FrontierChallenge: Evaluating Scientific Workflow Completion

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Website (Leaderboard) GitHub (Evaluation) Hugging Face (Dataset)

Abstract

Scientific agents increasingly analyze data, execute code, and produce research artifacts, yet most benchmarks emphasize final answers, isolated programs, or a single domain. We introduce FRONTIERCHALLENGE, a cross-domain benchmark comprising 300 end-to-end scientific workflows. In this paper, we release and evaluate 97 of these tasks, spanning quantum chemistry, molecular dynamics, materials characterization, analytical chemistry, life science, and electrochemistry/environment. Each task provides fixed inputs and specifies a bundle of required scientific deliverables. We evaluate twelve frontier models with three agent scaffolds. Pass Rate measures the fraction of tasks satisfying the full-completion criterion, while Avg. Score captures partial progress. Each of the best-performing configurations completed only 20 of the 97 released tasks, yielding a Pass Rate of 20.6%. Partial progress translated especially poorly into complete delivery in analytical chemistry and electrochemistry/environment: Avg. Scores reached 87.6 and 94.9, but the highest Pass Rates were only 4% and 0%. Among non-passing Claude Code trajectories, 75.5% still ended with language claiming completion. Complementary HDS6 process scores correlate strongly with task outcomes, supporting FRONTIERCHALLENGE as a benchmark of Heavy Duty Solver capabilities. These findings show that neither high partial scores nor confident claims of completion reliably indicate that a scientific task has been fully delivered, highlighting the need to evaluate end-to-end workflow execution and the completeness of scientific deliverables together.

1 Introduction

Language models are evolving from text generators into agents that can plan, call tools, execute code, and modify persistent files (Liu et al., 2024; Mialon et al., 2024; Xie et al., 2024). Alongside advances in agent scaffolding, continual pre-training has been explored as a way to scale general agent capabilities (Su et al., 2025). Recent systems suggest that agentic support can extend beyond isolated tasks such as literature retrieval or text translation to coordinating multi-stage research workflows with inspectable outputs (Lu et al., 2024). This shift changes what constitutes success on a scientific task. Producing a plausible conclusion is not enough: an agent may need to inspect heterogeneous inputs, select and run an analysis, validate intermediate results, and deliver mutually consistent code, tables, figures, and prose.

Existing benchmarks cover expert knowledge, general tool use, software interaction, code repair, paper replication, and scientific data analysis (Phan et al., 2025; Jimenez et al., 2024; Chen et al., 2025; Siegel et al., 2024; Starace et al., 2025). Their evaluation units, however, are often a final answer, an interaction trace, a single program, or a workflow from one discipline. These settings do not fully characterize whether an agent can complete heterogeneous scientific work whose success depends on several analytical stages and several required deliverables.

FRONTIERCHALLENGE therefore asks a focused question:

> *Given a specified scientific task and fixed data, can an agent independently complete the workflow from input processing to final deliverables and satisfy the complete task contract?*

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Reliable execution underpins a trustworthy scientific handoff: analyses and outputs must be inspectable, reproducible, and mutually consistent. FRONTIERCHALLENGE therefore targets a narrower capability than autonomous science: executing a specified scientific workflow after its objective, inputs, and required outputs are fixed. The agent is not asked to set the research agenda or formulate the problem.

We constructed a pool of 300 end-to-end scientific workflows grouped into six reporting domains: quantum chemistry, molecular dynamics, materials characterization, analytical chemistry, life science, and electrochemistry/environment. In this study, we evaluate and publicly release 97 tasks; the remaining 203 are retained as an internal held-out set. Representative tasks require agents to use domain software, including ORCA, CP2K, LAMMPS, AmberTools, and PLUMED; perform quantitative analysis, quality control, and visualization; and produce executable code and evidence-grounded reports. The unit of evaluation is the complete submitted artifact bundle rather than a single answer.

We evaluated twelve frontier models with three agent scaffolds on the 97 tasks. Our primary metric is Pass Rate, defined as the fraction of tasks for which the complete task contract is satisfied. Avg. Score is reported only as a complementary measure of partial progress; a high-scoring but incomplete submission is not counted as a pass.

To complement outcome-based evaluation, we examine how agents carry out these workflows. Following the HDS6 framework introduced in *Apodex Discovery* (Wang et al., 2026a), we assess Coherence, Evidence, Alternatives, Scope, Tools, and Repair in 1,164 frozen trajectories from 12 model–scaffold configurations. HDS6 process scores correlate strongly with both Avg. Score and Pass Rate (Section 4.4), providing convergent evidence that FRONTIERCHALLENGE tests Heavy Duty Solver capabilities through the execution and delivery of scientific workflows.

The central finding is a persistent gap between partial progress and complete scientific delivery. The best-performing configurations (i.e., GPT-5.6 Sol with Codex and Grok 4.6 with Claude Code) completed only 20 of 97 tasks, corresponding to a Pass Rate of 20.6%, despite the highest Avg. Score reaching 87.9. This gap was especially pronounced in analytical chemistry and electrochemistry/environment: Avg. Scores reached 87.6 and 94.9, respectively, while the highest Pass Rates were only 4% and 0%. Thus, although frontier systems can make substantial progress on complex scientific tasks, they remain far from reliable end-to-end execution.

This work makes three contributions:

1. **Cross-domain scientific workflow benchmark.** We construct a pool of 300 end-to-end workflows spanning six reporting domains, evaluate and publicly release 97 tasks, and retain 203 as an internal held-out set. Each task is defined by fixed inputs, a heterogeneous deliverable contract, and a task-specific Grader.
2. **Contract-level evaluation.** We use Pass Rate as the primary metric of complete workflow execution and Avg. Score to characterize partial progress across task-specific scientific rubrics.
3. **Frontier model study and failure analysis.** We evaluate twelve frontier models with multiple agent scaffolds, quantify domain-level completion gaps, compare machine-observable contract-breach signatures across domains, and analyze final-status and error behavior in 970 Claude Code trajectories.

