

Enriching Scientific Knowledge Graph with Entropy-driven Progressive Self-Feedback Fusion (Technical Report)

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Abstract

To support the reproducibility and scientific rigor of “Enriching Scientific Knowledge Graph with Entropy-driven Progressive Self-Feedback Fusion”, this technical report provides essential background and extended results. Key contents include in-depth descriptions of scientific knowledge fusion tasks, precise LLM prompt engineering strategies, and a broader array of experimental results across diverse scientific domains. This document acts as a primary reference for the implementation details and the expanded empirical evidence of the Self-Fusion methodology.

Keywords

AI for Science; Scientific Knowledge Graph Fusion; Entropy-driven Progressive Self-Feedback

A Methodology: Implementation Details

A.1 Entropy-driven Validity Estimation via Token Probability

In Section 4.3, we introduced the validity probability $P((v, r, \hat{v}) | \mathcal{G}_{local}^s(u_i^s))$ to filter high-entropy candidates. To ensure scientific rigor and avoid hallucinated confidence scores often associated with direct numeric output from LLMs, we utilize the model’s intrinsic uncertainty via *output token log-probabilities*.

For a candidate fact $f \in C_{meta}^g(u_i^s)$ and the local context $C_{ctx} = \mathcal{G}_{local}^s(u_i^s)$, we construct a validity query prompt x . We task the LLM to predict a binary verification token $y \in \{\text{"Yes"}, \text{"No"}\}$. The validity probability is calculated as the softmax-normalized probability of the positive token using the access to raw logits:

$$P(f | \mathcal{G}_{local}^s(u_i^s)) = \frac{\exp(\ell(\text{"Yes"}))}{\exp(\ell(\text{"Yes"})) + \exp(\ell(\text{"No"}))} \quad (1)$$

where $\ell(\cdot)$ denotes the logit value of the target token given the context x .

Furthermore, during the *Fusion Scene Generation* (Section 4.3.2), we quantify the **Generation Entropy** to measure the model’s hesitation in grounding the graph structure into natural language. Given the generated description sequence $y = (y_1, \dots, y_T)$, the sequence-level entropy is computed as: $\mathcal{H}_{gen}(y | F_{new}) = -\frac{1}{T} \sum_{t=1}^T \sum_{w \in \mathcal{V}} P(w | y_{<t}, F_{new}) \log P(w | y_{<t}, F_{new})$, where $P(w | \cdot)$ is the probability

distribution over the vocabulary \mathcal{V} at step t . A lower \mathcal{H}_{gen} indicates that the fused scientific facts F_{new} are deterministic enough to induce a coherent and unambiguous scientific description. Facts resulting in $\mathcal{H}_{gen} > \tau_{ent}$ are flagged as high-entropy noise and discarded.

A.2 Core Prompt Details

To ensure reproducibility, we detail the core prompts used in the Self-Fusion framework. We define a standardized prompt template to simulate scientific peer review.

Prompt 1: Validity Verification (Entropy Filter)

Role: You are an expert scientist in [Target Domain, e.g., Molecular Biology].

Context: We have a specialized Scientific Knowledge Graph (SKG) with the following local mechanism:

{Local_SKG_Structure}

Task: We have mined a candidate fact from a General Knowledge Graph:

{Candidate_Fact}

Instruction: Determine if this candidate fact is scientifically rigorous enough to be integrated into the SKG context.

- (1) Does it align with the specific granularity of the context? (e.g., specific protein pathways vs. general associations).
- (2) Does it contradict existing rigorous mechanisms?

Output: Answer strictly with "Yes" or "No".

Prompt 2: Scene Generation (Graph → Text)

Input: A set of scientific facts (Triples):

{Fused_Facts_Set}

Instruction: Synthesize these facts into a coherent, rigorous scientific abstract. The text must logically connect the entities and reflect the causal mechanisms implied by the relations. If the facts are disconnected or ambiguous, explicitly acknowledge the uncertainty in the text.

