 ± 0.00	2.87 ± 0.00	4.57 ± 0.00	16.00 ± 0.00	4.49 ± 0.00	3.16 ± 0.00	4.51 ± 0.00	14.96 ± 0.00	4.46 ± 0.00	3.00 ± 0.00	4.52 ± 0.00
	SABK	19.61 ± 0.00	4.33 ± 0.00	3.12 ± 0.00	4.43 ± 0.00	17.24 ± 0.00	4.48 ± 0.00	2.85 ± 0.00	4.56 ± 0.00	26.00 ± 0.00	4.52 ± 0.00	3.02 ± 0.00	4.58 ± 0.00	20.00 ± 0.00	4.45 ± 0.00	2.95 ± 0.00	4.53 ± 0.00
Llama 3.3 70B	FBK	16.99 ± 2.47	3.54 ± 0.03	3.61 ± 0.04	3.53 ± 0.05	19.87 ± 1.03	3.65 ± 0.03	3.02 ± 0.01	3.55 ± 0.03	18.00 ± 1.00	3.53 ± 0.09	3.60 ± 0.01	3.42 ± 0.08	19.84 ± 0.29	3.59 ± 0.02	3.61 ± 0.02	3.51 ± 0.01
	NBK	21.57 ± 2.59	3.54 ± 0.03	3.61 ± 0.04	3.53 ± 0.05	18.27 ± 0.03	3.65 ± 0.03	3.02 ± 0.01	3.55 ± 0.03	18.00 ± 1.00	3.53 ± 0.09	3.60 ± 0.01	3.42 ± 0.08	19.84 ± 0.29	3.59 ± 0.02	3.61 ± 0.02	3.51 ± 0.01
	SBK	14.14 ± 0.00	3.64 ± 0.00	3.57 ± 0.00	3.54 ± 0.00	18.59 ± 0.00	3.63 ± 0.00	3.02 ± 0.00	3.43 ± 0.00	14.43 ± 0.00	3.4						

Table 4: Different versions of Gemini, OpenAI, Claude Sonnet, Llama, Qwen, and Deepseek evaluated on different question formats. Best values within each family are highlighted. **Conf.** := Confidence Score; **Diff.** := Difficulty Level; **Feas.** := Feasibility Score.