2 Related Work

General capability and long-horizon agent benchmarks. Humanity's Last Exam (HLE) probes the limits of expert knowledge with difficult, checkable questions (Phan et al., 2025). AgentBench, GAIA, OSWorld, and SWE-bench extend evaluation to tool use, computer interaction, and software engineering (Liu et al., 2024; Mialon et al., 2024; Xie et al., 2024; Jimenez et al., 2024). Agents' Last Exam (ALE) evaluates long-horizon professional work, while Frontier-Bench collects difficult, verifiable tasks near the frontier of agent capability (Sun et al., 2026b; Harbor Framework, 2026). These benchmarks establish

Table 1: Core design characteristics of related benchmarks. A solid dot indicates that the characteristic is part of the benchmark's primary design; a dash indicates otherwise.

Benchmark	Scientific workflow core	Fixed scientific inputs	End-to-end execution	Multiple artifacts	Executable evaluation	Cross-domain science
HLE (Phan et al., 2025)	–	–	–	–	–	●
ALE (Sun et al., 2026b)	–	–	●	●	●	–
Frontier-Bench (Harbor Framework, 2026)	–	–	●	●	●	–
BLADE (Gu et al., 2024)	●	●	–	–	●	●
ScienceAgentBench (Chen et al., 2025)	●	●	●	–	●	●
CORE-Bench (Siegel et al., 2024)	●	●	●	●	●	●
PaperBench (Starace et al., 2025)	●	●	●	●	●	–
BioAgent Bench (Fa et al., 2026)	●	●	●	●	●	–
BiomniBench (Qu et al., 2026)	●	●	●	●	●	–
NatureBench (Wang et al., 2026b)	●	●	●	●	●	●
AstaBench (Bragg et al., 2025)	●	●	●	–	●	●
FRONTIERCHALLENGE	●	●	●	●	●	●

the importance of evaluating completed work, but they are not centered on cross-domain scientific workflows.

Scientific knowledge and data analysis. LAB-Bench evaluates knowledge and reasoning required for biological research (Laurent et al., 2024). BixBench, BioMysteryBench, and CompBioBench use biological data to construct open-ended or objectively verifiable problems (Mitchener et al., 2025; Anthropic, 2026; Nair et al., 2026). BLADE represents open-ended data analysis through expert-recognized analytical decisions, while ScienceAgentBench asks agents to produce executable analyses derived from the scientific literature (Gu et al., 2024; Chen et al., 2025). These benchmarks substantially increase scientific realism, but many evaluate an answer, a decision set, or a single self-contained program rather than a heterogeneous deliverable set.

End-to-end scientific workflows. CORE-Bench and PaperBench evaluate computational reproduction and full research replication (Siegel et al., 2024; Starace et al., 2025). ScienceBoard, SciAgentArena, and SciAgentGym assess scientific software use, interactive research environments, and multi-step tool use (Sun et al., 2026a; Liu et al., 2026; Shen et al., 2026). BioAgent Bench and BiomniBench evaluate end-to-end artifacts or processes in bioinformatics and biomedicine (Fa et al., 2026; Qu et al., 2026). NatureBench and AstaBench broaden the scope to paper-level methods and cross-domain research tasks (Wang et al., 2026b; Bragg et al., 2025). FRONTIERCHALLENGE is complementary: it focuses on reliable completion after the scientific objective and inputs are fixed, while combining cross-domain coverage, multi-artifact outputs, and task-specific executable evaluation.

3 FrontierChallenge

3.1 Task Collection, Curation, and Packaging

Task collection. We collected tasks from scientific and engineering settings, focusing on realistic workflows that require domain knowledge, specialized software, experimental data, or engineering environments. The tasks originate from analysis, computation, simulation, and research-delivery processes performed in domain practice, rather than from expanded question answering or isolated coding exercises. We prioritized workflows in which an agent must understand a professional objective, use domain tools correctly, execute interdependent steps, and produce verifiable scientific artifacts. The complete collection contains 300 scientific workflows; in this paper, we release and evaluate 97.

Figure 1: Domain and workflow-family composition of the 97 released tasks; center bars show the retained Hard/Medium split.

Screening and quality control. We curated tasks according to four design principles:

- **Representativeness.** The workflow, software, and methods must reflect plausible professional practice.
- **Complexity.** The task must require an end-to-end, dependency-aware process culminating in a substantive deliverable, rather than a single command, tool call, or local edit.
- **Diversity.** The collection must vary in scientific knowledge, workflow type, and difficulty, rather than repeat templates with only inputs or parameters changed.
- **Verifiability.** Outputs must be assessable through files, numerical values, quantitative measures, or explicit acceptance criteria, thereby supporting repeatable automated evaluation.

We also checked that every included task had fixed inputs, a defined execution environment, a complete deliverable contract, and an executable evaluation procedure. Tasks centered on isolated facts or single-step operations, tasks with purely subjective outputs, and tasks lacking the materials needed for reproducible scoring were excluded before the final 300-workflow collection was formed.

Standardization and packaging. After curation, we organized each task as a self-contained package with five aligned elements: a *task description* defining the scientific objective; fixed *inputs*, including data and necessary context; the *software and tools* available in the execution environment; an *output contract* listing the required deliverables; and an *evaluation procedure* defining successful completion. Deliverables may include scientific reports, structured tables, diagnostic figures, executable analysis code, simulation products, or multiple artifacts that must remain mutually consistent. Completion therefore depends on the entire artifact bundle, not on whether the agent returns a plausible final answer.

Each package contains task metadata, agent-facing instructions, input data, expected-output or reference

material, a stepwise scoring rubric, an executable Grader, and documentation for reproduction and scoring. Environment specifications, domain tools, auxiliary references, and execution traces are included when required by the workflow. Agent-visible instructions and inputs are separated from evaluator-side references and scoring components. This standardized organization allows each task to be rerun under fixed conditions and scored consistently across evaluated systems.