Algorithm 1: Entropy-driven Progressive Self-Feedback Fusion

```

117 Input : Scientific KG  $G^s$ , General KG  $G^g$ , Thresholds  $\tau, \theta$ 
118 Output : Fused Facts  $F_{final}$ 
119
120 1 Initialize  $F_{final} \leftarrow \emptyset$ 
121 2 Transform  $G^s, G^g$  to Meta-knowledge Line Graphs  $\mathcal{G}^s, \mathcal{G}^g$ 
122 3 for each fact node  $u_i^s \in \mathcal{G}^s$  do
123     /* Phase 1: Fuzzy Retriever (Entropy
124        Maximization) */ *
125     Compute Semantic Candidates  $C_{node}^{sema}(u_i^s)$ 
126     Compute Structural Candidates  $C_{meta}^g(u_i^s)$ 
127     /* Phase 2: Progressive Fusion (Entropy
128        Reduction) */ *
129
130    Initialize feedback constraints  $I_{neg} \leftarrow \emptyset$ 
131     $F_{new} \leftarrow \emptyset$ 
132
133    while not converged and  $t < MaxIter$  do
134        // Step 2.1: Entropy-driven Filtering
135        9 for  $f \in C_{meta}^g(u_i^s)$  do
136            10 Calculate  $P(f | \mathcal{G}_{local}^s, I_{neg})$  via Token Logprobs
137            11 if  $P(f) \geq \tau$  then
138                12      $F_{new} \leftarrow F_{new} \cup \{f\}$ 
139
140        // Step 2.2: Scene Generation (Graph → Text)
141        15  $S_{desc} \leftarrow \text{SceneGen}(F_{new}, \mathcal{G}_{local}^s)$ 
142        // Step 2.3: Reconstruction (Text → Graph)
143        16  $F_{recon} \leftarrow \text{Recon}(S_{desc})$ 
144        // Step 2.4: Cycle Consistency Check
145        17  $F_{valid} \leftarrow F_{recon} \cap F_{new}$ 
146        18  $F_{mismatch} \leftarrow F_{recon} \setminus F_{new}$ 
147        19 if  $F_{mismatch} == \emptyset$  then
148            20      $F_{final} \leftarrow F_{final} \cup F_{valid}$ 
149            21     break           // Entropy minimized
150
151        22 else
152            23      $I_{neg} \leftarrow \text{UpdateConstraints}(F_{mismatch})$ 
153            24      $\tau \leftarrow \tau + \delta$            // Increase strictness
154
155    25 return  $F_{final}$ 
156
157
158
159
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```

Prompt 3: Reconstruction (Text → Graph)

Input: A scientific abstract:

{Generated_Scene_Text}

Instruction: Extract all deterministic scientific facts from the text. Return them strictly as triples (Head, Relation, Tail). Do not infer information not present in the text.

A.3 Self-Fusion Workflow

The overall training procedure of Self-Fusion is summarized in Algorithm 1. The framework alternates between the fuzzy retrieval phase (Exploration) and the progressive self-feedback phase (Crytallization).

Table B1: Statistics of the SciFusion-Bench. “# F_{fused} ”: Fused facts from GKG to SKG. “Str. Sim.”: average entity neighbor structure similarity[9]. “#Rel. O.”: The proportion of overlapping relations in SKG and GKG.

Cluster	Dataset	Domain	# F_{fused}	Str. Sim. \downarrow	Rel. O. \downarrow
LS	SKGF(W-Bio)	Biomedical	12,430	8.2%	0%
	SKGF(W-Plant)	Botany	8,120	13.2%	0%
NS	SKGF(W-Mat)	Materials	11,440	5.7%	0%
	DKG(W-I)	Politics	796,254	15.4%	0%
	DKG(Y-I)	Politics	451,158	14.0%	0%