Model	Experimental Setup	MCQ						Numerical						Free form					
		Calibration (1-5)			Calibration (1-5)			Calibration (1-5)			Calibration (1-5)			Calibration (1-5)					
		Accuracy (%)	Conf.	Diff.	Feas.	Accuracy (%)	Conf.	Diff.	Feas.	Accuracy (%)	Conf.	Diff.	Feas.	Partial	Full	Conf.	Diff.	Feas.	
Gemini 3-pro	NBK	36.21 ± 1.78	4.42 ± 0.03	3.45 ± 0.01	3.89 ± 0.06	12.80 ± 2.58	4.19 ± 0.05	4.01 ± 0.03	2.46 ± 0.11	37.70 ± 1.65	22.39 ± 2.45	4.62 ± 0.01	3.01 ± 0.03	4.19 ± 0.09					
	BK	42.39 ± 1.55	4.46 ± 0.01	3.36 ± 0.05	3.96 ± 0.02	12.80 ± 1.36	4.16 ± 0.03	4.03 ± 0.02	2.47 ± 0.06	36.04 ± 0.78	21.12 ± 2.33	4.62 ± 0.03	2.90 ± 0.05	4.25 ± 0.03					
	SBK	37.04 ± 0.00	4.52 ± 0.00	3.17 ± 0.00	4.15 ± 0.00	10.71 ± 0.00	4.19 ± 0.00	3.98 ± 0.00	2.77 ± 0.00	38.90 ± 0.00	23.66 ± 0.00	4.71 ± 0.00	2.78 ± 0.00	4.47 ± 0.00					
	SABK	41.36 ± 0.00	4.55 ± 0.00	3.17 ± 0.00	4.15 ± 0.00	12.50 ± 0.00	4.24 ± 0.00	3.91 ± 0.00	2.75 ± 0.00	35.90 ± 0.00	21.37 ± 0.00	4.69 ± 0.00	2.76 ± 0.00	4.39 ± 0.00					
Claude Opus 4.5	FBK	38.89 ± 0.00	4.41 ± 0.00	3.34 ± 0.00	3.81 ± 0.00	8.93 ± 0.00	4.14 ± 0.00	4.04 ± 0.00	2.28 ± 0.00	36.41 ± 0.00	19.85 ± 0.00	4.62 ± 0.00	2.98 ± 0.00	4.10 ± 0.00					
	NBK	33.54 ± 0.71	3.78 ± 0.05	3.88 ± 0.02	3.16 ± 0.01	13.99 ± 0.52	2.18 ± 0.03	4.59 ± 0.04	2.00 ± 0.02	34.69 ± 0.43	17.81 ± 1.17	3.74 ± 0.00	3.64 ± 0.01	3.50 ± 0.03					
	BK	39.09 ± 0.94	3.90 ± 0.03	3.80 ± 0.05	3.27 ± 0.02	15.77 ± 2.73	2.11 ± 0.02	4.58 ± 0.01	1.96 ± 0.02	38.37 ± 0.62	22.65 ± 1.17	3.79 ± 0.01	3.60 ± 0.03	3.54 ± 0.02					
	SBK	36.88 ± 0.00	3.95 ± 0.00	3.77 ± 0.00	3.34 ± 0.00	15.18 ± 0.00	2.23 ± 0.00	4.52 ± 0.00	2.08 ± 0.00	35.13 ± 0.00	19.23 ± 0.00	3.81 ± 0.00	3.47 ± 0.00	3.61 ± 0.00					
Claude Sonnet 4.5	SABK	35.80 ± 0.00	3.98 ± 0.00	3.69 ± 0.00	3.54 ± 0.00	17.86 ± 0.00	2.33 ± 0.00	4.53 ± 0.00	2.15 ± 0.00	36.34 ± 0.00	20.61 ± 0.00	3.91 ± 0.00	3.42 ± 0.00	3.64 ± 0.00					
	FBK	37.04 ± 0.00	3.72 ± 0.00	3.85 ± 0.00	3.17 ± 0.00	16.96 ± 0.00	2.06 ± 0.00	4.59 ± 0.00	1.99 ± 0.00	34.88 ± 0.00	19.85 ± 0.00	3.80 ± 0.00	3.62 ± 0.00	3.52 ± 0.00					
	NBK	29.01 ± 1.63	4.22 ± 0.03	3.60 ± 0.05	3.65 ± 0.01	16.07 ± 0.89	3.59 ± 0.07	4.15 ± 0.05	2.38 ± 0.01	35.75 ± 2.22	20.10 ± 1.17	4.23 ± 0.01	3.42 ± 0.01	3.94 ± 0.03					
	BK	36.01 ± 1.28	4.26 ± 0.02	3.55 ± 0.05	3.80 ± 0.04	15.77 ± 2.58	3.56 ± 0.04	4.12 ± 0.02	2.33 ± 0.05	40.83 ± 0.40	25.19 ± 3.05	4.26 ± 0.01	3.35 ± 0.00	4.01 ± 0.04					
Claude Opus 4.1	SBK	25.62 ± 0.00	4.29 ± 0.00	3.50 ± 0.00	3.95 ± 0.00	11.93 ± 0.00	3.70 ± 0.00	4.11 ± 0.00	2.61 ± 0.00	36.26 ± 0.00	17.19 ± 0.00	4.23 ± 0.00	3.44 ± 0.00	3.95 ± 0.00					
	SABK	33.33 ± 0.00	4.27 ± 0.00	3.55 ± 0.00	3.82 ± 0.00	13.39 ± 0.00	3.65 ± 0.00	4.13 ± 0.00	2.56 ± 0.00	38.91 ± 0.00	23.66 ± 0.00	4.26 ± 0.00	3.39 ± 0.00	4.05 ± 0.00					
	FBK	29.63 ± 0.00	4.17 ± 0.00	3.67 ± 0.00	3.51 ± 0.00	14.29 ± 0.00	3.44 ± 0.00	4.12 ± 0.00	2.36 ± 0.00	39.25 ± 0.00	22.90 ± 0.00	4.12 ± 0.00	3.54 ± 0.00	3.90 ± 0.00					
	NBK	29.01 ± 2.83	4.15 ± 0.02	3.64 ± 0.02	3.38 ± 0.06	16.07 ± 1.79	3.75 ± 0.07	4.00 ± 0.03	2.28 ± 0.07	34.38 ± 0.37	19.08 ± 0.76	4.13 ± 0.01	3.47 ± 0.01	3.68 ± 0.01					
Gemini 3-Flash	BK	35.39 ± 0.36	4.18 ± 0.01	3.54 ± 0.05	3.55 ± 0.04	14.58 ± 2.25	3.79 ± 0.05	4.01 ± 0.03	2.25 ± 0.05	37.52 ± 1.14	22.39 ± 0.44	4.12 ± 0.03	3.38 ± 0.03	3.76 ± 0.01					
	SBK	28.75 ± 0.00	4.20 ± 0.00	3.52 ± 0.00	3.76 ± 0.00	17.27 ± 0.00	3.95 ± 0.00	3.96 ± 0.00	2.43 ± 0.00	34.63 ± 0.00	19.38 ± 0.00	4.22 ± 0.00	3.33 ± 0.00	3.98 ± 0.00					
	SABK	30.86 ± 0.00	4.22 ± 0.00	3.52 ± 0.00	3.79 ± 0.00	16.96 ± 0.00	3.89 ± 0.00	3.99 ± 0.00	2.45 ± 0.00	38.24 ± 0.00	22.90 ± 0.00	4.18 ± 0.00	3.31 ± 0.00	4.03 ± 0.00					
	FBK	30.25 ± 0.00	4.16 ± 0.00	3.63 ± 0.00	3.42 ± 0.00	15.18 ± 0.00	3.59 ± 0.00	4.07 ± 0.00	2.21 ± 0.00	32.03 ± 0.00	17.56 ± 0.00	4.08 ± 0.00	3.54 ± 0.00	3.63 ± 0.00					