3.2 Dataset Statistics

All 300 workflows in the curated collection passed the quality-control checks above. For this study, we randomly selected 97 tasks from the subset whose official evaluation does not require GPU resources, publicly released them, and used them for the reported experiments. The remaining 203 tasks form an internal held-out set, which also contains workflows whose official evaluation requires GPUs; none of these held-out tasks is included in the results reported in this paper. The released tasks comprise 74 Hard tasks and 23 Medium tasks. They begin from fixed public empirical data, public sequence or structural resources, or scientifically constrained synthetic data. These source types describe the inputs used to instantiate the workflows; they do not imply that every task begins from a direct laboratory measurement.

For analysis, we organize the 97 released tasks into six reporting domains: quantum chemistry (20 tasks), molecular dynamics (16), materials characterization (22), analytical chemistry (23), life science (10), and electrochemistry (6). Collectively, these tasks cover 21 workflow families and require heterogeneous deliverables, including scientific reports, structured data, figures, executable code, and simulation products. Figure 1 summarizes the domain counts, all 21 workflow families, and the within-domain Hard/Medium composition.

The six domains are descriptive slices of the released evaluation set, not probability samples of their corresponding scientific fields. Their sizes reflect the composition of the current release rather than a claim of balanced coverage. Accordingly, differences in model performance across domains should not be interpreted as intrinsic rankings of disciplinary difficulty.

4 Experiments

We conducted experiments to address four research questions:

1. **RQ1:** How reliably can current frontier models complete specified scientific workflows?
2. **RQ2:** How does scientific workflow performance vary across domains?
3. **RQ3:** Which observable contract breaches and trajectory behaviors most often accompany incomplete scientific handoffs?
4. **RQ4:** What process capabilities do frozen trajectories reveal under a Heavy Duty Solver assessment?

4.1 Agent Scaffolds and Models

Agent scaffolds. We used three advanced agent scaffolds. These were Codex (OpenAI, 2026a), Claude Code (Anthropic, 2026a), and Frontier Agent (ApodexAI, 2026). Codex was used with GPT-5.6 Sol and GPT-5.6 Terra (max), whereas Claude Code served as the common scaffold for ten models. Frontier Agent was evaluated with Apodex 1.1 in the Agent Team configuration.

Models. We evaluated twelve frontier models. These comprised GPT-5.6 Sol and GPT-5.6 Terra (max) (OpenAI, 2026b), Grok 4.6 (xAI, 2026), Kimi K3 (Kimi Team, 2026), Claude Opus 5 (Anthropic, 2026b), and Qwen 3.8 Max (Alibaba Group, 2026). We also included Qwen3.5-397B-A17B (Qwen Team, 2026), DeepSeek V4 Flash-0731 and DeepSeek V4 Pro-0813 (DeepSeek-AI, 2026), Apodex 1.1 (Apodex

Team et al., 2026), and GLM-5.2 (Z.ai, 2026), together with Gemini 3.7 Flash (Google DeepMind, 2026) using dynamic thinking. All models received the same 97 task objectives and task-visible inputs.

4.2 Task-specific Evaluation and Primary Metrics

Each task has a task-specific Grader that checks the required files, numerical results, formats, figures, code execution, and cross-artifact consistency. It returns a native score $s_{mi} \in [0, 100]$ for configuration m on task i. If a rubric-defined semantic criterion is delegated to a Judge, the Judge remains part of that task's Grader. We use GPT-5.6 Sol as the Judge and run each Judge-assessed criterion three times.

Let $N = 97$ denote the number of evaluated tasks. Because scores from three Judge passes are averaged, a submission satisfying the complete rubric can be reported slightly below 100. Following the frozen scoring rule, we therefore define the full-completion indicator as $f_{mi} = \mathbb{1}[s_{mi} \geq 99.9]$ and report:

$$\text{PassRate}_m = \frac{1}{N} \sum_{i=1}^{N} f_{mi}, \tag{1}$$

$$\text{Avg. Score}_m = \frac{1}{N} \sum_{i=1}^{N} s_{mi}. \tag{2}$$

Pass Rate is the primary metric and records tasks meeting this strict full-completion criterion. Avg. Score is the mean task score and measures partial completion. The 99.9 threshold only absorbs minor numerical variation introduced when the three Judge scores are averaged; it does not relax any rubric requirement. Because task-specific rubrics are heterogeneous, Avg. Score is a descriptive suite-level aggregate rather than a calibrated cross-task scale.

4.3 Overall performance

Strict completion remained rare across all configurations. Across the evaluated systems, Pass Rate ranged from 3.1% to 20.6%, whereas Avg. Score ranged from 67.5 to 87.9 (Fig. 2 and Table 2). Codex with GPT-5.6 Sol achieved the highest Avg. Score of 87.9 and shared the highest Pass Rate of 20.6% with Claude Code using Grok 4.6, which obtained an Avg. Score of 86.6. Claude Code with Kimi K3 and Claude Opus 5 each achieved a Pass Rate of 17.5%, with Avg. Scores of 85.5 and 84.9, respectively. Codex with GPT-5.6 Terra (max) followed with an Avg. Score of 84.7 and a Pass Rate of 15.5%.

Table 2: Pass Rate overall and by task difficulty.

Model	Agent Scaffold	Overall ↑	Medium ↑	Hard ↑
GPT-5.6 Sol	**Codex**	**20.6%**	39.1%	**14.9%**
Grok 4.6	**Claude Code**	**20.6%**	**43.5%**	13.5%
Kimi K3	Claude Code	17.5%	39.1%	10.8%
Claude Opus 5	Claude Code	17.5%	39.1%	10.8%
GPT-5.6 Terra (max)	Codex	15.5%	39.1%	8.1%
Qwen 3.8 Max	Claude Code	15.5%	34.8%	9.5%
DeepSeek V4 Pro-0813	Claude Code	13.4%	30.4%	8.1%
DeepSeek V4 Flash-0731	Claude Code	12.4%	34.8%	5.4%
Apodex 1.1	Frontier Agent (Agent Team)	12.4%	30.4%	6.8%
Gemini 3.7 Flash	Claude Code	10.3%	21.7%	6.8%
Apodex 1.1	Claude Code	10.3%	30.4%	4.1%
Qwen3.5-397B-A17B	Claude Code	4.1%	13.0%	1.4%
GLM-5.2	Claude Code	3.1%	4.3%	2.7%

Figure 2: Average score versus complete workflow pass rate.