SHS	SKGF(W-Music)	Musicology	5,057	16.8%	0%

B Supplementary Experiments

In this section, we present a comprehensive evaluation of our framework. We begin by detailing the experimental setup, followed by an in-depth analysis of the results to demonstrate the superiority of the proposed framework in multiple scientific scenarios.

B.1 Experimental Settings

B.1.1 Benchmark Datasets. To evaluate the robustness of Self-Fusion across diverse scientific disciplines, we construct SciFusion-Bench, a multi-domain benchmark encompassing six standardized datasets. As illustrated in Table B1, each dataset follows the prior criteria [29], where general knowledge from Wikidata (via Wikidata or YAGO) is selectively integrated into a specialized SKG. The benchmark is categorized into three major scientific clusters:

- **Life Science (LS):** This cluster covers biological systems and molecular mechanisms. SKGF(W-Bio) integrates general molecular attributes and genetic metadata from Wikidata into PrimeKG [4], a precision medicine KG. SKGF(W-Plant) fuses Wikipedia’s botanical descriptions into the specialized taxonomy and trait records of AgroLD [19].
- **Physical Science (PS):** This cluster emphasizes the properties of physical matter. SKGF(W-Mat) identifies chemical nomenclature and physical constants from Wikidata to enrich the experimental crystal structure data in the materials project [14].
- **Social & Humanistic Science (SHS):** This cluster captures human events and culture. It includes DKG(W-I) and DKG(Y-I), which selectively fuse background entity facts from Wikidata/YAGO into the temporal political event streams of ICEWS [29]. SKGF(W-Music) integrates artist biographies from Wikipedia into the musicology structures of MusicBrainz [12, 23].

Detailed statistics of the entities and fused facts are provided in Table B1.

B.2 Dataset Construction Details

To ensure the reproducibility of SciFusion-Bench and to facilitate future research in AI for Science, we provide a detailed elaboration on the dataset construction protocol. Following the methodology proposed in [29], our construction process adheres to a rigorous pipeline: *Source Selection* → *Entity Alignment* → *Scientific Relevance Filtering* → *Fusion Set Generation*.

Table B2: Main results on DKG(W-I) and DKG(Y-I). The best ACC/F1 results are highlighted in **bold, while the runner-up results are underlined. “*Sema.*, *Struc.*, *LLM*” indicate the use of semantics, structural information, and LLMs, respectively.**

Benchmark Configurations	Settings	DKGF(W-I)-S1					DKGF(Y-I)-S1					DKGF(W-I)-S2					DKGF(Y-I)-S2				
		<i>Sema.</i>	<i>Struc.</i>	<i>LLM</i>	ACC	P	R	F1	ACC	P	R	F1	ACC	P	R	F1	ACC	P	R	F1	ACC
<i>General-purpose</i>																					
Rule.	StringMatch-F	✓			0.496	0.160	0.002	0.004	0.498	0.286	0.003	0.005	0.498	0.192	0.002	0.003	0.498	0.308	0.003	0.005	0.498
	TF-IDF-F	✓			0.498	0.461	0.025	0.047	0.507	0.598	0.043	0.081	0.498	0.451	0.023	0.043	0.508	0.598	0.046	0.086	0.508
Trans.	TransE-F	✓	✓		0.649	0.668	0.596	0.630	0.588	0.782	0.244	0.372	0.637	0.662	0.560	0.607	0.575	0.772	0.212	0.332	0.772