OpenAI GPT-5.2	NBK	29.22 ± 2.85	4.38 ± 0.02	3.38 ± 0.01	4.30 ± 0.02	11.90 ± 1.03	4.18 ± 0.01	3.92 ± 0.03	4.02 ± 0.02	35.71 ± 1.56	22.39 ± 1.17	4.63 ± 0.02	3.03 ± 0.00	4.54 ± 0.04					
	BK	35.39 ± 1.28	4.44 ± 0.01	3.35 ± 0.02	4.32 ± 0.01	9.52 ± 1.86	4.18 ± 0.02	3.89 ± 0.02	4.03 ± 0.01	37.11 ± 3.11	22.14 ± 2.02	4.68 ± 0.03	2.92 ± 0.05	4.60 ± 0.02					
	SBK	31.06 ± 0.00	4.50 ± 0.00	3.24 ± 0.00	4.35 ± 0.00	12.61 ± 0.00	4.20 ± 0.00	3.84 ± 0.00	4.04 ± 0.00	33.56 ± 0.00	18.75 ± 0.00	4.72 ± 0.00	2.90 ± 0.00	4.65 ± 0.00					
	SABK	37.65 ± 0.00	4.49 ± 0.00	3.28 ± 0.00	4.37 ± 0.00	9.82 ± 0.00	4.22 ± 0.00	3.89 ± 0.00	4.05 ± 0.00	40.93 ± 0.00	25.95 ± 0.00	4.77 ± 0.00	2.79 ± 0.00	4.69 ± 0.00					
Human Baseline	FBK	33.33 ± 0.00	4.33 ± 0.00	3.43 ± 0.00	4.26 ± 0.00	14.29 ± 0.00	4.21 ± 0.00	3.89 ± 0.00	3.98 ± 0.00	36.75 ± 0.00	22.14 ± 0.00	4.59 ± 0.00	3.11 ± 0.00	4.50 ± 0.00					
	NBK	28.81 ± 3.40	3.95 ± 0.00	3.12 ± 0.03	3.95 ± 0.02	12.50 ± 2.36	2.77 ± 0.05	4.02 ± 0.01	2.84 ± 0.06	33.80 ± 1.00	17.30 ± 1.17	3.82 ± 0.02	3.21 ± 0.04	3.88 ± 0.02					
	BK	30.04 ± 0.49	3.98 ± 0.02	3.01 ± 0.01	4.01 ± 0.02	13.10 ± 3.72	2.94 ± 0.07	3.99 ± 0.02	3.04 ± 0.05	38.52 ± 1.46	22.14 ± 1.32	3.92 ± 0.03	3.11 ± 0.02	3.94 ± 0.03					
	SBK	26.54 ± 0.00	3.92 ± 0.00	2.96 ± 0.00	4.01 ± 0.00	13.39 ± 0.00	2.97 ± 0.00	3.91 ± 0.00	3.13 ± 0.00	29.33 ± 0.00	14.50 ± 0.00	3.90 ± 0.00	3.03 ± 0.00	4.00 ± 0.00					
OpenAI O3-mini	SABK	27.16 ± 0.00	4.07 ± 0.00	3.31 ± 0.00	3.99 ± 0.00	9.82 ± 0.00	3.92 ± 0.00	3.57 ± 0.00	4.02 ± 0.00	33.18 ± 0.00	17.56 ± 0.00	4.62 ± 0.00	2.95 ± 0.00	4.67 ± 0.00					
	FBK	25.31 ± 0.00	4.60 ± 0.00	2.75 ± 0.00	4.73 ± 0.00	10.71 ± 0.00	3.90 ± 0.00	3.72 ± 0.00	4.00 ± 0.00	32.70 ± 0.00	18.32 ± 0.00	4.44 ± 0.00	3.20 ± 0.00	4.43 ± 0.00					
	NBK	23.66 ± 1.43	4.70 ± 0.04	3.50 ± 0.01	4.37 ± 0.04	13.39 ± 0.00	3.85 ± 0.13	4.06 ± 0.10	4.17 ± 0.10	33.14 ± 0.81	18.58 ± 1.92	4.74 ± 0.02	3.34 ± 0.11	4.49 ± 0.03					
	BK	27.98 ± 4.20	4.72 ± 0.01	3.29 ± 0.07	4.45 ± 0.04	12.50 ± 2.36	3.98 ± 0.04	3.97 ± 0.17	4.18 ± 0.08	36.92 ± 1.16	22.65 ± 2.68	4.84 ± 0.02	3.20 ± 0.11	4.43 ± 0.08					
DeepSeek v3	SBK	25.00 ± 0.00	4.75 ± 0.00	3.41 ± 0.00	4.44 ± 0.00	8.04 ± 0.00	4.10 ± 0.00	4.14 ± 0.00	4.11 ± 0.00	34.21 ± 0.00	18.32 ± 0.00	4.76 ± 0.00	3.44 ± 0.00	4.51 ± 0.00					
	SABK	25.31 ± 0.00	4.73 ± 0.00	3.36 ± 0.00	4.46 ± 0.00	10.71 ± 0.00	3.96 ± 0.00	4.05 ± 0.00	4.13 ± 0.00	36.37 ± 0.00	21.37 ± 0.00	4.77 ± 0.00	3.32 ± 0.00	4.52 ± 0.00					
	FBK	29.01 ± 0.00	4.65 ± 0.00	3.33 ± 0.00	4.48 ± 0.00	13.39 ± 0.00	3.76 ± 0.00	4.09 ± 0.00	4.25 ± 0.00	32.92 ± 0.00	16.79 ± 0.00	4.76 ± 0.00	3.49 ± 0.00	4.45 ± 0.00					
	NBK	26.75 ± 0.71	3.92 ± 0.03	3.42 ± 0.02	3.83 ± 0.05	12.50 ± 0.89	2.73 ± 0.05	3.99 ± 0.02	2.67 ± 0.08	25.61 ± 1.94	12.47 ± 1.17	3.63 ± 0.08	3.74 ± 0.03	3.41 ± 0.01					
Llama 3.3 70B	BK	28.81 ± 0.36	4.01 ± 0.04	3.33 ± 0.02	3.92 ± 0.10	14.29 ± 1.79	2.84 ± 0.04	3.98 ± 0.03	2.82 ± 0.07	26.58 ± 1.46	13.49 ± 1.17	3.72 ± 0.00	3.64 ± 0.03	3.60 ± 0.05					
	SBK	24.68 ± 0.00	4.03 ± 0.00	3.35 ± 0.00	3.92 ± 0.00	10.19 ± 0.00	2.90 ± 0.00	3.99 ± 0.00	2.72 ± 0.00	24.00 ± 0.00	11.63 ± 0.00	3.64 ± 0.00	3.67 ± 0.00	3.48 ± 0.00					
	SABK	27.78 ± 0.00	4.07 ± 0.00	3.31 ± 0.00	3.99 ± 0.00	9.82 ± 0.00	2.89 ± 0.00	3.99 ± 0.00	2.90 ± 0.00	26.27 ± 0.00	13.74 ± 0.00	3.80 ± 0.00	3.58 ± 0.00	3.69 ± 0.00					
	FBK	27.16 ± 0.00	3.93 ± 0.00	3.51 ± 0.00	3.81 ± 0.00	13.39 ± 0.00	2.72 ± 0.00	3.99 ± 0.00	2.55 ± 0.00	25.05 ± 0.00	12.21 ± 0.00	3.59 ± 0.00	3.71 ± 0.00	3.39 ± 0.00					
OpenAI O3	NBK	21.40 ± 0.36	4.00 ± 0.01	2.97 ± 0.01	4.03 ± 0.02	11.31 ± 1.36	3.67 ± 0.03	3.29 ± 0.04	3.83 ± 0.02	35.69 ± 2.54	19.34 ± 3.09	3.99 ± 0.01	3.00 ± 0.02	4.03 ± 0.01					
	BK	29.22 ± 2.57	4.00 ± 0.01	2.96 ± 0.01	4.06 ± 0.01	12.80 ± 2.87	3.74 ± 0.08	3.19 ± 0.01	3.91 ± 0.01	37.99 ± 2.50	21.37 ± 2.75	3.99 ± 0.01	3.00 ± 0.01	4.03 ± 0.01					
	SBK	25.31 ± 0.00	4.02 ± 0.00	2.88 ± 0.00	4.12 ± 0.00	14.													

