Tool Selection Bias Amplifies in Multi-turn User–Agent Interactions

Nakyeong Yang [1 2] **Junseok Kim** [2] **Kyomin Jung** [2]

Abstract

Large language models (LLMs) are increasingly deployed as agents that interact with external tools via APIs. However, tool selection relies on natural language descriptions and is susceptible to bias from textual variations. Prior work has studied tool selection bias in single-turn settings, whereas its behavior in multi-turn interactions remains underexplored. In this work, we introduce TBMT, a novel benchmark to systematically evaluate tool selection bias in multi-turn settings. Using TBMT, we investigate multi-turn tool selection bias and demonstrate that prior tool choices influence subsequent selections, leading to repeated reuse. Furthermore, this effect persists despite intervening user-agent interactions and can even lead to incorrect tool selections. To resolve these problems, we propose a robust bias mitigation method, TBFAIR, which identifies and perturbs neurons contributing to biased behavior. Our approach significantly reduces bias and improves fairness by modifying only a small fraction of neurons ($\leq 1\%$), while preserving valid tool-calling functionality.

1. Introduction

Large language models (LLMs) have rapidly advanced, achieving remarkable performance across a wide range of real-world tasks (Yang et al., 2025a; Team et al., 2025; Singh et al., 2025). However, they remain inherently limited in their ability to interact with the external world. Specifically, they cannot obtain real-time information (e.g., weather, stock market data) or access external data (e.g., live product listings), as their knowledge is limited to pretraining data. Therefore, LLMs are evolving into autonomous agents capable of interacting with external environments through API tool use (Yao et al., 2022; Qin et al., 2023; Plaat et al., 2025).

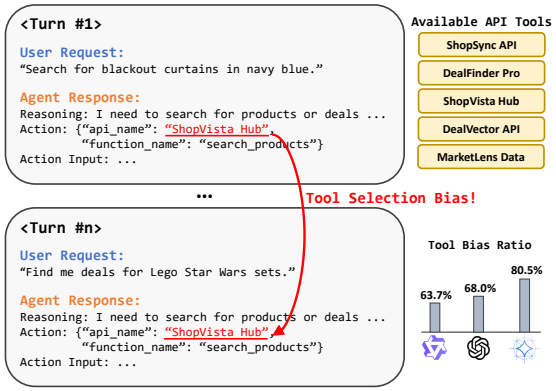

Figure 1. **Multi-turn Tool Selection Bias in LLMs.** After selecting a tool in Turn #1, the agent tends to reuse it in later turns.

However, in the agentic process, LLM agents are provided with a set of available tools described in natural language, making tool selection highly sensitive to subtle textual variations. As agents increasingly mediate access to external services, tool selection shapes the distribution of exposure across API providers (Rothschild et al., 2025; Chiu et al., 2025). Therefore, existing studies have characterized this phenomenon as tool selection bias and have investigated whether such tool usage is fair (Faghih et al., 2025; Blankenstein et al., 2025). Specifically, they investigate LLM biases in factors such as tool descriptions, familiarity, and positional effects. However, these studies primarily focus on single-turn agentic interactions, overlooking multi-turn dynamics. As realistic interactions between users and agents unfold over multiple turns, such biases can accumulate, potentially leading to unfair distribution of tool usage.

To analyze this phenomenon, we first introduce TBMT, a novel benchmark for investigating **T**ool selection **B**ias in **M**ulti-**T**urn settings. Our benchmark covers five tool usage categories (i.e., E-commerce, Finance, Music, Movies, and Travel) and reflects realistic user–agent interaction scenarios. In our experiments, we observe that widely used LLMs exhibit strong biases toward previously selected tools, often overlooking alternative options. Specifically, prior tool selection rates reach 63.7%, 80.5%, and 68.0% for Qwen3 30B, Gemma3 27B, and GPT-5, respectively. Since LLM

[1]Max Planck Institute for Software Systems [2]Seoul National University. Correspondence to: Nakyeong Yang <nyang@mpi-sws.org>, Kyomin Jung <kjung@snu.ac.kr>.

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agents already exhibit biases toward certain tools in single-turn settings (Faghih et al., 2025; Blankenstein et al., 2025), their accumulation across turns can significantly undermine fairness for tool providers. In addition, we show that tool selection biases persist even when intervening user–agent interactions between consecutive tool calls. Furthermore, we demonstrate that multi-turn tool selection biases can also lead to incorrect tool calls, beyond concerns of fairness.

To address these issues, we propose a robust method, TBFAIR, which identifies neurons contributing to tool selection bias and mitigates it by suppressing their influence. Specifically, we identify neurons driving tool selection bias via an attribution method (Yang et al., 2025b), and scale their activations to mitigate biased tool-calling tendencies. We demonstrate that our method significantly mitigates tool selection bias and improves the fairness of agentic LLMs by perturbing only a small portion of neurons ($\leq 1\%$), while preserving valid tool-calling functionality. In contrast, we observe that instruction or persona-based approaches provide limited fairness improvements, as LLMs fail to faithfully follow such guidance in multi-turn tool selection. We make the following contributions:

- We introduce TBMT, a novel benchmark for evaluating tool selection bias in multi-turn user–agent interactions
- We show that prior tool selections bias next decisions, persist despite intervening user-agent interactions, and can induce incorrect tool calls.
- We propose TBFAIR, which identifies and perturbs neurons underlying tool selection bias, and show that it mitigates bias in multi-turn settings.

2. Related Works

2.1. Tool Usage in Agentic LLMs

Recent advances in LLMs have enabled them to interact with external tools, APIs, and plugins, significantly extending their capabilities beyond static knowledge. Prior work has shown that LLMs can effectively orchestrate tool usage to solve complex, multi-step tasks across diverse domains (Parisi et al., 2022; Mialon et al., 2023; Schick et al., 2023; Song et al., 2023; Liang et al., 2024; Patil et al., 2024; He et al., 2025; Wang et al., 2025). More recently, efforts have focused on standardizing how LLMs interface with external tools. In particular, the Model Context Protocol (MCP) (Anthropic, 2024) has contributed to a growing ecosystem of tools and services accessible to agentic LLMs. This development has accelerated the adoption of tool-augmented agents, enabling more scalable integration of external functionalities.

2.2. Tool Selection Bias in LLMs

Recent work has identified tool selection bias as a reliability issue in tool-augmented LLMs. Faghih et al. (2025) have shown that tool preferences are highly sensitive to modifications in tool descriptions, with edits such as assertive cues, usage examples, and name-dropping significantly skewing selection behavior. Shi et al. (2025) have demonstrated prompt-injection attacks on tool selection in LLMs, showing that injecting malicious tool documents into the tool library can manipulate both tool retrieval and tool selection, forcing the LLM to choose attacker-controlled tools. Blankenstein et al. (2025) have further revealed biases toward specific API providers and tool ordering, and shown that factors such as metadata alignment and pretraining exposure can amplify these effects. While these works establish the presence of tool selection bias, they primarily focus on single-turn settings, overlooking how such biases accumulate and persist across multi-turn interactions.