	TransH-F	✓	✓		0.640	0.683	0.520	0.591	0.583	0.764	0.240	0.365	0.632	0.685	0.489	0.570	0.568	0.768	0.195	0.311	0.768
	DistMult-F	✓	✓		0.554	0.547	0.629	0.585	0.525	0.524	0.548	0.536	0.536	0.532	0.590	0.560	0.532	0.530	0.562	0.545	0.530
	ComplEx-F	✓	✓		0.553	0.546	0.632	0.586	0.526	0.525	0.567	0.545	0.544	0.539	0.609	0.572	0.515	0.514	0.546	0.530	0.530
GNN.	GCN-F		✓		0.485	0.487	0.572	0.526	0.501	0.501	0.793	0.614	0.493	0.494	0.582	0.534	0.498	0.499	0.796	0.613	0.499
	TransGNN-F	✓	✓		0.490	0.491	0.505	0.498	0.465	0.465	0.477	0.471	0.486	0.487	0.507	0.497	0.468	0.468	0.481	0.474	0.468
	Graph-Memba-F	✓	✓		0.485	0.487	0.572	0.526	0.503	0.502	0.794	0.615	0.493	0.494	0.582	0.534	0.499	0.501	0.796	0.615	0.501
Generative.	BERT-F	✓			0.532	0.531	0.549	0.540	0.586	0.599	0.523	0.558	0.530	0.531	0.507	0.519	0.569	0.561	0.631	0.594	0.561
	ICL-F	✓		✓	0.550	0.553	0.528	0.540	0.583	0.573	0.649	0.609	0.494	0.494	0.523	0.508	0.488	0.489	0.523	0.505	0.489
	Self-Consistency-F	✓	✓	✓	0.592	0.607	0.522	0.561	0.590	0.584	0.621	0.602	0.531	0.533	0.507	0.520	0.566	0.559	0.628	0.591	0.543
	Self-RAG-F	✓	✓	✓	0.576	0.589	0.506	0.544	0.594	0.623	0.477	0.540	0.544	0.544	0.545	0.545	0.577	0.595	0.481	0.532	0.577
<i>Cross-task Adaptation</i>																					
EA.	SimpleHHEA-F	✓	✓		0.490	0.492	0.507	0.499	0.493	0.493	0.503	0.498	0.492	0.492	0.507	0.500	0.477	0.477	0.481	0.479	0.477
	ChatAE-F	✓	✓	✓	0.596	0.551	0.581	0.566	0.649	0.727	0.477	0.576	0.592	0.611	0.507	0.554	0.592	0.619	0.481	0.541	0.541
KGC.	KG-BERT-F	✓	✓		0.523	0.522	0.546	0.534	0.516	0.515	0.531	0.523	0.507	0.507	0.515	0.511	0.503	0.503	0.481	0.492	0.503
	KG-LLaMA-F	✓	✓	✓	0.512	0.512	0.531	0.521	0.539	0.537	0.558	0.547	0.529	0.527	0.529	0.528	0.521	0.521	0.514	0.517	0.521
	KoPA-F	✓	✓	✓	0.558	0.556	0.577	0.566	0.561	0.556	0.602	0.578	0.549	0.547	0.564	0.556	0.541	0.543	0.522	0.532	0.543
	PRGC-F	✓	✓		0.503	0.503	0.508	0.505	0.507	0.507	0.515	0.511	0.504	0.504	0.507	0.506	0.503	0.503	0.481	0.492	0.503
RTE.	NoGen-BART-F	✓	✓		0.516	0.515	0.531	0.523	0.511	0.511	0.523	0.517	0.508	0.508	0.517	0.512	0.509	0.509	0.491	0.500	0.509
	NoGen-T5-F	✓	✓		0.510	0.510	0.522	0.516	0.507	0.507	0.515	0.511	0.509	0.509	0.519	0.514	0.504	0.504	0.509	0.506	0.504
D.	ExeFuse	✓	✓		0.680	0.673	0.708	0.690	0.661	0.615	0.717	0.662	0.655	0.627	0.683	0.654	0.633	0.634	0.682	0.657	0.657
	Self-Fusion (Ours)	✓	✓	✓	0.779	0.877	0.649	0.746	0.750	0.815	0.647	0.721	0.753	0.878	0.586	0.703	0.691	0.664	0.772	0.714	0.714

B.2.1 Construction Protocol. Phase 1: Domain-Specific Source Selection. We selected three representative authoritative scientific knowledge bases as the backbone for our SKGs:

- **Life Science (PrimeKG):** A precision medicine graph focusing on drug-disease-phenotype interactions. We utilize the subgraph related to *pharmacokinetics*.
- **Physical Science (Materials Project):** A database containing computed properties of inorganic crystals. We focus on the *crystal structure* and *thermodynamic stability* subsets.
- **Social Science (ICEWS):** As described in Section B, we use the temporal political event graph.