Table 5: Different versions of Gemini, OpenAI, Claude Sonnet, Llama, Qwen, and Deepseek evaluated on different levels of confidence, difficulty, and feasibility scores. Best values within each family are highlighted.

Table 6: Different versions of Gemini, OpenAI, Claude Sonnet, Llama, Qwen, and Deepseek evaluated on different levels of human-rated confidence, difficulty, and feasibility scores. Best values within each family are highlighted.

Model	Exp.	Confidence										Difficulty										Feasibility									
		L1		L2		L3		L4		L5		L1		L2		L3		L4		L5		L1		L2		L3		L4		L5	
		Acc (%)	# Quac.	Acc (%)	# Quac.	Acc (%)	# Quac.	Acc (%)	# Quac.	Acc (%)	# Quac.	Acc (%)	# Quac.	Acc (%)	# Quac.	Acc (%)	# Quac.	Acc (%)	# Quac.	Acc (%)	# Quac.	Acc (%)	# Quac.	Acc (%)	# Quac.	Acc (%)	# Quac.	Acc (%)	# Quac.	Acc (%)	# Quac.
Gemini 3-pro	NBK	17.33 ± 1.50	50	22.57 ± 2.41	90	26.45 ± 0.63	92	26.76 ± 4.16	147	41.60 ± 5.77	10	30.20 ± 3.87	65	29.84 ± 2.27	124	21.51 ± 0.41	141	17.95 ± 2.35	65	20.00 ± 0.00	65	20.34 ± 1.96	135	20.41 ± 5.40	49	28.97 ± 2.34	107	41.50 ± 5.89	49		
	BBK	17.33 ± 1.50	50	22.57 ± 2.41	90	26.45 ± 0.63	92	26.76 ± 4.16	147	41.60 ± 5.77	10	30.20 ± 3.87	65	29.84 ± 2.27	124	21.51 ± 0.41	141	17.95 ± 2.35	65	20.00 ± 0.00	65	20.34 ± 1.96	135	20.41 ± 5.40	49	28.97 ± 2.34	107	41.50 ± 5.89	49		
	DKB	17.33 ± 1.50	50	22.57 ± 2.41	90	26.45 ± 0.63	92	26.76 ± 4.16	147	41.60 ± 5.77	10	30.20 ± 3.87	65	29.84 ± 2.27	124	21.51 ± 0.41	141	17.95 ± 2.35	65	20.00 ± 0.00	65	20.34 ± 1.96	135	20.41 ± 5.40	49	28.97 ± 2.34	107	41.50 ± 5.89	49		
Claude Opus 4.5	NBK	14.00 ± 5.00	50	22.25 ± 3.04	90	25.72 ± 3.49	92	26.88 ± 3.71	140	40.00 ± 20.00	20	20.00 ± 0.00	65	27.96 ± 2.03	124	21.04 ± 0.41	141	13.84 ± 3.08	68	14.34 ± 1.54	68	16.93 ± 1.13	135	15.47 ± 2.07	49	27.21 ± 1.62	107	40.11 ± 1.85	49		
	BBK	14.00 ± 5.00	50	22.25 ± 3.04	90	25.72 ± 3.49	92	26.88 ± 3.71	140	40.00 ± 20.00	20	20.00 ± 0.00	65	27.96 ± 2.03	124	21.04 ± 0.41	141	13.84 ± 3.08	68	14.34 ± 1.54	68	16.93 ± 1.13	135	15.47 ± 2.07	49	27.21 ± 1.62	107	40.11 ± 1.85	49		
	DKB	14.00 ± 5.00	50	22.25 ± 3.04	90	25.72 ± 3.49	92	26.88 ± 3.71	140	40.00 ± 20.00	20	20.00 ± 0.00	65	27.96 ± 2.03	124	21.04 ± 0.41	141	13.84 ± 3.08	68	14.34 ± 1.54	68	16.93 ± 1.13	135	15.47 ± 2.07	49	27.21 ± 1.62	107	40.11 ± 1.85	49		
Claude Sonnet 4.5	NBK	21.33 ± 1.50	50	22.22 ± 1.20	90	21.01 ± 1.26	92	23.13 ± 1.80	147	30.00 ± 0.00	20	20.00 ± 0.00	65	22.31 ± 2.03	124	21.78 ± 0.41	141	18.46 ± 1.54	65	15.90 ± 0.89	65	20.09 ± 1.13	135	13.61 ± 2.36	49	29.04 ± 0.93	107	34.01 ± 4.25	49		
	BBK	21.33 ± 1.50	50	22.22 ± 1.20	90	21.01 ± 1.26	92	23.13 ± 1.80	147	30.00 ± 0.00	20	20.00 ± 0.00	65	22.31 ± 2.03	124	21.78 ± 0.41	141	18.46 ± 1.54	65	15.90 ± 0.89	65	20.09 ± 1.13	135	13.61 ± 2.36	49	29.04 ± 0.93	107	34.01 ± 4.25	49		
	DKB	21.33 ± 1.50	50	22.22 ± 1.20	90	21.01 ± 1.26	92	23.13 ± 1.80	147	30.00 ± 0.00	20	20.00 ± 0.00	65	22.31 ± 2.03	124	21.78 ± 0.41	141	18.46 ± 1.54	65	15.90 ± 0.89	65	20.09 ± 1.13	135	13.61 ± 2.36	49	29.04 ± 0.93	107	34.01 ± 4.25	49		
Claude Opus 4.1	NBK	16.67 ± 2.31	50	23.96 ± 2.08	90	21.74 ± 1.00	92	22.68 ± 2.83	147	26.07 ± 2.89	20	20.00 ± 0.00	65	28.13 ± 2.35	65	23.12 ± 0.93	124	21.04 ± 2.28	141	17.44 ± 0.49	65	17.44 ± 2.28	65	18.77 ± 2.14	135	12.93 ± 1.12	49	25.55 ± 1.08	107	40.11 ± 1.89	49
	BBK	16.67 ± 2.31	50	23.96 ± 2.08	90	21.74 ± 1.00	92	22.68 ± 2.83	147	26.07 ± 2.89	20	20.00 ± 0.00	65	28.13 ± 2.35	65	23.12 ± 0.93	124	21.04 ± 2.28	141	17.44 ± 0.49	65	17.44 ± 2.28	65	18.77 ± 2.14	135	12.93 ± 1.12	49	25.55 ± 1.08	107	40.11 ± 1.89	49
	DKB	16.67 ± 2.31	50	23.96 ± 2.08	90	21.74 ± 1.00	92	22.68 ± 2.83	147	26.07 ± 2.89	20	20.00 ± 0.00	65	28.13 ± 2.35	65	23.12 ± 0.93	124	21.04 ± 2.28	141	17.44 ± 0.49	65	17.44 ± 2.28	65	18.77 ± 2.14	135	12.93 ± 1.12	49	25.55 ± 1.08	107	40.11 ± 1.89	49
Gemini 3-Flash	NBK	18.67 ± 3.06	50	19.10 ± 0.60	90	25.36 ± 1.66	92	22.22 ± 2.19	147	31.60 ± 7.64	20	26.67 ± 5.77	65	20.97 ± 2.42	124	21.75 ± 0.41	141	22.56 ± 4.70	65	23.39 ± 3.20	65	20.25 ± 1.13	135	20.10 ± 2.04	49	27.74 ± 3.02	107	36.73 ± 3.53	49		
	BBK	18.67 ± 3.06	50	19.10 ± 0.60	90	25.36 ± 1.66	92	22.22 ± 2.19	147	31.60 ± 7.64	20	26.67 ± 5.77	65	20.97 ± 2.42	124	21.75 ± 0.41	141	22.56 ± 4.70	65	23.39 ± 3.20	65	20.25 ± 1.13	135	20.10 ± 2.04	49	27.74 ± 3.02	107	36.73 ± 3.53	49		
	DKB	18.67 ± 3.06	50	19.10 ± 0.60	90	25.36 ± 1.66	92	22.22 ± 2.19	147	31.60 ± 7.64	20	26.67 ± 5.77	65	20.97 ± 2.42	124	21.75 ± 0.41	141	22.56 ± 4.70	65	23.39 ± 3.20	65	20.25 ± 1.13	135	20.10 ± 2.04	49	27.74 ± 3.02	107	36.73 ± 3.53	49		
OpenAI GPT-5.2	NBK	18.67 ± 2.31	50	22.22 ± 1.19	90	19.84 ± 0.63	92	19.85 ± 3.07	147	30.00 ± 5.00	20	13.33 ± 5.77	65	27.18 ± 1.78	124	22.22 ± 1.24	141	17.95 ± 0.89	65	16.28 ± 0.85	65	20.14 ± 1.48	135	21.18 ± 1.95	49	39.36 ± 3.12	107	47.62 ± 5.14	49		
	BBK	18.67 ± 2.31	50	20.25 ± 1.27	79	19.84 ± 0.66	88	23.21 ± 2.40	140	38.89 ± 5.09	30	27.08 ± 3.61	65	30.88 ± 3.89	68	24.17 ± 2.20	120	19.05 ± 2.64	133	18.63 ± 3.06	68	13.33 ± 3.55	65	19.51 ± 0.86	135	12.93 ± 1.12	49	25.86 ± 3.78	107	47.62 ± 5.14	49
	DKB	18.67 ± 2.31	50	20.25 ± 1.27	79	19.84 ± 0.66	88	23.21 ± 2.40	140	38.89 ± 5.09	30	27.08 ± 3.61	65	30.88 ± 3.89	68	24.17 ± 2.20	120	19.05 ± 2.64	133	18.63 ± 3.06	68	13.33 ± 3.55	65	19.51 ± 0.86	135	12.93 ± 1.12	49	25.86 ± 3.78	107	47.62 ± 5.14	49
Human Baseline	NBK	12.00	50	12.50	90	17.39	92	28.57	147	30.00	20	30.00	65	13.88	124	13.48	65	14.41	92	65	3.08	65	5.93	13	12.24	49	27.10	107	75.51	49	
	BBK	14.00	50	10.13	79	18.18	88	27.85	133	30	31.25	65	16.33	68	26.67	120	14.29	133	8.82	68	3.08	65	5.19	13	12.24	49	28.97	107	75.51	49	
	DKB	14.00	50	10.13	79	18.18	88	27.85	133	30	31.25	65	16.33	68	26.67	120	14.29	133	8.82	68	3.08	65	5.19	13	12.24	49	28.97	107	75.51	49	
OpenAI O3-mini	NBK	16.00 ± 5.29	50	19.79 ± 1.30	90	14.49 ± 0.63	92	23.13 ± 0.68	147	30.00 ± 5.00	20	13.33 ± 5.77	65	27.18 ± 0.89	65	16.40 ± 0.47	124	20.33 ± 0.82	141	18.97 ± 6.22	65	10.77 ± 3.08	65	19.02 ± 2.26	135	16.33 ± 7.36	49	19.15 ± 1.95	107	38.78 ± 0.00	49
	BBK	12.67 ± 1.15	50	17.72 ± 0.20	79	15.86 ± 0.60	88	24.89 ± 3.24	130	35.85 ± 5.09	30	20.83 ± 6.31	65	36.27 ± 3.06	68	18.05 ± 1.67	120	19.05 ± 1.15	133	16.18 ± 1.47	68	9.74 ± 0.89	65	15.31 ± 1.13	135	20.41 ± 3.53	49	25.23 ± 3.12	107	46.26 ± 3.12	49
	DKB	12.67 ± 1.15	50	17.72 ± 0.20	79	15.86 ± 0.60	88	24.89 ± 3.24	130	35.85 ± 5.09	30	20.83 ± 6.31	65	36.27 ± 3.06	68	18.05 ± 1.67	120	19.05 ± 1.15	133	16.18 ± 1.47	68	9.74 ± 0.89	65	15.31 ± 1.13	135	20.41 ± 3.53	49	25.23 ± 3.12	107	46.26 ± 3.12	49
DeepSeek 3	NBK	14.00 ± 4.00	50	20.49 ± 3.08	90	16.67 ± 3.14	92	21.09 ± 2.45	147	23.33 ± 5.77	20	10.00 ± 0.00	65	22.08 ± 1.40	124	17.49 ± 0.47	141	17.44 ± 2.38	65	12.18 ± 3.08	65	13.11 ± 1.54	65	8.16 ± 0.00	65	24.30 ± 3.17	107	31.04 ± 1.18	49		
	BBK	14.00 ± 4.00	50	20.49 ± 3.08	90	16.67 ± 3.14	92	21.09 ± 2.45	147	23.33 ± 5.77	20	10.00 ± 0.00	65	22.08 ± 1.40	124	17.49 ± 0.47	141	17.44 ± 2.38	65	12.18 ± 3.08	65	13.11 ± 1.54	65	8.16 ± 0.00	65	24.30 ± 3.17	107	31.04 ± 1.18	49		
	DKB	14.00 ± 4.00	50	20.49 ± 3.08	90	16.67 ± 3.14	92	21.09 ± 2.45	147	23.33 ± 5.77	20	10.00 ± 0.00	65	22.08 ± 1.40	124	17.49 ± 0.47	141	17.44 ± 2.38	65	12.18 ± 3.08	65	13.11 ± 1.54	65	8.16 ± 0.00	65	24.30 ± 3.17	107	31.04 ± 1.18	49		
Llama 3.70B	NBK	10.67 ± 1.15	50	18.75 ± 1.50	90	9.6	12.68 ± 3.32	92	23.81 ± 0.86	147	18.33 ± 5.77	20	10.00 ± 0.00	65	21.74 ± 1.40	124	20.88 ± 0.40	141	9.74 ± 0.89	65	8.72 ± 2.35	65	13.11 ± 1.54	65	8.16 ± 0.00	65	24.30 ± 3.17	107	33.57 ± 1.18	49	
	BBK	10.67 ± 1.15	50	18.75 ± 1.50	90	9.6	12.68 ± 3.32	92	23.81 ± 0.86	147	18.33 ± 5.77	20	10.00 ± 0.00	65	21.74 ± 1.40	124	20.88 ± 0.40	141	9.74 ± 0.89	65	8.72 ± 2.35	65	13.11 ± 1.54	65	8.16 ± 0.00	65	24.30 ± 3.17	107	33.57 ± 1.18	49	
	DKB	10.67 ± 1.15	50	18.75 ± 1.50	90	9.6	12.68 ± 3.32	92	23.81 ± 0.86	147	18.33 ± 5.77	20	10.00 ± 0.00	65	21.74 ± 1.40	124	20.88 ± 0.40	141	9.74 ± 0.89	65	8.72 ± 2.35	65	13.11 ± 1.54	65	8.16 ± 0.00	65	24.30 ± 3.17	107	33.57 ± 1.18	49	
Gemini 2.5-pro	NBK	18.00 ± 2.00	50	16.32 ± 3.66	90	16.84 ± 2.26	92	13.63 ± 2.00	147	23.33 ± 2.89	20	13.33 ± 5.77	65	22.56 ± 4.44	65	18.82 ± 2.33	124	15.37 ± 3.35	141	12.31 ± 1.54	65	10.77 ± 1.54	65	10.37 ± 2.96	135	11.56 ± 5.56	49	20.25 ± 0.54			

Table 7: Different versions of Gemini, OpenAI, Claude Sonnet, Llama, Qwen, and Deepseek evaluated on their ability to answer questions based on required background knowledge needed to answer questions.