High Avg. Scores did not imply complete delivery. Eight configurations achieved Avg. Scores above 80, but none completed more than 20.6% of tasks under the strict criterion. Thus, high average scores often reflected artifact bundles that still missed at least one requirement. The two Apodex 1.1 configurations also varied substantially. Frontier Agent (Agent Team) obtained a higher Avg. Score and Pass Rate than Claude Code (74.5 and 12.4% versus 71.8 and 10.3%). This comparison is descriptive and does not isolate a pure scaffold effect.

4.4 Heavy Duty Solver Capability Assessment

Protocol and coverage. Following the HDS6 evaluation framework introduced in *Apodex Discovery* (Wang et al., 2026a), we assess six Heavy Duty Solver capabilities independently of final-task success. We apply this framework through the archived FrontierChallenge HDS6 campaign from September 7, 2026. This is a retrospective process assessment of frozen trajectories, complementing the artifact-based completion metrics in Section 4.2. It covers 12 model–scaffold configurations on all 97 tasks (1,164 scorecards). Apodex 1.1 is included only with Claude Code: the Frontier Agent runs lack the structured ATIF trajectories required by this assessment. The partially covered GLM-5.3 configuration is also excluded. These results therefore do not constitute an HDS6 assessment of every scaffold in the main benchmark.

The six dimensions are *Coherence* (long-horizon state and cross-artifact consistency), *Evidence* (fidelity to executed observations), *Alternatives* (hypothesis and method management), *Scope* (boundary and failure reasoning), *Tools* (tool use and execution-state management), and *Repair* (self-correction under verification). Each task uses 13 shared rubric items plus 6–10 task-specific items with 0/1/2 anchors; the archived scorer reports overall and capability scores on a 1–4 base scale. A reviewed opportunity matrix determines which capabilities are applicable. Missing opportunities are excluded rather than assigned zero: Alternatives and Repair are marked not applicable on 47 tasks each. The judge consumes converted trajectories and task packs, without direct access to the verifier's reference outputs. Private reasoning channels are stripped for all configurations. The archived TERRA panel uses GPT-5.6 Terra as judge and reviewer, GPT-5.6 Luna as sweeper, and Claude Opus 5 as arbiter.

Aggregation. Let A_m be the available runs for configuration m, and $V_m \subseteq A_m$ its graded runs passing the HDS6 integrity gate. This gate is distinct from the benchmark's task-completion threshold. For archived overall score h_{mi}, we reproduce the campaign's coverage-adjusted score:

$$H_m = \left(\frac{1}{|V_m|} \sum_{i \in V_m} h_{mi} \right) \sqrt{\frac{|V_m|}{|A_m|}}. \tag{3}$$

Table 3: Exploratory Heavy Duty Solver (HDS6) process assessment. Scores are coverage-adjusted; higher is better. C: Coherence; E: Evidence; A: Alternatives; S: Scope; T: Tools; R: Repair. V/N denotes gate-passing graded runs / available runs.

Model	Scaffold	HDS6	C	E	A	S	T	R	V/N
Claude Opus 5	Claude Code	3.768	3.890	3.951	3.823	3.508	3.704	3.653	97/97
GPT-5.6 Sol	Codex	3.670	3.874	3.919	3.431	3.341	3.641	3.533	96/97
Qwen 3.8 Max	Claude Code	3.624	3.845	3.842	3.472	3.186	3.601	3.607	96/97
GPT-5.6 Terra (max)	Codex	3.612	3.818	3.876	3.413	3.184	3.582	3.560	95/97
Grok 4.6	Claude Code	3.562	3.777	3.853	3.436	3.196	3.523	3.338	92/97
DeepSeek V4 Pro-0813	Claude Code	3.536	3.787	3.857	3.367	3.003	3.536	3.427	97/97
DeepSeek V4 Flash-0731	Claude Code	3.506	3.774	3.767	3.226	3.056	3.488	3.434	92/97
Kimi K3	Claude Code	3.496	3.776	3.815	3.316	2.996	3.523	3.252	95/97
Apodex 1.1	Claude Code	3.293	3.460	3.544	3.262	2.853	3.304	3.300	82/92
GLM-5.2	Claude Code	3.152	3.302	3.532	3.176	2.652	3.232	2.950	89/97
Gemini 3.7 Flash	Claude Code	3.016	3.258	3.451	2.854	2.438	3.098	2.499	90/97
Qwen3.5-397B-A17B	Claude Code	2.643	2.822	2.998	2.341	2.185	2.683	2.410	69/97

Tasks receive equal weight. For each capability, we average its available scores within V_m and apply the same configuration-level multiplier. Gate failures remain in A_m but do not contribute to the score mean. Five Apodex 1.1 runs containing only an API authentication failure have no process grade and are removed from both sets, giving $|A_m| = 92$ for that configuration and 97 for every other configuration. The original outcome metrics retain their original 97-task denominator. Coverage adjustment can reduce a score below the base scale's lower bound; it is not a pass rate.

Results and interpretation. The HDS6 ranking broadly agrees with the outcome-based ranking reported above. Across the 12 configurations, HDS6 correlates strongly with Avg. Score (Pearson $r = 0.874$, Spearman $\rho = 0.762$) and Pass Rate ($r = 0.828$, $\rho = 0.799$). The association also holds within individual tasks: the mean Pearson correlation between process score and task score is 0.475 across 94 eligible tasks, with positive correlations on 85% of them. Because HDS6 assesses agents' actions and their observed results independently of the artifact grader, this agreement provides evidence that success on FRONTIERCHALLENGE reflects Heavy Duty Solver capabilities. The benchmark's scientific workflows require agents to sustain coherent execution, ground outputs in evidence, manage tools, and verify their work, making FRONTIERCHALLENGE a substantive test of these capabilities.