Phase 2: Cross-Graph Entity Alignment. To bridge the specialized SKGs with General KGs (Wikidata/YAGO), we performed Entity Alignment (EA). Unlike traditional EA tasks that assume a 1-to-1 mapping, we adopted a *high-precision filtering strategy*. We used curated scientific identifiers (e.g., PubChem CID for chemicals, DOI for papers, GeoNames for locations) to establish rigid anchor links. For entities lacking explicit IDs, we employed a strict string matching protocol constrained by type consistency (e.g., a node in SKG must be of type “Protein” to match a Wikidata node).

Phase 3: Iterative Degree-based Masking (IDS). To rigorously simulate data scarcity in scientific domains, we employed the *Iterative Degree-based Sampling (IDS)* strategy [29]. Specifically, we systematically masked 50% of the aligned entities and their **incident triples** within the SKG. This procedure establishes a challenging “incompleteness gap”, thereby compelling the model to

actively retrieve and fuse external knowledge to restore scientific connectivity.

Phase 4: Scientific Relevance Filtering. A naive integration of Wikidata introduces massive noise (e.g., a scientist’s birth place is irrelevant to their research output). To construct the ground truth F_{fused} , we manually defined a set of *scientifically valid relation types* for each domain (e.g., for SKGF(W-Mat), we strictly retained relations like *has_band_gap*, *crystal_system*, excluding generic ones like *instance_of*).

B.2.2 Benchmark Configurations. Since SKGF is a nascent task with no pre-existing specialized scientific solutions, a primary contribution of this work is to establish a comprehensive and standardized evaluation suite to facilitate future research. Following [29], we systematically adapted 22 representative methods from related fields (e.g., KGC, EA) to the SKGF setting using a unified fusion scoring protocol. These configurations are categorized as follows:

- **General-purpose Configurations.** To establish benchmark performance using universal architectures, this category employs broadly applicable methods (e.g., TransE, GNN, BERT, LLMs) rather than task-specific designs. This category of configurations is mainly based on current advanced and classic general methods, including rule-based methods (i.e., “Rule.”), such as StringMatch-F [7] and TF-IDF-F [16]; Translation-based methods (i.e., “Trans.”) such as TransE-F [3], TransH-F [17], DistMult-F [22], and ComplEx-F [18]; GNN-based methods (i.e., “GNN”) like GCN-F [5, 28], TransGNN-F [26], and Graph-Memba-F [2];

349 Generative methods (i.e., “Generative.”) like BERT-F [6], ICL-
 350 F [10, 21], Self-Consistency-F [15, 20], and Self-RAG-F [1];

- 351 • **Cross-task Adaptation Configurations.** This category of con-
 352 figuration mainly involves improving representative methods
 353 from current related research tasks to adapt to the DKGF task, in-
 354 cluding entity alignment (i.e., “EA.”), such as SimpleHHEA-F [9]
 355 and ChatEA-F [8]; knowledge graph completion (i.e., “KGC.”),