3. Preliminary

Agentic LLM. LLM-based agents are expected to perform iterative planning and interact with their environment over multiple steps. We adopt the formulation of a tool-augmented LLM agent inspired by Yao et al. (2022) and Qin et al. (2023). At each time step t, the agent observes a signal $o_t \in \mathcal{O}$ and selects an action $a_t \in \mathcal{A}$ according to a policy $\pi(a_t \mid c_t)$, where O includes all of the signals that can be obtained from the user and the environment and A contains LLM responses including reasoning and decision makings. The context $c_t = (o_1, a_1, \ldots, o_{t-1}, a_{t-1}, o_t)$ summarizes the full interaction history up to time t.

Tool-calling LLM Agent. We assume access to a set of tools $\mathcal{T} = \{\tau_1, \ldots, \tau_N\}$, where each tool τ_i is associated with a tool description d_i and a parameter schema s_i. At each time step t, the agent selects an action a_t from an augmented action space:

$$\hat{\mathcal{A}} = \mathcal{A} \cup \{(\tau_i, \alpha) \mid \tau_i \in \mathcal{T},\ \alpha \in \mathcal{S}_i\},$$

where $\mathcal{S}_i$ denotes the set of valid arguments defined by the schema s_i of tool τ_i. The agent follows a policy $\pi(a_t \mid c_t, \mathcal{T})$, conditioned on the interaction history c_t and the available tool set $\mathcal{T}$. If $a_t \in \hat{\mathcal{A}}$ corresponds to a tool invocation, the environment executes the selected tool and returns an observation $o_{t+1} = \tau_i(\alpha_t)$, updating the context as $c_{t+1} = (c_t, a_t, o_{t+1})$. In contrast, when $a_t \in \mathcal{A}$ is a non-tool action, the agent produces a direct response to the current observation.

4. TBMT Benchmark

4.1. Problem Definition

Building upon the formulation of tool-using agents, we study *tool selection bias* in multi-turn interactions. To simulate it, we denote user queries as q_i and tool observations as o_i. Accordingly, the trajectory can be expressed as an interleaved sequence of user queries, agent actions, and tool observations as $c = (q_1, a_1, o_1, \ldots, q_t)$. In this study, we analyze how prior tool usage within a trajectory affects subsequent tool selection decisions under the following three setups:

General Tool Calling Setup. We consider a trajectory $c = (q_1, a_1, o_1, q_2)$, where $a_1 = (\tau_1, \alpha_1)$, and refer to the previously selected tool τ_1 as the **anchor tool**. Given the subsequent query q_2, the agent aims to select a correct tool from the valid tools $\mathcal{T}$, including τ_1. Accordingly, the agent generates an action $a_2 = (\tau_j, \alpha_2)$ conditioned on the trajectory c. We characterize tool selection bias as the tendency to reuse the anchor tool (i.e., $\tau_j = \tau_1$), even when multiple valid tools are available.

Tool Calling with Interleaved Noise. In practice, user interactions may include queries that do not require tool usage. To account for this, we introduce intermediate non-tool interactions between two tool-calling steps. Specifically, we consider a trajectory $c = (q_1, a_1, o_1, q_2, a_2, \ldots, q_n, a_n, q_{n+1})$, where $a_1 = (\tau_1, \alpha_1)$ corresponds to a tool invocation, and $a_2, \ldots, a_n \in \mathcal{A}$ denote non-tool actions (e.g., casual conversations). Given the subsequent query q_{n+1} that requires tool use, the agent generates an action $a_{n+1} = (\tau_j, \alpha_{n+1})$ conditioned on the trajectory c. We characterize tool selection bias as a tendency to reuse the anchor tool, i.e., when $\tau_j = \tau_1$, despite the presence of intervening non-tool interactions.

Tool Calling with an Incorrect Anchor Tool. We consider a trajectory $c = (q_1, a_1, o_1, q_2)$, where $a_1 = (\tau_1, \alpha_1)$. Given the subsequent query q_2, the agent is expected to select an appropriate tool from the tool set $\mathcal{T}$, where the previously selected tool τ_1 is not suitable for q_2. The agent then generates an action $a_2 = (\tau_j, \alpha_2)$ conditioned on the trajectory c. We identify a critical failure case when the agent reuses the incorrect anchor tool, i.e., when $\tau_j = \tau_1$, despite its incompatibility with the current query.

4.2. Data Collection

Tool Collections. Based on the problem definition, we construct a new dataset TBMT. We build our dataset by referring to real APIs collected in the ToolLLM benchmark (Qin et al., 2023). We determine five categories: (1) *E-commerce*, (2) *Finance*, (3) *Movies*, (4) *Music*, and (5) *Travel*, and manually evaluate all the tools in the categories to determine whether a tool is appropriate to utilize. To preserve realistic tool-use patterns while enabling controlled evaluation, we synthesize our dataset based on 73 functions collected from 18 real-world APIs.

User Query Generation. We generate realistic user queries for each tool function under the following constraints: (1) queries do not include exact API or function names, (2) queries are user-friendly and exclude internal system identifiers (e.g., "product ID 12345"), and (3) domain-specific reference numbers (e.g., "flight AA100") are allowed. To enforce these constraints, we include them in the system prompt and provide GPT-5 with the tool name, tool description, and available functions, prompting it to generate aligned and realistic queries. The detailed prompt for the query generation process is provided in Figure 6. We generate 100 queries for each category, manually evaluate them, and verify their correctness.

Synthetic Tools and Functions Generation. In this study, we aim to demonstrate that previously selected tools can be preferentially reused in the subsequent tool-calling step. We control for exogenous factors—such as tool name familiarity reported in prior work (Faghih et al., 2025; Shi et al., 2025; Blankenstein et al., 2025)—by generating synthetic tool and function names using GPT-5. Specifically, given a real tool name, we prompt GPT-5 to generate 20 realistic alternative tool names for each dataset category. Similarly, for each real function name, we generate 5 realistic pairs of function names and descriptions. The detailed prompts for the synthetic tool and function generation process are provided in Figure 7 and 8. All generated synthetic tools and functions are manually evaluated and verified for correctness.