Table 3 reveals both overall performance differences and specific capability profiles. Claude Opus 5 achieves the highest HDS6 score (3.768), followed by GPT-5.6 Sol (3.670), Qwen 3.8 Max (3.624), and GPT-5.6 Terra (3.612). Evidence is the highest or nearly highest dimension for every configuration, whereas Scope is consistently the lowest (2.185–3.508), identifying boundary checks and failure reasoning as a common weakness. Apodex 1.1 with Claude Code scores 3.293, above Qwen3.5-397B-A17B (2.643), GLM-5.2 (3.152), and Gemini 3.7 Flash (3.016), but below Kimi K3 (3.496) and DeepSeek V4 Flash-0731 (3.506). Its largest gaps relative to Claude Opus 5 are in Scope (2.853 versus 3.508) and Alternatives (3.262 versus 3.823), highlighting boundary/failure reasoning and hypothesis management as concrete targets for improvement.

4.5 Domain-level performance

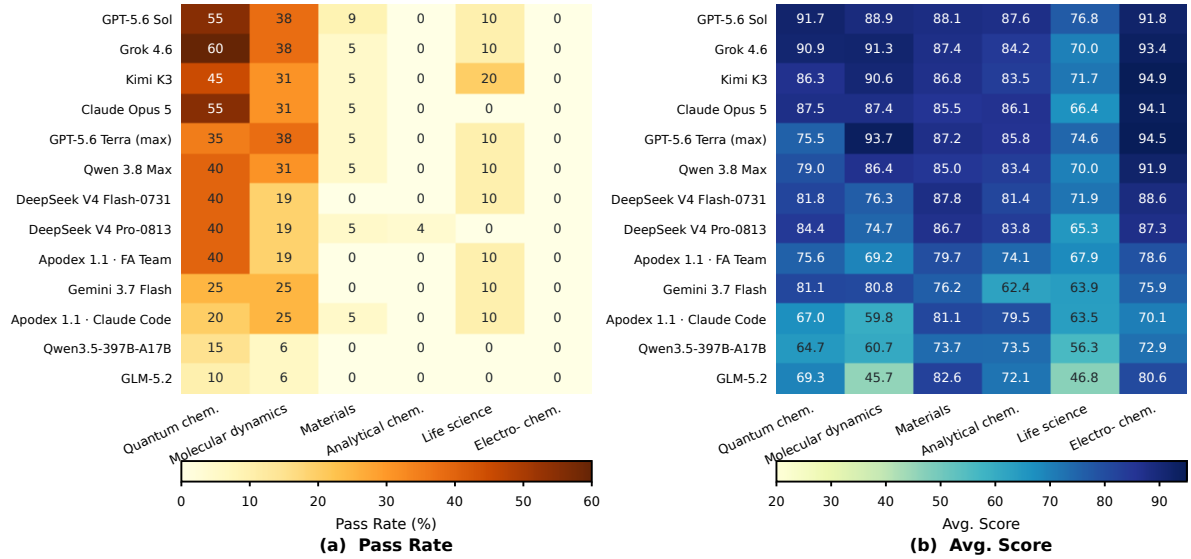

Figure 3: Domain performance.

Pass Rates were highest in two domains. Domain-level Avg. Score and Pass Rate were available for every evaluated system (Fig. 3). In quantum chemistry, Claude Code with Grok 4.6 achieved the highest Pass Rate of 60%, followed by Codex with GPT-5.6 Sol and Claude Code with Claude Opus 5 at 55%. In molecular dynamics, GPT-5.6 Sol, GPT-5.6 Terra (max), and Grok 4.6 each achieved a Pass Rate of 38%, while Terra obtained the highest Avg. Score of 93.7.

High domain-level Avg. Scores often coexisted with near-zero Pass Rates. In materials characterization, Avg. Scores reached 88.1, but no configuration exceeded a Pass Rate of 9%. The divergence was stronger in analytical chemistry and electrochemistry/environment. The highest Avg. Score in analytical chemistry was 87.6, yet only DeepSeek V4 Pro-0813 completed any task in that domain, with a Pass Rate of 4%. Electrochemistry/environment reached a maximum Avg. Score of 94.9, but its Pass Rate remained 0% for every configuration. Life-science tasks showed lower Avg. Scores overall; GPT-5.6 Sol achieved the highest Avg. Score of 76.8, whereas Kimi K3 achieved the highest Pass Rate of 20%.

Representative configurations showed distinct domain profiles. GPT-5.6 Sol had the broadest leading profile, with the highest Avg. Score in quantum chemistry, materials characterization, analytical chemistry, and life science. Grok 4.6 achieved the highest quantum-chemistry Pass Rate (60%) and shared the highest molecular-dynamics Pass Rate (38%). The strongest Apodex 1.1 configuration, Frontier Agent (Agent Team), was more competitive in quantum chemistry (40% Pass Rate) than in molecular dynamics (19%) and did not complete a task in materials characterization, analytical chemistry, or electrochemistry/environment. Terra's aggregate deficit to Sol was concentrated in quantum chemistry: it scored 75.5 versus 91.7 and completed 35% versus 55% of tasks, whereas Terra exceeded Sol in molecular-dynamics Avg. Score (93.7 versus 88.9) and electrochemistry/environment Avg. Score (94.5 versus 91.8). Gemini 3.7 Flash also varied across domains: its Avg. Score ranged from 62.4 in analytical chemistry to 81.1 in quantum chemistry, and it completed 25% of tasks in both quantum chemistry and molecular dynamics but none in materials characterization, analytical chemistry, or electrochemistry/environment. These profiles show that the aggregate ranking did not capture domain-specific strengths and weaknesses.

4.6 Resource use and execution time

Reported token use varied by more than sixfold. Among the twelve configurations with token records, reported input use ranged from 2.183 million tokens per task for Grok 4.6 with Claude Code to 13.730 million for Apodex 1.1 with Claude Code. GPT-5.6 Sol used 6.327 million reported input tokens and 23.1 thousand output tokens per task. GPT-5.6 Terra (max) used 7.039 million input tokens and 38.6 thousand output tokens per task. Their reported cache shares were 98.8% and 98.5%, respectively. Provider-specific tokenizers, caching, and reporting conventions preclude a hardware-normalized efficiency interpretation. Gemini 3.7 Flash used 6.599 million reported input tokens and 25.8 thousand output tokens per task, with a 75.3% cache share (Fig. 4a).