 356 such as KG-BERT-F [24, 27], KG-LLaMA-F [25, 27], KoPA-F [27]
 357 and PRGC-F [13]; and relation triple extraction (i.e., “RTE.”), like
 358 NoGen-BART-F [11], and NoGen-T5-F [11]; and domain-specific
 359 knowledge graph fusion (i.e., “D.”), like ExeFuse [29].

360
 361 **B.2.3 Baseline Implementation.** To ensure fair comparison, we
 362 adapted all baselines to the SKGF task under a **Unified Information**
 363 **Setting.**

364 **Adaptation for Embedding Models (e.g., TransE-F, GCN-F).**
 365 Since these models are designed for Link Prediction within a single
 366 graph, we merged the SKG and GKG into a unified graph $\mathcal{G}_{\text{unified}} =$
 367 $\mathcal{G}^s \cup \mathcal{G}^g$ via the alignment anchors. The models were trained to
 368 score the plausibility of triples (h^s, r^s, t^g) or (h^g, r^s, t^s) .

- 369 • **Hyperparameters:** We performed a grid search for the em-
 370 bedding dimension $d \in \{128, 256, 512\}$ and learning rate $\eta \in$
 371 $\{1e - 3, 5e - 4, 1e - 4\}$. The batch size was fixed at 1024.
- 372 • **Negative Sampling:** We used strict negative sampling where
 373 we corrupted the head or tail entity with a random entity from
 374 the *same domain* to enforce domain constraints.

375 **Adaptation for LLM Baselines (e.g., ChatEA, SelfRAG).** For
 376 method relying on Large Language Models, we constructed prompts
 377 that included the local neighborhood subgraph as context.

- 378 • **Model Version:** Unless otherwise stated in the ablation, we used
 379 gpt-3.5-turbo-1106 for efficient inference and gpt-4-0125-preview
 380 for the reported “Best” numbers.
- 381 • **Temperature:** Set to 0.2 to reduce randomness while allowing
 382 slight creativity for reasoning.

386 **B.3 Main Results**

387 **B.3.1 Performance on Standard Benchmarks (SHS).** As presented
 388 in Table B2, Self-Fusion consistently outperforms all 22 baseline
 389 configurations on the widely-used ICEWS datasets (DKGF(W-I)
 390 and DKGF(Y-I)). Specifically, Self-Fusion achieves a substantial
 391 improvement of **15.0%** in F1-score compared to the strongest gener-
 392 ative baseline, Self-RAG-F. A closer inspection reveals that general-
 393 purpose methods (e.g., TransE-F, GCN-F) struggle to bridge the
 394 semantic gap due to their reliance on shallow structural features.
 395 Similarly, LLM-based cross-task adaptation methods (e.g., ChatEA-
 396 F), while semantically powerful, often introduce high-entropy noise
 397 due to hallucinations. In contrast, Self-Fusion effectively mitigates
 398 these issues by coupling the *fuzzy retriever* with *progressive self-*
 399 *feedback*, ensuring that only scientifically relevant and structurally
 400 compatible facts are fused.

401 **B.3.2 Generalization across Scientific Disciplines (LS & NS).** To fur-
 402 ther validate the *scientific rigor* of our framework in “AI for science”
 403 scenarios, we extended the evaluation to the diverse disciplines
 404 in SciFusion-Bench, including biomedical (SKGF(W-Bio)), and

405 **Table B3: Diagnostic analysis on the auxiliary task “Relevant**