Model	# Corr.	# Ques.	Acc (%)
Gemini 3-pro	1268	1350	93.93
Claude Opus 4.5	1277	1344	95.01
Claude Sonnet 4.5	1232	1316	93.62
Claude Opus 4.1	1228	1327	92.54
Gemini 3-Flash	1279	1350	94.74
OpenAI GPT-5.2	1276	1350	94.52
OpenAI O3-mini	1250	1350	92.59
DeepSeek v3	1234	1353	91.20
Llama 3.3 70B	1132	1350	83.85
OpenAI O3	1261	1350	93.41
Qwen 3 32B	1149	1342	85.62
Gemini 2.5-pro	1246	1350	92.30
Qwen 3 235B	1222	1350	90.52
OpenAI O4-mini	1252	1350	92.74
Llama 3.1 8B	955	1329	71.86

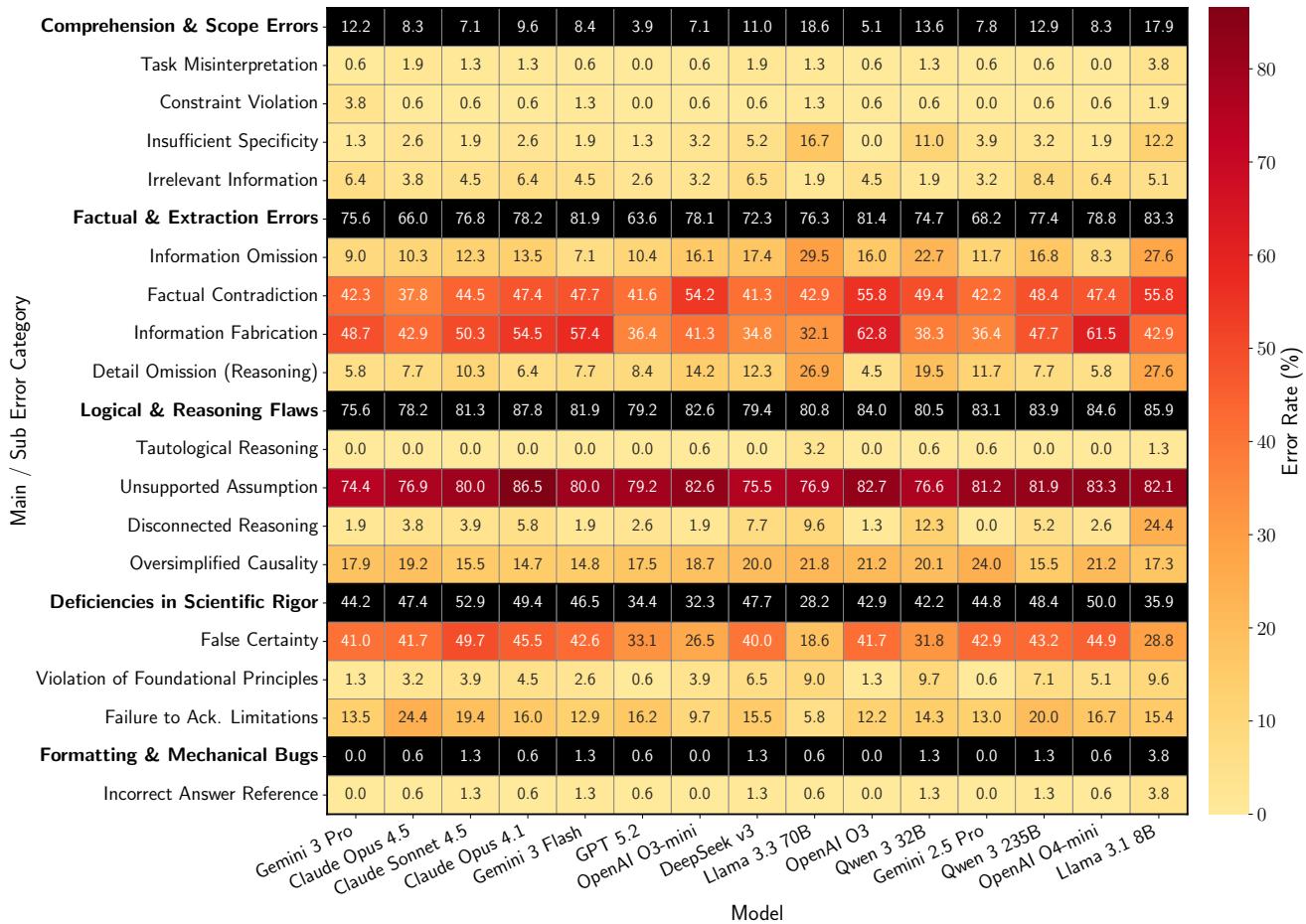


Figure 13: **Analysis of model errors for high feasible questions.** We employ an LLM judge to systematically classify errors in model predictions according to a hierarchical taxonomy spanning five top-level (in black background) categories and 16 specific error types. The heatmap shows the percentage of incorrect responses containing each error type for each evaluated model. Error categories progress from surface-level issues (Comprehension & Scope) to deeper reasoning failures (Logical & Reasoning Flaws) to fundamental scientific deficiencies (Deficiencies in Scientific Rigor). Models can exhibit multiple error types simultaneously, so accumulative percentage scores within top-level categories may exceed 100%. SciPredict tasks contribute to top-level category percentages if flagged with at least one underlying error type. Error analysis only considers the questions human experts marked as feasible to answer without running the practical experiment.

## D. Prompts

Prompt used for errors analysis judge

[SYS]

Fields: domain, field

Instructions: You are acting as a judge evaluating a 'suggested\_answer' to a scientific 'question' (of type 'question\_type') which corresponds to the prediction of the outcome of a scientific experiment in {domain} and the field of {field}. Your goal is to identify the reason(s) why the provided answer is flawed or incorrect when compared to the 'ground\_truth\_answer' and the provided 'experimental\_setup', 'measurements\_taken', and 'background\_knowledge'. Carefully review the provided materials and provide your judgment based on the rigorous definitions below. Your judgment should be based on a detailed analysis of the 'suggested\_answer's reasoning and factual claims.

Evaluation Materials and Terminology:

- 'question': The scientific question posed to the responder for prediction of the experimental outcome.
- 'experimental\_setup': Details of the experimental design, conditions, and procedures relevant to the 'question' provided to the responder for prediction of the experimental outcome.
- 'measurements\_taken': Information about the measurements taken relevant to the 'question' provided to the responder for prediction of the experimental outcome.
- 'background\_knowledge' (if any): Additional scientific context or principles relevant to the 'question' provided to the responder for prediction of the experimental outcome.
- 'suggested\_answer': The responder's answer to the 'question', including any reasoning or justification provided.
- 'ground\_truth\_answer': The ground truth answer to the 'question', representing the correct prediction of the experimental outcome based on the provided materials.

Question Types:

- Multiple-Choice (MCQ): Includes a set of possible answers from which one (1) OR more (>1) must be selected.
- Free-Form: Requires a comprehensive but concise explanation of the expected experimental results.
- Numerical: Requires a specific numerical value prediction based on the provided data for the outcome of the experiment described in the question.

Error Analysis Categories:

1. Comprehension & Scope Errors: The answer fails because it fundamentally misunderstands the user's question or violates its core constraints. This is the primary error if the answer, regardless of its correctness, is for the wrong question.
2. Factual & Extraction Errors: The answer fails because it incorrectly handles explicit information from the provided 'experimental\_setup', 'measurements\_taken', or 'background\_knowledge'. It omits, fabricates, or directly contradicts facts that are clearly stated.
3. Logical & Reasoning Flaws: The answer fails because the argument is logically unsound, even if the individual facts cited are correct. The connections between evidence and conclusion are invalid.
4. Deficiencies in Scientific Rigor: The answer fails because it lacks the necessary nuance and rigor expected in scientific communication. It may be factually correct but is presented with false certainty or violates a core scientific principle.
5. Formatting & Mechanical Bug: The answer fails due to a non-substantive formatting error.