Tool Calling and Observations Generation. An LLM selects and executes a tool given a user query, receiving observations from the execution. To emulate this process, we generate realistic tool-calling results using GPT-5. Specifically, we generate tool calls, observations, and agent responses for the first tool-calling step (anchor tool selection), and then construct full trajectories including them. The detailed prompts for tool calling results generation are provided in Figure 9. Note that our primary focus is on examining whether previously selected tools are reused in subsequent tool-calling steps. Accordingly, we prioritize generating sufficiently realistic tool-calling observations, rather than ensuring their perfect fidelity. For example, although an LLM-generated stock price for a company such as Google may deviate from the true value, such variations are unlikely to affect our analysis. Nevertheless, we conduct human evaluation on all generated tool calls, observations, and agent responses to ensure dataset realism and

reliability.

Human Evaluation. We recruit crowd workers fluent in English through the university's online community and ask them to evaluate all tool calling results for realism and reliability. They are instructed to judge the correctness of each output and provide justifications, considering structural validity, contextual consistency with the query, and alignment with function parameter definitions. As a result, we conclude that our benchmark is realistic and properly constructed, as no significant errors that could affect the experimental results were identified. While minor issues were occasionally observed, these were corrected to ensure overall consistency. Further details of the human evaluation are provided in Appendix A.1.

4.3. Multi-turn Tool Selection Bias Dataset

Following the problem definitions in Section 4.1, we first sample one synthetic tool–function pair, $\tau_1 = (\text{API}_1, f_1)$. We then sample a query q_1 associated with τ_1 from the generated query set. Note that each query is originally constructed from a real tool–function pair, and the synthetic tool and function names are built based on the corresponding real ones. In addition, each instance includes the corresponding function description and tool execution results. Therefore, each sampled data point consists of six components: query, tool name, function name, function description, tool call, observation, and agent response. From these components, we construct a trajectory defined as $c = (q_1, a_1, o_1, q_2)$, where $a_1 = (\tau_1, \alpha_1)$. α_1 denotes the generated synthetic tool call, and o_1 represents the corresponding observation and agent response. Table 14 presents the prompt template, including the user–agent interaction trajectory, used to analyze anchoring bias. Note that q_2 is sampled using different strategies for the SAME and DIFF datasets, as follows:

SAME Dataset. The SAME dataset measures anchoring bias when the objective of tool selection remains consistent across turns. For each category, we construct SAME samples as follows: (1) Randomly sample two different queries (q_1, q_2) from the same $\tau_1 = (\text{API}_1, f_1)$ pair without replacement. (2) Provide the sampled queries as a sequential user–agent interaction, where q_1 is presented at turn 1 and q_2 at turn 2. Note that we provide a_1 and o_1 corresponding to q_1 before presenting q_2. (3) Evaluate whether the API selected at turn 1 is reused at turn 2. We also add four randomly sampled API tools as selection options; thus, selecting one out of five yields a fair selection rate of 0.2.

DIFF Dataset. The DIFF dataset evaluates whether anchoring bias persists when the objective of tool selection differs across turns, requiring the agent to adapt to a new functional requirement. We construct DIFF samples as follows: (1) Randomly sample two distinct tool functions, f_1 and f_2, from the same tool name, API_1, without replacement. (2) Independently sample one query from each function to obtain (q_1, q_2). (3) Present (q_1, q_2) as consecutive turns in a user-agent interaction sequence. (4) Evaluate whether the API invoked at turn 1 is reused at turn 2, despite the change in required function. We also add four randomly sampled API tools as selection options; thus, the fair selection rate would be 0.2 accuracy per option.

NOISE Dataset. Based on the SAME and the DIFF datasets, we add some noisy conversations between turn 1 and turn 2 using the Alpaca dataset (Taori et al., 2023) to determine whether the tool selection biases persist against the added noises. Specifically, we sample n query-response pairs from Alpaca and add those pairs between turn 1 and turn 2 pairs, which are already constructed in the SAME and the DIFF datasets. We add $n \in \{1, 3, 5, 10\}$ number of noises to demonstrate the bias persistence. We also add four randomly sampled API tools as selection options; thus, the fair selection rate would be 0.2 accuracy per option.

WRONG Dataset. The WRONG dataset evaluates whether anchoring bias leads to definitively incorrect tool selection when prior tool usage becomes misleading. This dataset is a stricter variant of the DIFF dataset, where the tool selected at turn 1 should not be used at turn 2. We construct WRONG samples as follows: (1) Randomly sample a query q_1 associated with a tool function (API_1, f_1). (2) Sample a second query q_2 whose correct solution requires a different tool $\text{API}_2 \neq \text{API}_1$. (3) Present (q_1, q_2) as consecutive turns in a user-agent interaction sequence, and evaluate whether the API invoked at turn 1 is incorrectly reused at turn 2, where such reuse is strictly invalid.

4.4. Dataset Summary

We construct a multi-domain benchmark including five categories: *E-commerce*, *Finance*, *Movies*, *Music*, and *Travel*. For each category, we generate 100 queries, resulting in a total of 500 queries. The dataset covers 18 distinct APIs comprising 73 functions in total, with detailed statistics summarized in Table 5. For each category, we generate 20 synthetic tool names. For each real-world function, we generate 5 synthetic function names with corresponding descriptions. We further generate associated tool-calling results for each query-function pair. Examples of the generated tool names, function names, queries, and tool-calling results are shown in Table 10.

For evaluation, we construct multiple datasets to analyze tool selection behavior under different conditions. First, for both SAME and DIFF settings, we generate 100 samples per category, resulting in 500 samples for each dataset.

Model	E-commerce		Finance		Music		Movies		Travel	
	SAME	DIFF	SAME	DIFF	SAME	DIFF	SAME	DIFF	SAME	DIFF
Qwen3-4B	0.89 (+0.69)	0.91 (+0.71)	0.73 (+0.53)	0.62 (+0.42)	0.78 (+0.58)	0.72 (+0.52)	0.61 (+0.41)	0.58 (+0.38)	0.61 (+0.41)	0.46 (+0.26)
Qwen3-30B	0.76 (+0.56)	0.89 (+0.69)	0.59 (+0.39)	0.57 (+0.37)	0.72 (+0.52)	0.65 (+0.45)	0.54 (+0.34)	0.54 (+0.34)	0.57 (+0.37)	0.54 (+0.34)
Gemma3-12B	0.76 (+0.56)	0.92 (+0.72)	0.89 (+0.69)	0.75 (+0.55)	0.87 (+0.67)	0.82 (+0.62)	0.66 (+0.46)	0.72 (+0.52)	0.77 (+0.57)	0.50 (+0.30)
Gemma3-27B	0.78 (+0.58)	0.98 (+0.78)	0.86 (+0.66)	0.78 (+0.58)	0.84 (+0.64)	0.85 (+0.65)	0.63 (+0.43)	0.83 (+0.63)	0.73 (+0.53)	0.77 (+0.57)
GPT-5	0.50 (+0.30)	0.65 (+0.45)	0.82 (+0.62)	0.73 (+0.53)	0.79 (+0.59)	0.67 (+0.47)	0.68 (+0.48)	0.72 (+0.52)	0.60 (+0.40)	0.64 (+0.44)

Table 1. **Tool selection bias amplifies in multi-turn user-agent interactions.** We evaluate anchoring bias for the SAME and DIFF datasets across each category. The values highlighted in red indicate the deviation from the random sampling baseline (= 0.2).