406 Scientific Entity Discovery (RSED).“

Models	DKGF(W-I)-S1			DKGF(Y-I)-S1		
	ACC	F1	Avg.	ACC	F1	Avg.
DistMult-F	0.975	0.835	0.905	0.946	0.787	0.866
Self-RAG-F	0.970	0.785	0.878	0.936	0.721	0.829
ChatEA-F	0.973	0.806	0.889	0.938	0.719	0.828
ExeFuse	0.982	0.871	0.927	0.958	0.823	0.890
Self-Fusion	0.986	0.892	0.939	0.965	0.848	0.907

413 materials science (SKGF(W-Mat)). As shown in Figure B1, Self-Fusi
 414 on exhibits superior generalization capabilities across all domains.

415 **Insight: “Hard Science” Demands Entropy Reduction.** Crucially,
 416 we observe that the performance gap between Self-Fusion and LLM-based baselines (e.g., ChatEA-F) widens in “hard science”
 417 domains (LS & NS) compared to humanities (SHS).

- 418 • On **SKGF(W-Mat)** (materials science), Self-Fusion achieves a
 419 **13.1%** gain over the runner-up. material discovery requires strict
 420 adherence to physical laws; vague associations from GKGs (e.g.,
 421 matching a material solely by name) often lead to erroneous
 422 crystal structure predictions. Our *entropy-driven* mechanism ef-
 423 fectively filters this “scientific noise”.
- 424 • On **SKGF(W-Bio)** (biomedical), where precision is paramount
 425 to avoid false biological pathways, our model outperforms Self-
 426 RAG-F by over **27%**.

427 This suggests that while LLMs can handle the ambiguity of social
 428 sciences (e.g., SKGF(W-Music)), they fail to capture the *deterministic*
 429 *mechanisms* required by rigorous scientific domains without the
 430 explicit entropy reduction constraints imposed by Self-Fusion.

431 **B.4 Relevant Scientific Entity Discovery (RSED)**

432 Accurate identification of specialized, scientific domain-relevant
 433 entities serves as the cornerstone for effective knowledge fusion.
 434 We evaluate this capability through the diagnostic **RSED** task [29].
 435 As shown in Table B3, Self-Fusion consistently outperforms both
 436 the retrieval baseline (Self-RAG-F) and the previous SOTA domain
 437 fusion method (ExeFuse).

438 Notably, while ExeFuse achieves high accuracy, Self-Fusion
 439 yields a significant improvement in F1-score (e.g., **0.892** vs. 0.871 on
 440 DKGF(W-I)). This indicates that our *Entropy-driven Fuzzy Retriever*
 441 effectively balances precision and recall, capturing latent structural
 442 isomorphisms that rigid alignment methods miss. Crucially, this
 443 superior capability in “finding the right needle in the haystack”
 444 directly correlates with the main results in Table B2, where Self-Fu-
 445 sion achieves a 15.0% performance gain. The *Data Self-Feedback*
 446 loop plays a pivotal role here, iteratively filtering out high-entropy
 447 noise (irrelevant entities) that would otherwise propagate errors to
 448 the downstream fusion stage.

449 **B.5 Performance in Low-Resource Settings**

450 Scientific data is often scarce. We evaluated Self-Fusion and key
 451 baselines on **SKGF(W-Bio)** by varying the training data ratio from

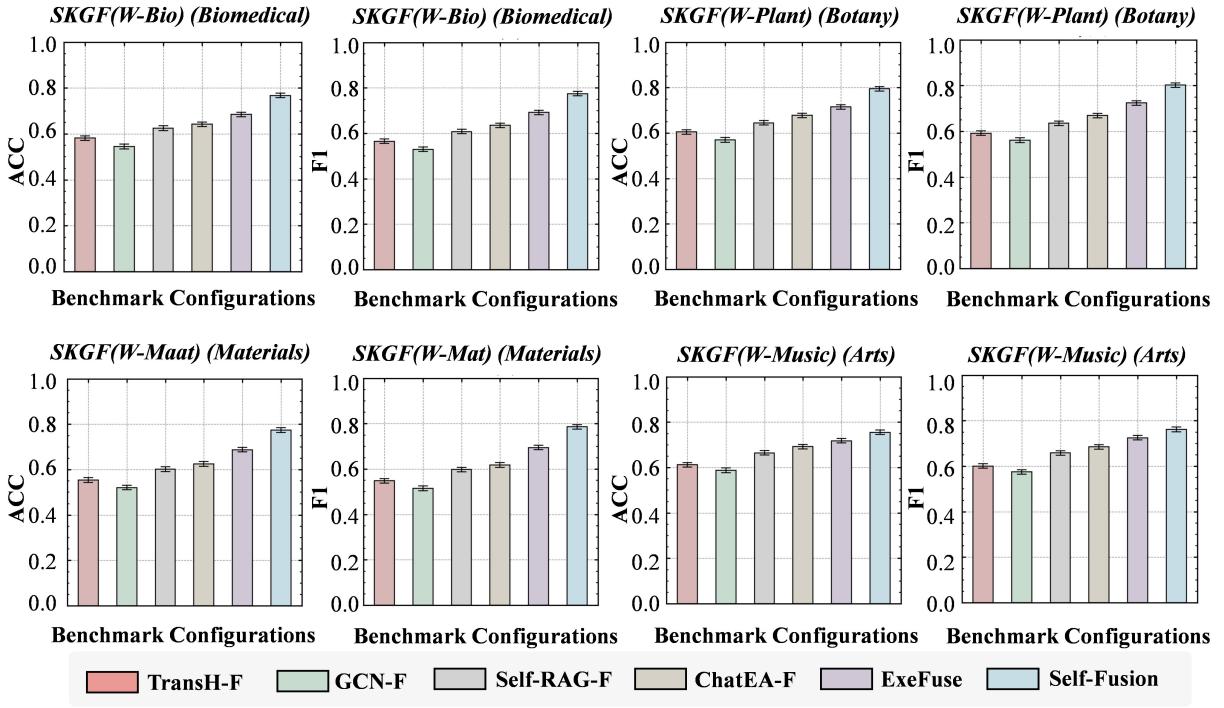