Detailed Analysis Flags:

First, choose a PRIMARY ERROR CATEGORY from the five main categories above that best explains WHY the 'suggested\_answer' is flawed or incorrect. For this choice of the primary error category, provide a

comprehensive justification (4-5 sentences) explaining your judgment.

Second, for EACH flag below (INCLUDING from ALL categories, NOT just the one you selected), choose YES, NO, or N/A based on the strict definitions provided:

1. Comprehension & Scope Errors

- 'flag\_task\_misinterpretation':
  - Evidence Source: 'question', 'suggested\_answer'.
  - Definition: Whether the 'suggested\_answer' addresses a fundamentally different question than the one posed.
  - Prerequisite: None.
  - 'YES': The answer's core purpose is different from the question's intent or it addresses a different scientific question than was asked.
  - 'NO': The conditions for 'YES' are NOT satisfied.
- 'flag\_constraintViolation':
  - Evidence Source: 'question', 'suggested\_answer'.
  - Definition: Whether the 'suggested\_answer' ignores a specific instruction or constraint mentioned in the 'question'.
  - Prerequisite: The 'question' contains an explicit constraint.
  - 'YES': The answer violates an explicit constraint in the question.
  - 'NO': The prerequisite IS met, but the conditions for 'YES' are NOT satisfied.
  - 'N/A': The prerequisite is NOT met.
- 'flag\_insufficient\_specificity':
  - Evidence Source: 'question', 'suggested\_answer', 'ground\_truth\_answer'.
  - Definition: Whether the 'suggested\_answer' is overly generic or lacks the required detail.
  - Prerequisite: None.
  - 'YES': The answer is too high-level and omits details that are necessary to fully address the question, as evidenced by the 'ground\_truth\_answer'.
  - 'NO': The conditions for 'YES' are NOT satisfied.
- 'flag\_irrelevant\_information':
  - Evidence Source: 'question', 'suggested\_answer', 'ground\_truth\_answer'.
  - Definition: Whether the 'suggested\_answer' includes factually correct but non-essential information.
  - Prerequisite: None.
  - 'YES': The answer contains information that does not help answer the specific 'question'.
  - 'NO': The conditions for 'YES' are NOT satisfied.

2. Factual & Extraction Errors

- 'flag\_information\_omission':
  - Evidence Source: 'experimental\_setup', 'measurements\_taken', 'background\_knowledge', 'suggested\_answer'.
  - Definition: Whether the 'suggested\_answer' fails to extract or reports as "missing" a REQUIRED piece of data explicitly present in the provided materials.
  - Prerequisite: The information is explicitly stated in the 'experimental\_setup', 'measurements\_taken', or 'background\_knowledge' AND the information is REQUIRED for answering the question.
  - 'YES': A key fact, value, or condition from the provided materials is missing from, or was ignored in the 'suggested\_answer'.
  - 'NO': The prerequisite IS met, but the conditions for 'YES' are NOT satisfied.
  - 'N/A': The prerequisite is NOT met.
- 'flag\_factual\_contradiction':
  - Evidence Source: 'experimental\_setup', 'measurements\_taken', 'background\_knowledge', 'suggested\_answer'.
  - Definition: Whether the 'suggested\_answer' directly misrepresents or contradicts facts, values, or relationships stated in the provided materials.
  - Prerequisite: None.

- 'YES': A statement in the 'suggested\_answer' is verifiably FALSE when checked against the provided materials.
- 'NO': The conditions for 'YES' are NOT satisfied.
- 'flag\_information\_fabrication':
  - Evidence Source: 'experimental\_setup', 'measurements\_taken', 'background\_knowledge', 'suggested\_answer'.
  - Definition: Whether the 'suggested\_answer' invents data, formulas, or external "facts" not supported by the provided materials.
  - Prerequisite: None.
  - 'YES': The answer includes specific information that cannot be found in or reasonably inferred from the provided materials.
  - 'NO': The conditions for 'YES' are NOT satisfied.
- 'flag\_detail\_omission\_in\_reasoning':
  - Evidence Source: 'experimental\_setup', 'measurements\_taken', 'background\_knowledge', 'suggested\_answer'.
  - Definition: Whether the reasoning in the 'suggested\_answer' omits a CRITICAL piece of evidence from the provided materials that is necessary to logically support its OWN conclusion.
  - Prerequisite: The 'suggested\_answer' presents a logical argument or reasoning.
  - 'YES': The argument or reasoning provided for the answer is incomplete because a necessary premise from the provided materials is missing.
  - 'NO': The prerequisite IS met, but the conditions for 'YES' are NOT satisfied.
  - 'N/A': The prerequisite is NOT met.

3. Logical & Reasoning Flaws

- 'flag\_tautological\_reasoning':
  - Evidence Source: 'suggested\_answer'.
  - Definition: Whether the justification restates the conclusion without providing independent evidence.
  - Prerequisite: The 'suggested\_answer' provides a justification or reasoning.
  - 'YES': The reasoning is circular, using the conclusion as its own evidence.
  - 'NO': The prerequisite IS met, but the conditions for 'YES' are NOT satisfied.
  - 'N/A': The prerequisite is NOT met.
- 'flag\_unsupported\_assumption':
  - Evidence Source: 'experimental\_setup', 'measurements\_taken', 'background\_knowledge', 'suggested\_answer'.
  - Definition: Whether the reasoning relies on a significant, unstated assumption that is NOT supported by the provided materials.
  - Prerequisite: The 'suggested\_answer' presents a logical argument or reasoning.
  - 'YES': The logical leap from evidence to conclusion requires an assumption that is NOT provided or justified by the provided materials.
  - 'NO': The prerequisite IS met, but the conditions for 'YES' are NOT satisfied.
  - 'N/A': The prerequisite is NOT met.
- 'flag\_disconnected\_reasoning':
  - Evidence Source: 'suggested\_answer'.
  - Definition: Whether the 'suggested\_answer' lists correct facts but fails to logically connect them to the final conclusion.
  - Prerequisite: The 'suggested\_answer' presents more than one (>1) piece of evidence in its reasoning.
  - 'YES': NO logical connection is made between the evidence presented and the conclusion drawn.
  - 'NO': The prerequisite IS met, but the conditions for 'YES' are NOT satisfied.
  - 'N/A': The prerequisite is NOT met.
- 'flag\_oversimplified\_causality':
  - Evidence Source: 'experimental\_setup', 'measurements\_taken', 'background\_knowledge', 'suggested\_answer'.
  - Definition: Whether the reasoning focuses on a minor cause while ignoring a more critical or explicitly stated factor impacting the conclusion to be made from the provided materials.

- Prerequisite: The provided materials present multiple potential causal factors.
- 'YES': The reasoning incorrectly prioritizes a secondary factor over the primary factor described in the provided materials.
- 'NO': The prerequisite IS met, but the conditions for 'YES' are NOT satisfied.
- 'N/A': The prerequisite is NOT met.

#### 4. Deficiencies in Scientific Rigor

- 'flag\_false\_certainty':
  - Evidence Source: 'experimental\_setup', 'measurements\_taken', 'background\_knowledge', 'suggested\_answer'.
  - Definition: Whether the 'suggested\_answer' presents a probabilistic, correlational, or uncertain outcome as a definitive fact.
  - Prerequisite: The outcome described in the provided materials or 'ground\_truth\_answer' is NON-deterministic.
  - 'YES': The answer uses absolute language where uncertainty or probability is warranted.
  - 'NO': The prerequisite IS met, but the conditions for 'YES' are NOT satisfied.
  - 'N/A': The prerequisite is NOT met.
- 'flag\_violation\_of\_foundational\_principles':
  - Evidence Source: 'suggested\_answer'.
  - Definition: Whether the reasoning in the 'suggested\_answer' is scientifically invalid because it violates a fundamental, universally accepted scientific principle.
  - Prerequisite: The 'suggested\_answer' invokes reasoning related to a known scientific principle.
  - 'YES': The reasoning makes a statement that is verifiably FALSE according to a FOUNDATIONAL scientific principle.
  - 'NO': The prerequisite IS met, but the conditions for 'YES' are NOT satisfied.
  - 'N/A': The prerequisite is NOT met.
- 'flag\_failure\_to\_acknowledge\_limitations':
  - Evidence Source: 'experimental\_setup', 'suggested\_answer'.
  - Definition: Whether the 'suggested\_answer' presents a conclusion without acknowledging critical limitations or uncertainties evident from the 'experimental\_setup'.
  - Prerequisite: The 'experimental\_setup' contains CLEAR limitations or sources of error.
  - 'YES': The answer presents its conclusion as robust WITHOUT mentioning the known limitations.
  - 'NO': The prerequisite IS met, but the conditions for 'YES' are NOT satisfied.
  - 'N/A': The prerequisite is NOT met.