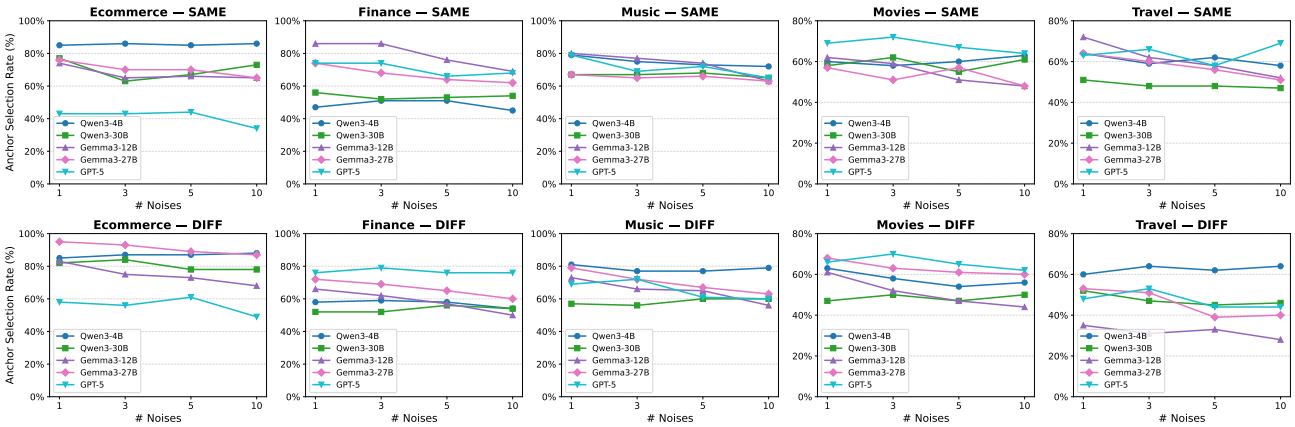

Figure 2. **Tool selection bias persists in multi-turn user-agent interactions with noisy conversation.**

Second, the NOISE dataset augments the SAME and DIFF samples by inserting irrelevant intermediate interactions. Specifically, for each noise level $n \in \{1, 3, 5, 10\}$, we construct 100 samples per category. In the SAME, DIFF, and NOISE settings, the agent must select one API from a candidate set of five. Finally, the WRONG dataset is constructed as a stricter variant of DIFF, where reusing the previously selected tool leads to an invalid solution. Following the same construction protocol, we generate 100 samples per category. In this setting, the agent selects between two candidate APIs, where only one API yields a valid solution.

5. Tool Selection Bias Exists in Multiple User-agent Interactions

5.1. Experimental setups

We select Qwen3 (4B & 30B) (Yang et al., 2025a), Gemma3 (12B & 27B) (Team et al., 2025), and GPT-5 (Singh et al., 2025), chosen due to their strong performance in NLP tasks and widespread use. We utilize their instruction-tuned variants to better reflect real-world deployment scenarios of LLMs. Since prior work has reported significant position bias in tool selection (Blankenstein et al., 2025), we randomize the position of available tools to mitigate this effect. Detailed experimental setups are described in Appendix B.

5.2. The SAME and DIFF dataset results

We conduct experiments on the SAME and DIFF datasets to determine whether tool selection bias exists. Specifically, we measure the anchor tool selection rate, defined as the proportion of cases in which the previously selected tool is chosen again. Under fair selection (i.e., random sampling from five options), this value should be close to 0.2. The experimental results are shown in Table 1. Notably, all models exhibit significant bias toward the anchor tool (i.e., selected in the previous turn) in human–agent interaction scenarios, with anchor tool selection rates consistently exceeding the baseline ($= 0.2$). These results indicate that LLM agents tend to follow previously selected tools in subsequent decisions. This behavior raises concerns about fairness, as it may lead to unequal exposure among tool providers and can be further amplified through bias accumulation.

5.3. The NOISE dataset results

We conduct experiments on the NOISE dataset to examine whether tool selection bias persists when noise is introduced between tool-calling steps. Specifically, we use query–response pairs from the Alpaca dataset (Taori et al., 2023) as noise interactions, and measure the anchor tool selection rate while varying the number of inserted noise interactions (i.e., $n \in \{1, 3, 5, 10\}$). The experimental results are shown in Figure 2. The results indicate that the anchor tool selection bias persists even in the presence of

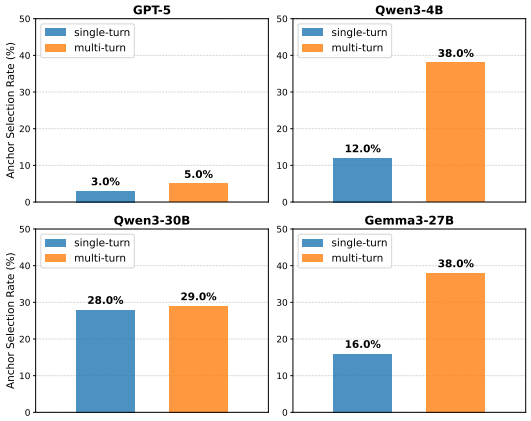

Figure 3. **Tool selection bias occasionally induces incorrect tool selection.** The y-axis shows the ratio of cases in which the wrong anchor tool is selected over the correct tool. *single-turn* and *multi-turn* denote w/o and w/ prior anchor tool selection, respectively.

noise interactions. Although the bias shows a slight decrease as the number of inserted interactions increases, the anchor tool selection rate remains substantially above the random baseline across all settings.

5.4. The WRONG dataset results

We conduct experiments on the WRONG dataset to examine whether tool selection bias can lead to incorrect tool selection. Specifically, we compare settings with and without prior tool selection (i.e., single-turn vs. multi-turn), and further examine how the bias is amplified as interactions progress over turns. The experimental results are presented in Figure 3 and 5. We first observe that models exhibit non-zero rates of incorrect tool selection even in the single-turn setting. However, in the E-commerce category (Figure 3), LLM agents tend to confuse incorrect APIs with correct ones, resulting in a relatively higher anchor tool selection rate in multi-turn settings. In this setting, when an initial bias is already present, prior tool selection further amplifies this bias, which can ultimately lead to incorrect tool selection. These results suggest that tool selection bias can reinforce semantically incorrect API choices. Even occasional errors can adversely affect the reliability of agentic LLMs, highlighting the practical importance of this issue in real-world deployments.