Execution times varied substantially and showed long tails. Across the evaluated systems, mean execution time ranged from 21.8 to 112.8 minutes per task. Frontier Agent (Agent Team) had the longest mean time at 112.8 minutes, with a median of 54.9 minutes and a 90th percentile of 272.2 minutes. Terra (max) had a higher median than Sol (14.0 versus 7.8 minutes) but a lower mean (21.8 versus 22.8), lower 90th percentile (35.0 versus 46.1), fewer trajectories over 60 minutes (5 versus 7), and fewer total machine hours (35.3 versus 36.9), indicating a shorter observed tail. Gemini 3.7 Flash averaged 28.4 minutes per task, with a median of 16.9 minutes, a 90th percentile of 71.9 minutes, and 11 trajectories exceeding 60 minutes. These aggregate summaries describe observed runtimes rather than isolated model speed.

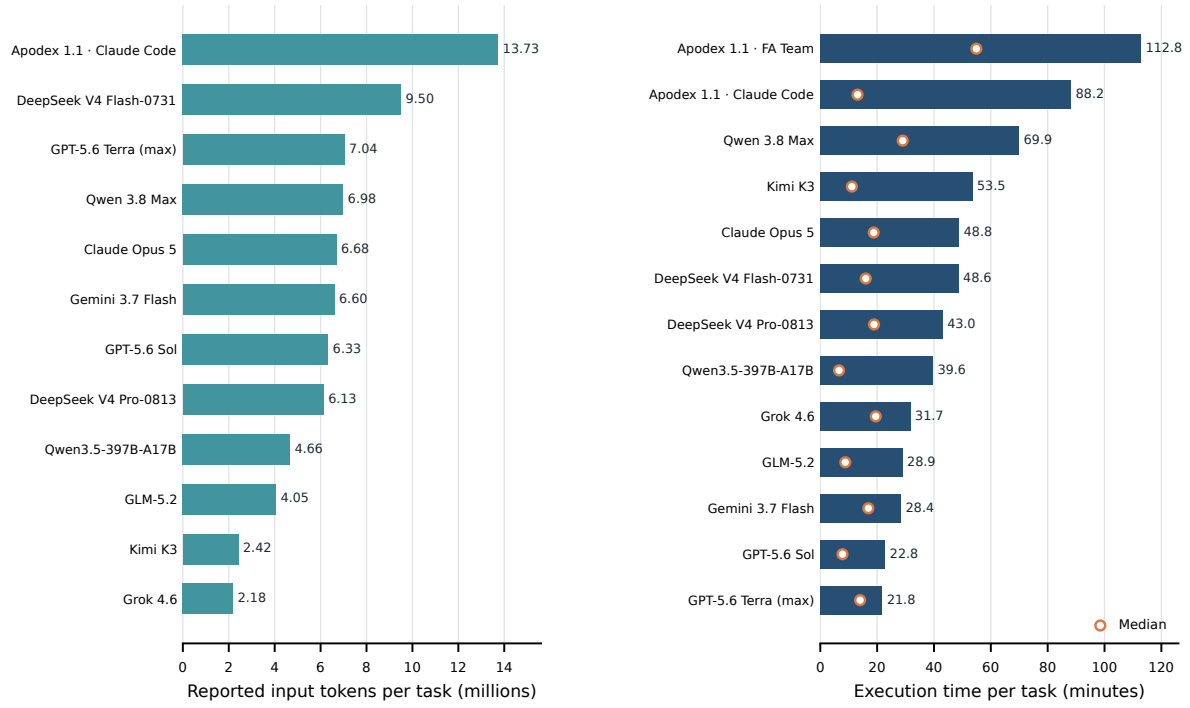

Figure 4: Resource use.

4.7 Failure Mode Analysis

Figure 5 summarizes incomplete scientific handoffs from three complementary views: the prevalence and domain distribution of machine-observable contract-breach signatures, completion language in final messages, and raw tool errors. The signatures can overlap, and the trajectory comparisons are restricted to Claude Code, for which a common event schema was available across models. These analyses are descriptive and do not assign a unique cause to any run.

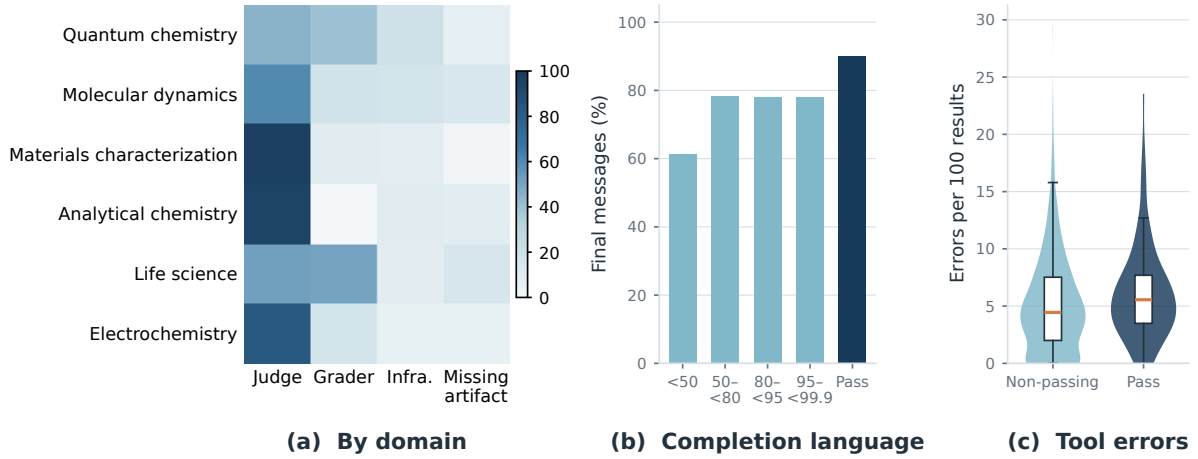

Figure 5: Failure analysis.