Figure B1: Comprehensive evaluation across diverse scientific disciplines in SciFusion-Bench.

20% to 100%. As shown in Table B4, Self-Fusion maintains high performance even with limited data. Notably, at 15.0% training data, Self-Fusion surpasses ChatEA-F (trained on 100% data), demonstrating that our *entropy-driven* mechanism learns generalized scientific logic rather than relying on memorization.

Table B4: Performance (F1-score) w.r.t. Training Data Ratio on SKGF(W-Bio). “Δ” denotes improvement over the best baseline.

Method	20%	40%	60%	80%	100%
TransH-F	0.352	0.415	0.488	0.542	0.565
GCN-F	0.320	0.395	0.462	0.510	0.530
ChatEA-F	0.485	0.542	0.589	0.620	0.635
Self-Fusion	0.654	0.702	0.738	0.765	0.775
Improvement (Δ)	+34.8%	+29.5%	+25.3%	+23.4%	+22.0%

B.6 Impact of LLM Backbones

To verify that our performance gain stems from the proposed framework rather than the underlying LLM capability, we tested Self-Fusion with different backbones on SKGF(W-Mat). Table B5 shows that Self-Fusion powered by the open-source Llama-3-70B outperforms ChatEA-F powered by the proprietary GPT-4. This confirms the effectiveness of our *Progressive Self-Feedback* design.

B.7 Parameter Sensitivity Analysis

We investigate two critical hyperparameters in Self-Fusion: the entropy threshold τ (which controls fusion strictness) and the structural weight α .

Table B5: Ablation of LLM Backbones on SKGF(W-Mat) (F1-score).

Backbone	ChatEA-F	Self-RAG-F	Self-Fusion
GPT-3.5-Turbo	0.582	0.565	0.742
Llama-3-8B (Open)	0.545	0.532	0.695
Llama-3-70B (Open)	0.605	0.588	0.768
GPT-4-Turbo	0.638	0.615	0.786

Table B6 (represented as table data for clarity) illustrates the F1-score variations on DKG(W-I).

- **Entropy Threshold τ :** Performance peaks at $\tau = 0.7$. Lower values ($\tau < 0.5$) introduce noise (high recall, low precision), while aggressive filtering ($\tau > 0.85$) discards valid scientific cues.
- **Structural Weight α :** The optimal α is around 0.4, indicating that structural isomorphism is slightly more important than semantic similarity in defining scientific validity.

Table B6: Sensitivity Analysis on DKG(W-I) (F1-score).

Metric	0.1	0.3	0.5	0.7	0.9
Threshold τ	0.582	0.645	0.712	0.746	0.685
Struct. Weight α	0.665	0.735	0.746	0.710	0.625

C Case Study

To intuitively understand the “Scientific Rigor,” we present a case from SKGF(W-Bio).

- **Query:** Drug Metformin.

- **Candidate from Wikidata:** (*Metformin, treats, Cancer*).
- **Baseline (ChatEA-F):** Accepts the fact. (Result: Too generic, low scientific value).
- **Self-Fusion:**
 - (1) *Fuzzy Retrieval:* Identifies structural isomorphism between Metformin's pathway and the mTOR pathway.
 - (2) *Entropy Check:* The direct link "treats" has high entropy.
 - (3) *Self-Feedback:* Reconstructs the chain: (*Metformin, activates, AMPK*) → (*AMPK, inhibits, mTOR*).
 - (4) *Final Fusion:* Fuses the specific mechanism chain instead of the generic edge.

This demonstrates how Self-Fusion crystallizes vague general knowledge into deterministic scientific mechanisms.

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