6. Neuron Intervention to Mitigate Tool Selection Bias

We present TBFAIR, a robust method that identifies neurons associated with **T**ool selection **B**ias and selectively intervenes on them to improve **FAIR**ness. We employ an attribution method to identify neurons related to the bias and mitigate it by scaling the activations of the identified neurons.

6.1. Quantifying Tool Selection Bias

Attribution Method. We utilize an attribution method (Yang et al., 2025b) to quantify the importance of neurons for specific undesirable bias patterns in LLMs. Formally, suppose we have $P_\theta(y|x) = \prod_{t=1}^{T} P_\theta(y_t|x, y_1, ..., y_{t-1})$ that represents a language model. The contribution of an i-th neuron to the representation h in a particular layer, in predicting an answer y given a question x using P_θ, is defined as follows:

$$A_{\theta_i,k}^{(x,y)} = h_{\theta_i,k} \times \frac{\partial P_\theta(y|x)}{\partial h_{\theta_i,k}}, \tag{1}$$

where $h_{\theta_i,k}$ denotes the representation of the i-th neuron for the k-th token, computed by P_θ, and $\partial P_\theta(y|x)/\partial h_{\theta_i,k}$ represents the gradient of the output probability with respect to $h_{\theta_i,k}$. We analyze transformer models by computing representations and gradients for each token at a given layer. Given an input sequence of length K, this results in K attribution scores per neuron. Following Yang et al. (2025b), we define a neuron as an individual scalar element in the hidden representation h.

Bias Quantification. To quantify the bias relevance of each neuron, we first construct a trajectory $c = (q_1, a_1, o_1, q_2)$ and feed it into the prompt in Table 14 to form the input x, with the output defined as $y = \text{API}_1$, where $a_1 = (\text{API}_1, f_1, \alpha_1)$. Therefore, the attribution computed for this (x, y) pair corresponds to the amount of tool selection bias knowledge. The final tool selection bias score S_{θ_i} is computed as follows:

$$S_{\theta_i} = \mathbb{E}_{(x,y)\sim\mathcal{D}}[\max_k A_{\theta_i,k}^{(x,y)}], \tag{2}$$

where $\mathcal{D}$ is a set of tool selection bias pairs. In this research, we utilize only ten samples for $\mathcal{D}$ since they are sufficient to quantify the bias knowledge pattern. In addition, we aggregate attributions of tokens by using *max pooling* to acquire a single neuron attribution.

6.2. Scaling Tool Selection Bias Neuron

This section describes how to mitigate the influence of the detected bias neurons. We first sort neurons of the whole layers by the bias attribution scores; then, we scale the top-n neurons by degrading their activation values as follows:

$$\tilde{h}_{\theta_i,k} = (1 - \mathbb{1}[i \in \mathcal{I}_n](1 - \beta))\, h_{\theta_i,k}, \tag{3}$$

where $h_{\theta_i,k}$ denotes the original activation of the i-th neuron, $\tilde{h}_{\theta_i,k}$ is the modified activation after intervention, $\mathcal{I}_n$ represents the set of top-n neurons selected based on the bias scores S_{θ_i}, $\mathbb{1}[\cdot]$ is the indicator function that equals 1

Model	Method	E-commerce		Finance		Music		Movies		Travel	
		ANCHOR	VALID	ANCHOR	VALID	ANCHOR	VALID	ANCHOR	VALID	ANCHOR	VALID
Qwen3-4B	DEFAULT	0.90	1.0	0.68	1.0	0.75	1.0	0.60	1.0	0.54	1.0
	PERSONA	0.90 (+0.00)	1.0	0.67 (-0.01)	1.0	0.75 (+0.00)	1.0	0.59 (+0.01)	1.0	0.54 (+0.00)	1.0
	INSTRUCT	0.90 (+0.00)	1.0	0.67 (-0.01)	1.0	0.75 (+0.00)	1.0	0.57 (-0.03)	1.0	0.54 (+0.00)	1.0
	DIRECT	0.85 (-0.05)	1.0	0.63 (-0.05)	1.0	0.70 (-0.05)	1.0	0.49 (-0.11)	1.0	0.46 (-0.08)	1.0
	TBFAIR	**0.19** (-0.71)	1.0	**0.43** (-0.25)	1.0	**0.56** (-0.19)	1.0	**0.50** (-0.10)	1.0	**0.32** (-0.22)	1.0
Qwen3-30B	DEFAULT	0.83	1.0	0.58	1.0	0.69	1.0	0.54	1.0	0.56	1.0
	PERSONA	0.82 (-0.01)	1.0	0.59 (+0.01)	1.0	0.69 (+0.00)	1.0	0.53 (-0.01)	1.0	0.55 (-0.01)	1.0
	INSTRUCT	0.80 (-0.03)	1.0	0.60 (+0.02)	1.0	0.67 (-0.02)	1.0	0.54 (-0.00)	1.0	0.54 (-0.02)	1.0
	DIRECT	0.75 (-0.08)	1.0	0.39 (-0.19)	1.0	0.62 (-0.07)	1.0	0.42 (-0.12)	1.0	0.36 (-0.20)	1.0
	TBFAIR	**0.17** (-0.66)	1.0	**0.16** (-0.42)	1.0	**0.25** (-0.44)	1.0	**0.20** (-0.34)	1.0	**0.31** (-0.25)	1.0
Gemma3-27B	DEFAULT	0.88	1.0	0.82	1.0	0.85	1.0	0.73	1.0	0.75	1.0
	PERSONA	0.89 (+0.01)	1.0	0.83 (+0.01)	1.0	0.85 (+0.00)	1.0	0.73 (+0.00)	1.0	0.76 (+0.01)	1.0
	INSTRUCT	0.88 (+0.01)	1.0	0.83 (+0.01)	1.0	0.85 (+0.00)	1.0	0.73 (+0.00)	1.0	0.75 (+0.00)	1.0
	DIRECT	0.78 (-0.10)	1.0	0.72 (-0.10)	1.0	0.78 (-0.07)	1.0	0.65 (-0.08)	1.0	0.71 (-0.04)	1.0
	TBFAIR	**0.22** (-0.66)	1.0	**0.31** (-0.51)	1.0	**0.24** (-0.61)	1.0	**0.21** (-0.52)	1.0	**0.29** (-0.46)	1.0

Table 2. **Tool Selection Bias Mitigation Results.** We report the averaged results across SAME and DIFF. Values in parentheses indicate the change in bias relative to the default score, where negative and positive values denote decreases and increases, respectively. The individual results for SAME and DIFF are provided in Table 15 and 16.

if the condition holds and 0 otherwise, and $\beta \in [0, 1]$ is the scaling factor controlling the degree of attenuation.