#### 5. Formatting & Mechanical Bugs

- 'flag\_incorrect\_answer\_reference':
  - Evidence Source: 'question', 'suggested\_answer', 'ground\_truth\_answer'.
  - Definition: Whether the provided justification or reasoning identifies the correct answer option(s), BUT then a different option letter is given as the final answer.
  - Prerequisite: The 'question' IS a multiple-choice question (MCQ).
  - 'YES': The justification or reasoning provided refers to one option letter while discussing the content of another.
  - 'NO': The prerequisite IS met, but the conditions for 'YES' are NOT satisfied.
  - 'N/A': The prerequisite is NOT met.

Output: Provide your evaluation in the specified JSON format, including the single 'primary\_error\_category' and the choice ('YES', 'NO', or 'N/A') for every 'flag\_'. Note that for some flags the ONLY possible choices are 'YES' and 'NO' (NOT 'N/A'). For each flag, include a brief but clear justification (1-2 sentences) explaining your provided judgment.

[USER]

Fields: outcome\_prediction\_question, pq\_format, experimental\_setup, measurement\_taken, required\_background\_knowledge, answer, reasoning\_for\_answer, clean\_gta

Given the following 'experimental\_setup' and 'measurements\_taken' and 'background\_knowledge' (if any):

- 'experimental\_setup':
 

```
"""
{experimental_setup}
"""
```
- 'measurements\_taken':
 

```
"""
{measurement_taken}
"""
```
- 'background\_knowledge':
 

```
"""
{required_background_knowledge}
"""
```

And for the following 'question' (of type 'question\_type') and its 'ground\_truth\_answer':

- 'question\_type': {pq\_format}
- 'question' (along with choices if applicable):
 

```
"""
{outcome_prediction_question}
"""
```
- 'ground\_truth\_answer':
 

```
"""
{clean_gta}
"""
```

Evaluate the following 'suggested\_answer' with respect to the provided materials as instructed:

- 'suggested\_answer':
 

```
"""
{answer}
"""
```
- REASONING: {reasoning\_for\_answer}
 

```
"""
"""
```

Prompt for generating responses with background knowledge

[SYS]

Fields: domain, field, experimental\_setup, measurement\_taken, required\_background\_knowledge

Instructions: You are tasked with predicting the outcome of a scientific experiment in {domain} and the field of {field} given the provided 'experimental\_setup' and 'measurements\_taken'. You must analyze the user's scientific 'question' very carefully, and forecast the results AS ACCURATELY AS POSSIBLE given the inputs provided. Each question will have a type (multiple-choice, free-form, numerical) that you must consider when formulating your predictions. Ensure that your predictions are well-reasoned and based on the data provided.

Inputs :

- 'domain': {domain}
- 'field': {field}
- 'experimental\_setup': {experimental\_setup}
- 'measurements\_taken': {measurement\_taken}

- 'required\_background\_knowledge': {required\_background\_knowledge}

Question Types:

- Multiple-Choice: Choose the most likely outcome from the list of provided options.
- Free-Form: Provide a comprehensive but concise explanation of the expected results.
- Numerical: Predict a specific numerical value of the outcome based on the provided data.

Output: Depending on the 'question\_type' provided by the user and based on the provided background knowledge, output the appropriate prediction in the following output fields:

- 'answer'
  - Multiple-Choice: Write ONLY the letter(s) corresponding to the most likely outcome in the 'answer' field (e.g., "X"). If choosing multiple letters (items) is allowed by the 'question' and desired, separate them with commas (e.g., "X, Y, Z").
  - Free-Form: Provide a comprehensive but concise explanation of the expected results.
  - Numerical: Write ONLY the predicted numerical value in the 'answer' field (e.g., "1.234").
- 'reasoning\_for\_answer': A detailed explanation of how you arrived at your prediction, including any relevant calculations, assumptions, or scientific principles applied.
- 'confidence': Choose between the levels provided. "Confidence" refers to how certain you are about the accuracy of your prediction based on the information provided.
- 'difficulty': Choose between the levels provided. "Difficulty" refers to the complexity of accurately predicting the outcome of the experiment based on the information provided.
- 'feasibility': Choose between the levels provided. "Feasibility" refers to the practicality of predicting the outcome of the experiment WITHOUT conducting it, based on the information provided.
- 'reasoning\_for\_feasibility': A detailed explanation of how you arrived at your feasibility assessment, considering factors such as experimental design, measurement accuracy, and potential sources of error.

Ensure that your predictions are clear, concise, and directly address the user's scientific 'question'.

[USER]

Fields: pq\_format, outcome\_prediction\_question

Answer the following 'question' as accurately as possible:

- 'question\_type': {pq\_format}
- 'question': {outcome\_prediction\_question}

Prompt for generating responses without background knowledge

[SYS]

Fields: domain, field, experimental\_setup, measurement\_taken

Instructions: You are tasked with predicting the outcome of a scientific experiment in {domain} and the field of {field} given the provided 'experimental\_setup' and 'measurements\_taken'. You must analyze the user's scientific 'question' very carefully, and forecast the results AS ACCURATELY AS POSSIBLE given the inputs provided. Each question will have a type (multiple-choice, free-form, numerical) that you must consider when formulating your predictions. Ensure that your predictions are well-reasoned and based on the data provided.

Inputs :

- 'domain': {domain}
- 'field': {field}
- 'experimental\_setup': {experimental\_setup}
- 'measurements\_taken': {measurement\_taken}

Question Types:

- Multiple-Choice: Choose the most likely outcome from the list of provided options.
- Free-Form: Provide a comprehensive but concise explanation of the expected results.

- Numerical: Predict a specific numerical value of the outcome based on the provided data.

Output: Depending on the 'question\_type' provided by the user, output the appropriate prediction in the following output fields:

- 'answer'
- Multiple-Choice: Write ONLY the letter(s) corresponding to the most likely outcome in the 'answer' field (e.g., "X"). If choosing multiple letters (items) is allowed by the 'question' and desired, separate them with commas (e.g., "X, Y, Z").
- Free-Form: Provide a comprehensive but concise explanation of the expected results.
- Numerical: Write ONLY the predicted numerical value in the 'answer' field (e.g., "1.234").
- 'reasoning\_for\_answer': A detailed explanation of how you arrived at your prediction, including any relevant calculations, assumptions, or scientific principles applied.
- 'confidence': Choose between the levels provided. "Confidence" refers to how certain you are about the accuracy of your prediction based on the information provided.
- 'difficulty': Choose between the levels provided. "Difficulty" refers to the complexity of accurately predicting the outcome of the experiment based on the information provided.
- 'feasibility': Choose between the levels provided. "Feasibility" refers to the practicality of predicting the outcome of the experiment WITHOUT conducting it, based on the information provided.
- 'reasoning\_for\_feasibility': A detailed explanation of how you arrived at your feasibility assessment, considering factors such as experimental design, measurement accuracy, and potential sources of error.

Ensure that your predictions are clear, concise, and directly address the user's scientific 'question'.

[USER]

Fields: pq\_format, outcome\_prediction\_question

Answer the following 'question' as accurately as possible:

- 'question\_type': {pq\_format}
- 'question': {outcome\_prediction\_question}

Prompt used for judge

[SYS]

Fields: domain, field, rubric\_criteria\_lines

Instructions: You are acting as an impartial judge evaluating a suggested answer ('suggested\_answer') to a scientific prediction question in the {domain} domain and the field of {field}. Your goal is to determine how well the 'suggested\_answer' aligns with the 'ground\_truth\_answer' based on a set of specific 'rubric\_criteria' (a list of >=1 criterion items). Each criterion will need to be evaluated independently. Your evaluation must be objective, rigorous, and strictly based on the provided information. The 'question' was asked given the context information of a scientific experiment as defined by the provided 'experimental\_setup' and 'measurements\_taken'.