Failure signatures varied substantially by domain. Judge-assessed artifact shortfalls appeared in 97% of non-passing materials-characterization submissions, 95% of analytical-chemistry submissions, and 85% of electrochemistry/environment submissions, compared with 43% in quantum chemistry. Deterministic Grader diagnostics were more common in life science (50%) and quantum chemistry (40%) than in the other domains (Fig. 5a). These contrasts partly reflect differences in task contracts and evaluator composition and therefore do not establish intrinsic domain-specific causes.

Completion language did not reliably indicate successful delivery. Among the 970 Claude Code trajectories, 641 of the 849 non-passing runs (75.5%) had a final message containing lexical completion language; only 13 (1.5%) explicitly indicated that work was still running, waiting, or in progress. Completion language was less frequent among runs scoring below 50 (61.2%) but remained above 78% in each non-passing band above 50; it appeared in 90.1% of passing runs (Fig. 5b). Final self-reporting is therefore not a reliable substitute for evaluating the submitted artifact bundle.

Raw tool errors did not predict success. At least one tool error occurred in 80.7% of non-passing and 94.2% of passing Claude Code trajectories. Median error rates were 4.4 and 5.6 per 100 tool results, respectively (Fig. 5c). Successful trajectories can encounter and recover from tool errors; the presence of an error alone does not identify the eventual contract breach.

5 Conclusion

FRONTIERCHALLENGE evaluates whether scientific agents can complete specified, multi-stage workflows and deliver mutually consistent artifacts rather than merely produce plausible answers. The benchmark comprises 300 workflows; this study releases and evaluates 97 across six scientific domains using task-specific executable Graders. Across the evaluated models and agent scaffolds, Pass Rate ranged from 3.1% to 20.6%, despite Avg. Scores of 67.5 to 87.9. GPT-5.6 Sol with Codex achieved the highest Avg. Score and shared the highest Pass Rate with Grok 4.6 using Claude Code. Partial progress translated especially poorly into complete delivery in analytical chemistry and electrochemistry/environment, and the distinct domain profiles show that aggregate rankings do not capture every scientific setting. Failure analysis further showed that 75.5% of non-passing Claude Code trajectories ended with completion language, while tool errors were frequent in both passing and non-passing runs. Final self-reports and the mere presence of errors are therefore weak indicators of successful delivery. The findings are limited to the released task set, evaluated configurations, Claude Code trajectory scope, provider-specific resource accounting, and single runs. Within these bounds, the results establish complete, contract-level delivery as a distinct and unresolved capability. More reliable scientific agents will require explicit contract

tracking, cross-artifact validation, and evidence-based completion checks.

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Appendix

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B Illustrative Task Case

The following three cases illustrate the benchmark unit at the level visible to an evaluated system: a scientific objective, a frozen input bundle, a required workflow, and an artifact contract. They intentionally disclose neither model submissions nor scores, evaluator code, hidden checks, expected outputs, or reference artifacts. Accordingly, the examples characterize what must be done and handed off, not the answer to any task.

B.1 Cell-migration wound-healing assay

Task and visible evidence. This case is an image-analysis and statistical workflow built from 18 supplied bright-field microscopy images. The frozen input crosses two groups (control and experimental), three time points (0, 12, and 24 hours), and three biological replicates. In every image, the experimenter has already marked the closed boundary of the unmigrated region in white. Figure 6 shows one complete time course from each group exactly as provided to the system; the outlines are part of the source images, not generated results.