6.3. Experimental Setups

Dataset and Metrics. We use the SAME and the DIFF datasets to evaluate the tool bias neuron intervention results. As in the previous experimental setups (Section 4.4), we provide five API tools and investigate whether an LLM agent selects the anchor tool (the first selected API) or not. We select two metrics for evaluation. **(1) ANCHOR:** This metric measures the anchor tool selection ratio. This should be close to the random selection ratio of 0.2. **(2) VALID:** This metric measures the proportion of tool selections among the five available options, reflecting whether the model consistently maintains its tool selection behavior. After intervening in neurons, an LLM should retain the ability to contextually predict the tool for the user query.

Baselines. We select two baselines to show the challenges in pursuing the tool selection fairness. **(1) PERSONA:** We inject a persona *"You are a fair tool-usage agent"* in the system prompt to enhance the tool selection fairness of an LLM agent. **(2) INSTRUCT:** We add an instruction *"You should not be restricted to a single tool, but instead be able to use a variety of tools."* in the system prompt to enhance the tool selection fairness of an LLM agent. **(3) DIRECT:** We add a more direct instruction *"You must never reuse any tool that has been used before."* to the system prompt as a direct tool selection restriction. Although such an instruction may not realistically reflect practical use cases, we include it as a strong control condition to evaluate whether explicit restrictions can effectively mitigate tool selection bias. These three baselines are simple but explicit ways to adjust an agent's behavior. Detailed setups are described in Appendix C.

Implementation Details. We evaluate Qwen3 (4B & 30B) and Gemma3 (27B) to evaluate the tool selection bias mitigation effect of our method, TBFAIR. Our method targets neurons in both the self-attention components (Q,K,V,O) and the feed-forward networks (FFNs) across all transformer layers. We use only 10 samples for the bias attribution quantification. We utilize the scaling factor $\beta = 0.7$, and the detailed experiments for the hyperparameter search are shown in Appendix C.

To identify the optimal number of neurons for scaling, we perform binary search over a discretized search space $n \in \{0, 100, \ldots, 20000\}$, requiring at most 8 steps in the worst case. Note that 20000 neurons corresponds to 1.72% of the entire neurons in the case of Qwen3-4B. We utilize 20 data samples as a validation dataset for the binary search evaluation. We stop the binary search process when two conditions are satisfied: (1) the VALID score retains the original VALID score, and (2) the ANCHOR score becomes under the random tool selection baseline of 0.2. If the ANCHOR score can not reach 0.2, we select the highest number of neurons showing the original VALID score as the optimal number.

6.4. TBFAIR Mitigates the Anchor Tool Bias

We intervene in identified bias neurons to mitigate the anchor tool bias, and the experimental results are shown in Table 2. Surprisingly, the injection of the persona and instructions fail to mitigate the anchor tool bias, demonstrating that prompt-based approaches can not resolve the problem. However, TBFAIR successfully mitigates biases without degrading the tool selection performance, especially more in the bigger models. Models with a larger number

Model	Method	E-commerce		Finance		Music		Movies		Travel	
		ANCHOR	VALID	ANCHOR	VALID	ANCHOR	VALID	ANCHOR	VALID	ANCHOR	VALID
Qwen3-4B	DEFAULT	0.90	1.0	0.68	1.0	0.75	1.0	0.60	1.0	0.54	1.0
	TBFAIR(E-commerce)	0.19 (-0.71)	1.0	0.20 (-0.48)	1.0	0.23 (-0.52)	1.0	0.21 (-0.39)	1.0	0.33 (-0.21)	1.0
	TBFAIR(Travel)	0.81 (-0.09)	1.0	0.34 (-0.34)	1.0	0.55 (-0.20)	1.0	0.48 (-0.12)	1.0	0.32 (-0.22)	1.0
Qwen3-30B	DEFAULT	0.83	1.0	0.58	1.0	0.69	1.0	0.54	1.0	0.56	1.0
	TBFAIR(E-commerce)	0.17 (-0.66)	1.0	0.30 (-0.28)	1.0	0.27 (-0.42)	1.0	0.20 (-0.34)	1.0	0.16 (-0.40)	1.0
	TBFAIR(Travel)	0.41 (-0.42)	1.0	0.29 (-0.29)	1.0	0.25 (-0.44)	1.0	0.18 (-0.36)	1.0	0.31 (-0.25)	1.0
Gemma3-27B	DEFAULT	0.88	1.0	0.82	1.0	0.85	1.0	0.73	1.0	0.75	1.0
	TBFAIR(E-commerce)	0.22 (-0.66)	1.0	0.24 (-0.58)	1.0	0.40 (-0.45)	1.0	0.25 (-0.48)	1.0	0.26 (-0.49)	1.0
	TBFAIR(Travel)	0.40 (-0.48)	1.0	0.27 (-0.55)	1.0	0.41 (-0.44)	1.0	0.30 (-0.43)	1.0	0.29 (-0.46)	1.0

Table 3. **Tool Selection Bias Transfer Experiments.** We report the average results over the SAME and DIFF datasets. The detailed results for each dataset are provided in Tables 17 and 18.

Model	E-commerce	Finance	Music	Movies	Travel
Qwen3-4B	0.79%	0.69%	0.86%	0.56%	0.71%
Qwen3-30B	0.48%	0.13%	0.35%	0.50%	0.78%
Gemma3-27B	0.38%	0.46%	0.18%	0.16%	0.23%

Table 4. **Proportion of Neurons Removed.** We report the averaged results across SAME and DIFF.

of parameters tend to exhibit more fine-grained functional specialization across neurons, which enables more precise identification of neurons associated with bias. In addition, we investigate how many neurons are required to mitigate anchor tool bias, as shown in Table 4. We demonstrate that only a small number of neurons is sufficient to mitigate bias, requiring under 1% of neurons.

6.5. Bias Knowledge Can Transfer

We examine whether the quantified bias knowledge can be transferred to other domains. Specifically, we quantify the bias knowledge and search for the optimal bias neurons using the E-commerce and the Travel datasets, and evaluate the results on the other domain datasets. Table 3 and 19 show the experimental results on the other domain datasets. We report the average score for the SAME and the DIFF datasets. The results show that the identified bias neurons consistently reduce anchor tool selection bias even in domains that were not used during neuron discovery.