Evaluation Requirements:

1. First, carefully read and understand the scientific context (domain, field) and the specific 'question'. Use the provided 'experimental\_setup' and 'measurements\_taken' to inform your understanding.
2. Compare the 'suggested\_answer' with the 'ground\_truth\_answer' and reason about the overall correctness and completeness of the 'suggested\_answer'.
3. For EACH criterion (INDEPENDENTLY) provided in the 'rubric\_criteria' list (could be 1 or more criterion items), you must meticulously assess if the 'suggested\_answer' satisfies it ("true" or "false"). The ground truth answer should be used as the reference as the overall correct answer to the 'question'. Provide the output in the corresponding '\_satisfied' fields.
4. Your judgment must be objective. Do not introduce external knowledge or make assumptions beyond the provided text.
5. Provide a concise yet clear justification for EACH criterion's determined satisfaction status ("true"/"false") in the corresponding '\_reasoning' field.

Inputs:

- 'domain': {domain}
- 'field': {field}
- 'rubric\_criteria': Provided below as a list.

Evaluation Criteria:  
 {rubric\_criteria\_lines}

Output Format:

You MUST provide your evaluation in a strict JSON format. For each criterion, you will output two fields: one boolean ('\_satisfied') and one string ('\_reasoning').

[USER]

Fields: outcome\_prediction\_question, predicted\_answer, clean\_gta, experimental\_setup, measurement\_taken

Given the following 'experimental\_setup' and 'measurements\_taken':

- 'experimental\_setup':

```
"""
{experimental_setup}
"""
```

- 'measurements\_taken':

```
"""
{measurement_taken}
"""
```

Evaluate the following 'question' with respect to the provided 'suggested\_answer' and 'ground\_truth\_answer' as instructed:

- 'question': {outcome\_prediction\_question}
- 'suggested\_answer': {predicted\_answer}
- 'ground\_truth\_answer': {clean\_gta}

Prompt to generate responses for questions on background knowledge

[SYS]

Fields: domain, field

Instructions: You are tasked with answering questions about a scientific knowledge/facts in the {domain} domain and the field of {field}. You will be provided with the experimental setup ('experimental\_setup') and the measurements taken ('measurement\_taken') as additional context that are relevant to the questions. Using this information, you must answer the provided question ACCURATELY and COMPLETELY.

Output: Provide your accurate and complete answer to each provided question clearly and concisely. Provide your reasoning for the provided answers in the corresponding output fields.

[USER]

Fields: bkg\_to\_qa, experimental\_setup, measurement\_taken

Given the following 'experimental\_setup' and 'measurements\_taken':

- 'experimental\_setup':

```
"""
{experimental_setup}
"""
```

- 'measurements\_taken':

```
"""
{measurement_taken}
"""
```

Answer each of the following questions (each question has a unique hash identifier):  
{bkg\_to\_qa}

Prompt to generate questions on background knowledge

[SYS]

Fields: domain, field

You are tasked with converting a list of scientific knowledge/fact items in the {domain} domain and the field of {field} into a set of clear, answerable questions. You will be provided with the description of the experimental setup and the measurements taken, the purpose of the given scientific knowledge/fact items is to help predict the outcome of the experiment. You must create EXACTLY ONE question where the original knowledge/fact is the complete and direct answer. DO NOT MAKE any direct references to the experimental setup, and the measurements taken in the questions.

Output the list of questions and the corresponding original facts in the required JSON format.

[USER]

Fields: experimental\_setup, measurement\_taken, required\_background\_knowledge\_hashed

Given the following 'experimental\_setup' and 'measurements\_taken':

- 'experimental\_setup':

""

{experimental\_setup}

""

- 'measurements\_taken':

""

{measurement\_taken}

""

List of knowledge/fact items to convert:

{required\_background\_knowledge\_hashed}

Prompt for generating synthetic background knoweldge

[SYS]

Fields: domain, field

Instructions: You are tasked with generating relevant background knowledge required for predicting the outcome of the provided scientific experiment in the {domain} domain and the field of {field}. Based on the provided domain, field, experimental setup, and measurements, identify and list 3-6 key scientific principles, facts, or concepts that are essential for predicting the outcome.

Output: Your output must match the required JSON format. Output ONLY a single background knowledge item as an element of the output list (multiple items in the list collectively resulting in multiple pieces of background knowledge). Do NOT output ANY additional comments or text outside in addition to the actual pieces of background knowledge.

Example Output:

```
{  
  "generate_bkg": [  
    "Background sentence 1.",  
    "Background sentence 2."  
  ]}
```

```

    ]
}

[USER]
Fields: domain, field, experimental_setup, measurement_taken
```

Please generate the background knowledge for the following experimental direction:

- Domain: {domain}
- Field: {field}
- Experimental Setup: {experimental\_setup}
- Measurements Taken: {measurement\_taken}

Prompt for judging answers to questions on background knowledge

[SYS]  
Fields: domain, field

Instructions: You are acting as an impartial judge evaluating a list of answers ('answers') to questions and if those answers capture the corresponding ground truth facts ('ground\_truth\_facts') for that question in the context of a scientific experiment in the {domain} and the field of {field}. You will also be provided with the experimental setup ('experimental\_setup') and measurements taken ('measurements\_taken') as additional context that are relevant to the questions. Your goal is to determine if each answer is factually correct and complete (using a coverage metric) based on the provided ground truth facts.

Output: Output your evaluation in the provided JSON format. Each corresponding answer/fact pair is guaranteed to match with a unique hash identifier. For completeness coverage, output a number strictly in the range [0, 1] representing the fraction of ground truth facts that are covered by the answer. For correctness, output "true" if the answer is factually correct with respect to the ground truth facts, and "false" otherwise. Provide a concise yet clear justification for each judgment in the corresponding 'reasoning' fields.

[USER]  
Fields: answer\_bkg\_qa, experimental\_setup, measurement\_taken, required\_background\_knowledge\_hashed

Given the following 'experimental\_setup' and 'measurements\_taken':

- 'experimental\_setup':  
"""
   
{experimental\_setup}  
"""
- 'measurements\_taken':  
"""
   
{measurement\_taken}  
"""

And the following 'ground\_truth\_facts' (IDs provided in the start of the lines):  
{required\_background\_knowledge\_hashed}

Provide your judgments strictly matching the above criteria on the correctness and completeness coverage of each ANSWER against the ground truth (ANSWERs need to be evaluated NOT the ground truth facts):  
{answer\_bkg\_qa}

Prompt for converting mcq to ff

[SYS]

Fields: domain, field

Instructions: You are an task with converting multiple-choice questions (MCQ) provided in the {domain} domain and the field of {field} to a free-form question format. You will be provided with the original questions, the multiple-choice options, and the correct answer(s) (potentially multiple), as well as the experimental setup and the measurements taken for the experiment.

Output: Provide the corresponding free-form output question and provide a clear but concise reasoning for the choice and writing of the question. The question must NOT include ANY part from the final MCQ answer and must also not be dependent on the experimental setup or measurements as much as possible. The goal is to have a responder answer the output free-form question, and for a judge to then be able to check whether the free-form question was answered correctly and completely or not based on the original correct answer(s) to the original MCQ question. You should also provide an explanation of how a judge would then be able to verify the correctness AND completeness of an answer to the output free-form question given ONLY the original MCQ question and correct answer(s) as well as experimental setup and measurements taken. Questions MUST be clear in scope (not too broad or too narrow), unambiguous, targeted, and end with a question mark.

[USER]

Fields: outcome\_prediction\_question, experimental\_setup, measurement\_taken, clean\_gta

Given the following 'experimental\_setup' and 'measurements\_taken':

- 'experimental\_setup':

""

{experimental\_setup}

""

- 'measurements\_taken':

""

{measurement\_taken}

""

Convert the following multiple-choice question into a free-form question based on the provided instructions.  
{outcome\_prediction\_question}

Correct answer(s) for this question (NOT to be included in the output free-form question):

{clean\_gta}

Provide your output in the specified JSON format, including the new free-form question, your reasoning for constructed it that way, and the explanation for how a judge would verify the correctness and completeness of an answer to the free-form question.