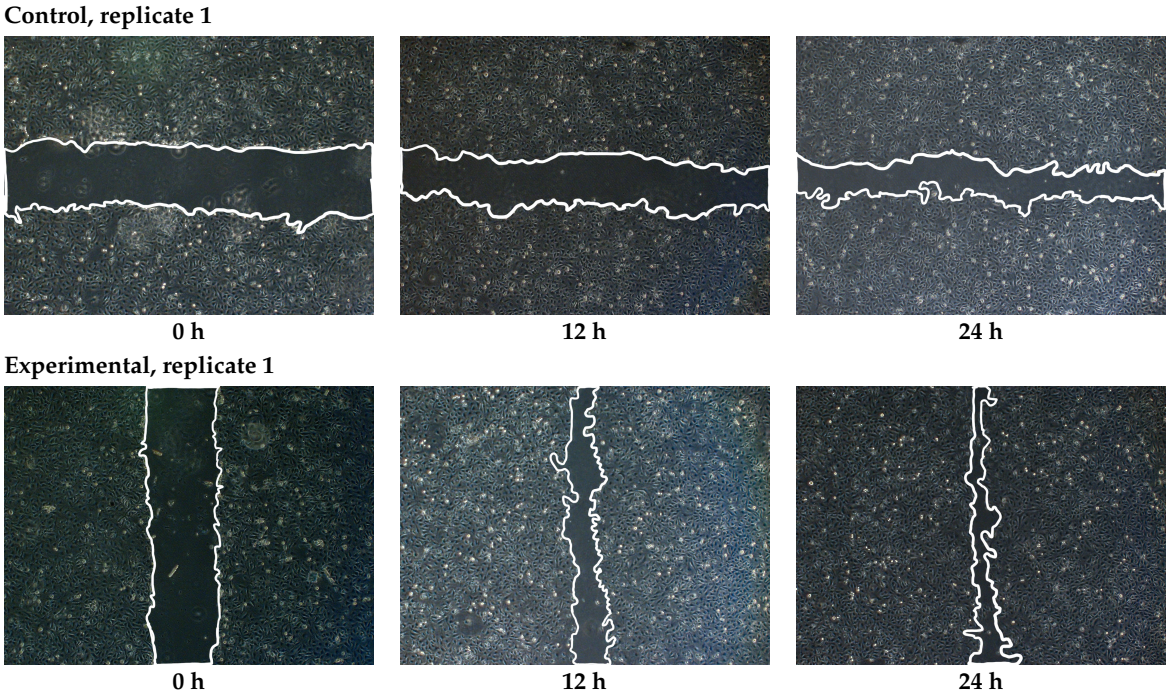


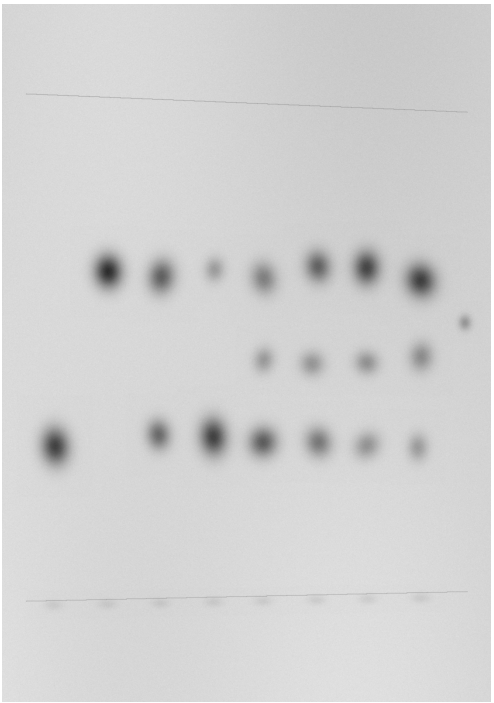
Figure 6: Agent-visible input from the wound-healing case. Columns are the three supplied time points; rows show one biological replicate from each group. White contours were drawn by the experimenter in the original images to delineate the unmigrated region. The remaining twelve images supply two additional replicates for every group–time combination.

Expected handoff. The system must segment the marked unmigrated region in all 18 images, inspect segmentation quality, pair time points by group and replicate, and compute the 12-hour and 24-hour migration rates relative to the matching 0-hour image. It then performs separate between-group tests at both follow-up times. The checkable handoff consists of a reproducible analysis script, an image-level table, a group-statistics table, two labeled summary plots, and a methodological report. No measured area, migration rate, test statistic, or conclusion is shown here.

B.2 TLC monitoring of a Suzuki coupling

Task and visible evidence. This case is an analytical-chemistry image workflow centered on a supplied UV254 thin-layer chromatography plate. Its eight lanes comprise starting- material and product standards, a co-spot, and reaction samples collected at 0, 15, 30, 60, and 120 minutes. The frozen input also supplies the plate map, compound-reference Rf windows and response factors, sampling metadata, image geometry, integration settings, and the endpoint rule. The spotting line and solvent front are intentionally tilted, so Rf must be computed from the local geometry at each lane.

Expected handoff. The system must detect and integrate spots after local background correction, assign compounds using the standards and co-spot, calculate lane-specific Rf values, apply the declared response correction, reconstruct reaction progress, and recommend an endpoint under the supplied rule. Its handoff includes a reproducible script; plate-QC, spot-level, lane-composition, reaction-progress, and endpoint tables; an annotated plate; lane profiles; and a report. Figure 7 is the unmodified agent-visible plate image and contains no derived annotations, integrated intensities, conversion values, or endpoint.



Agent-visible plate map

Lane	Sample	Time
L01	Starting-material standard	–
L02	Product standard	–
L03	Co-spot	–
L04	Reaction sample	0 min
L05	Reaction sample	15 min
L06	Reaction sample	30 min
L07	Reaction sample	60 min
L08	Reaction sample	120 min

Dark UV-quenching spots are the measured image signal. Lane centers, approximate line endpoints, compound search windows, response factors, and the endpoint criterion are supplied separately as structured input.

Figure 7: Unmodified agent-visible TLC input for the Suzuki- coupling case, shown with the supplied lane map. The plate contains standards, a co-spot, and a five-time-point reaction series. No detected spot boundary, Rf assignment, corrected intensity, composition, or endpoint decision is displayed.

B.3 Reaction-calorimetry safety assessment

Task and visible evidence. This case is a hard process-chemistry and thermal-safety workflow. Its frozen input contains electrical calibration pulses, blank-dosing experiments, reaction runs, run and

protocol metadata, and a configuration containing the screening rules. The left side of Figure 8 plots three representative raw input traces exactly as supplied; no baseline correction, integration, derived metric, or protocol decision is displayed.

Expected handoff. The analysis must calibrate and correct heat flow, derive run-level metrics, summarize replicates by protocol, and apply the declared screening criteria. A reproducible script must produce mutually traceable calibration, correction, time-series, run-metric, protocol-summary, and decision tables, together with diagnostic figures and a report. The right side of Figure 8 shows this audit chain rather than its outcome.

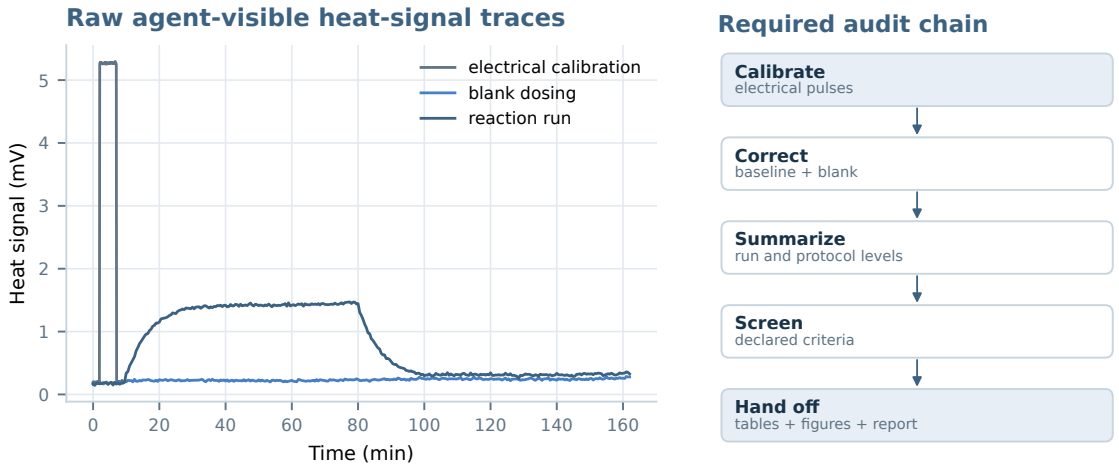


Figure 8: Answer-free view of the reaction-calorimetry case. Raw agent-visible signal traces provide visual context, while the schematic records the required path from calibration evidence to a complete handoff.

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