6.6. Random Neuron Intervention Experiments

We further compare our method with a random neuron selection baseline to evaluate whether the mitigation effect arises specifically from the identified bias-related neurons. We conduct experiments on the SAME and DIFF datasets using the E-commerce and Travel categories for Qwen3-30B and Gemma3-27B. Figure 4 shows the experimental results for random neuron intervention. In the random baseline, we randomly select the same number of neurons and apply activation scaling with a factor of 0.7 to the selected neurons. To reduce randomness, we repeat the random neuron selection process three times and report the averaged results. The results show that random neuron selection fails to meaningfully reduce tool selection bias, with the anchor tool selection rate remaining close to the original level. This result suggests that the effectiveness of our approach does not come from generic activation perturbation, but from selectively intervening on neurons that are specifically associated with tool selection bias.

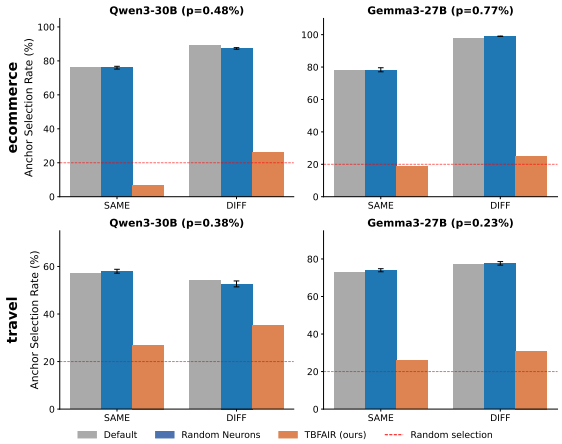

Figure 4. **Comparison with random neuron intervention.** We compare TBFAIR with random neuron selection. Both methods apply activation scaling with a factor of 0.7 to the same number of neurons. For the random neuron baseline, we report the mean and standard deviation over three trials. *Default* denotes the original LLM behavior, and the red dotted line indicates the random selection baseline among five tools.

7. Conclusion

This work investigates tool selection bias in agentic LLMs from a multi-turn perspective. To analyze this, we first introduce TBMT, a novel benchmark for examining tool selection bias in realistic multi-turn settings. In our experiments, we observe that widely used LLMs exhibit strong bias toward previously selected tools, which persists even across intervening user–agent interactions, and can lead to incorrect tool calls beyond fairness concerns. To mitigate this, we propose TBFAIR, a neuron-level intervention that identifies and suppresses bias-inducing neurons. Our approach effectively reduces bias and improves fairness while modifying only a small fraction of neurons, preserving valid tool-calling functionality.

Impact Statements

The dataset constructed in this work includes information about real-world entities, such as airlines, movies, and companies. During the data generation process, GPT-5 may introduce hallucinations related to these entities. However, they do not materially impact our analysis, which focuses on tool selection behavior.

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A. Details of Dataset Construction

We utilize GPT-5 for the dataset construction. We generate diverse natural language queries along with their corresponding function names, given a tool specification that includes the tool name, description, and available functions. Table 6 shows the prompt for the query generation process. As a tool description for the query generation, we use the description of the original API tool, provided in the ToolLLM benchmark. Statistics for the source data are described in Table 5.

Category	# queries	# APIs	# functions
E-commerce	100	5	10
Finance	100	3	29
Movies	100	4	13
Music	100	4	14
Travel	100	2	7
Total	500	18	73

Table 5. **Source Data Statistics.**

To minimize unintended exogenous influences inherent in existing tool names, we generate synthetic tool names for each dataset category. Table 7 presents the prompt used for synthetic API name generation. To ensure realism, we provide a description for each category during the generation process as follows: **(1) E-commerce:** *"online shopping, product search, deals, e-commerce APIs"*, **(2) Finance:** *"financial data, stock market, investment, trading APIs"*, **(3) Music:** *"music streaming, song search, artist info, chart APIs"*, **(4) Movies:** *"movie, TV show, anime, entertainment content APIs"*, **(5) Travel:** *"flight search, airport, ticket booking, travel APIs"*. Furthermore, we generate function names and descriptions by using the prompt, shown in Table 8.

In addition, we generate tool-calling results for each query and its corresponding tool–function pair. Table 9 presents the prompt used for this process. For each instance, we provide GPT-5 with a query, the associated tool–function pair, and the parameter definitions of the function. GPT-5 then generates three components: function_calling, tool observation, and agent response. The function_calling and observation are constrained to JSON format, while the agent response is a natural language answer to the user's query based solely on the observation.

Examples of the generated tool names, function names, queries, and tool calling results are provided in Table 10.

A.1. Details of Human Evaluation

We conduct human evaluation to assess both the correctness of tool calls, the realism of tool observations, and the correctness of responses, following the criteria in Table 11. We find that all tool calls are structurally valid, indicating that GPT-5 reliably generates correct function names and arguments. In contrast, we observe a small number of minor inconsistencies in the tool observations. For example, in rare cases, the deal price exceeds the original price, or the number of returned items is fewer than specified due to our display constraints (at most three items). Importantly, these inconsistencies do not affect the structural correctness of tool usage or the agent's decision-making process, which are the primary focus of our analysis. Therefore, we treat them as negligible for our study. To further improve data quality, we manually correct detected inconsistencies. However, we intentionally retain certain deviations from real-world values (e.g., stock prices, URLs, or airing periods), as exact realism is not required for evaluating tool selection behavior. Examples of the above-mentioned errors are provided in Table 12.

B. Details of Tool Selection Bias Analysis

All our experiments for tool selection bias follow the prompt specified in Table 14. We evaluate tool selection bias in a two-turn tool-use setting. In the first turn, instead of letting the agent generate its own actions, we provide a pre-constructed trajectory for the initial query q_1, including the selected API function, corresponding arguments, and a synthesized observation and response. In the second turn, the agent is presented with a subsequent query q_2 requiring tool use, along with a valid tool set $\mathcal{T}$, which includes the previously selected tool τ_1. The agent is then required to select an appropriate tool from $\mathcal{T}$ by generating the API name, function name, and corresponding input arguments. We provide reasoning that is designed to have minimal influence on the agent's tool selection. The reasoning texts used for each category are shown in Table 13.

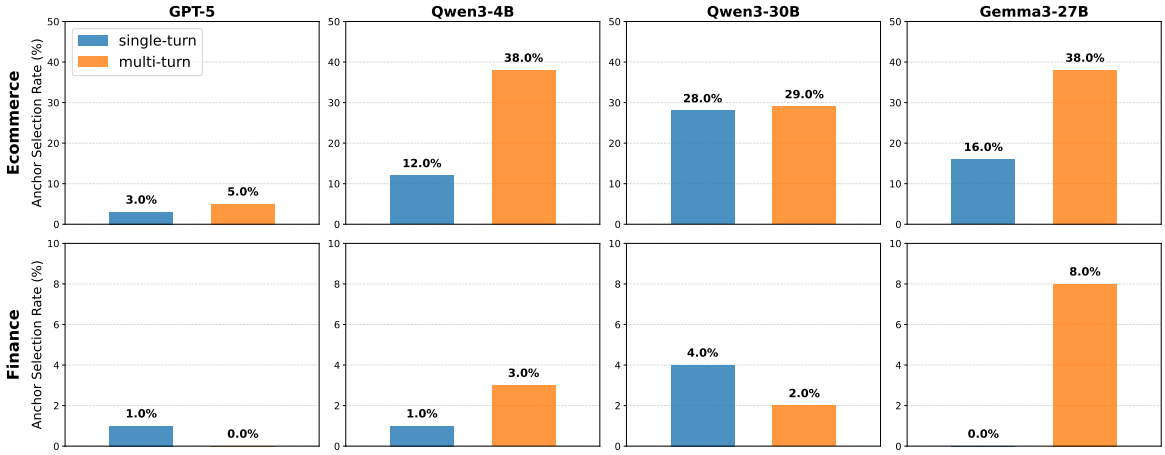

Figure 5. **Tool selection bias occasionally induces incorrect tool selection.** *Single* denotes no prior anchor tool selection, while *Multi* assumes prior anchor tool selection. The values highlighted in red indicate the deviation between the *Single* and *Multi* settings.

The same prompt is used across all datasets (i.e., SAME, DIFF, NOISE, and WRONG). In the NOISE dataset, additional noise conversations are inserted between Turn 1 and Turn 2. To ensure reproducibility, we adopt greedy decoding for generation. To mitigate position bias, we randomize the ordering of the available tools for each instance.

C. Details of Neuron Intervention Experimental Setups

To compute attributions and identify the appropriate number of neurons, we construct a validation set of 20 samples and use it to guide the mitigation of tool selection bias. For neuron steering, we explore scaling factors of 0.5 and 0.7. Since our search procedure selects the number of neurons under the constraint of preserving valid tool selection performance, a scaling factor of 0.5 often fails to satisfy this condition due to overly aggressive steering. As a result, it tends to select suboptimal configurations, leading to degraded overall performance. The comparison between two scaling factors can be found in Figure 6.

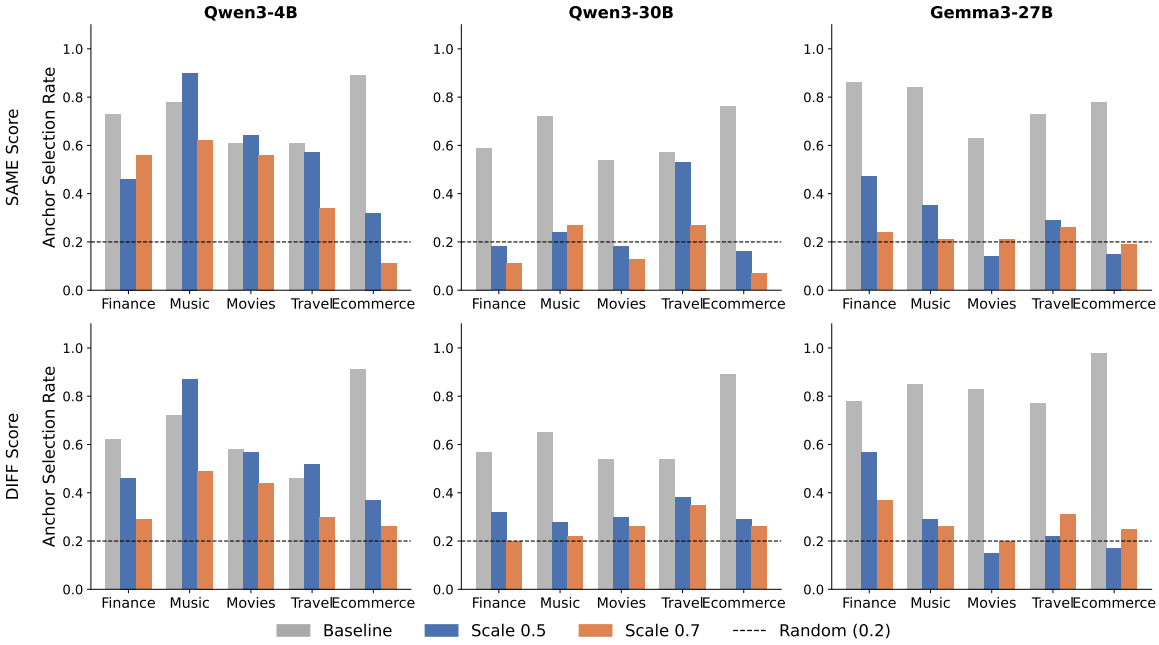

Figure 6. **Scaling factors Comparison for TBFAIR.**

[System Prompt]
You are a helpful query generation assistant. Your job is to generate realistic, diverse user queries for a given API tool.

Rules:
1. Each query must be answerable by calling EXACTLY ONE function from the given tool.
2. Do NOT mention any tool name, brand name, or API name in the query.
3. Write queries as a real user would — natural, task-focused language.
4. Distribute queries across functions as evenly as possible.
5. Include concrete details (ticker symbols, artist names, city names, dates, etc.) to make queries realistic.
6. Output ONLY a JSON array — no markdown, no explanation.

Query realism guidelines:
- NEVER use internal system IDs (e.g., "product ID 123456", "node id 987654") since real users do not know these.
- Stock ticker symbols (AAPL, TSLA, BTC) are acceptable since real users know these.
- Train/flight/booking reference numbers users would realistically receive (e.g., PNR "AB1234", flight "AA100") are acceptable.
- ALWAYS refer to things by their real-world names: product names, artist names, movie titles, company names, city names, etc.
- If a function requires an ID to look up details, generate a query that describes what the user wants by name or context — NOT by ID number.
- BAD: "Get details for the product with ID 123456."
- GOOD: "Show me details for the Wayfair sectional sofa in beige."
- BAD: "What are the details for the anime with ID 4567?"
- GOOD: "What are the details for the anime Attack on Titan?"

[User Prompt]
Generate {n_queries} diverse natural language user queries for the following API tool.

Tool Information
Tool: {tool_name}
Description: {tool_description}

Available Functions ({n_functions} total)
{available_functions}

Output Format
Return a JSON array of exactly {n_queries} objects. Each object must have:
- "query": the natural language user query (no tool/brand names)
- "func_name": the exact function name from the list above

Distribute the {n_queries} queries as evenly as possible across all {len(functions)} functions.

Example:
[{"query": "What is the current price of Apple stock?", "func_name": "real_time_price"},
{"query": "Show me the income statement for Microsoft from last quarter.", "func_name": "income_statement"}]

Table 6. **Prompt template for query generation.** Given a tool specification—including the tool name, description, and available functions—the model generates diverse natural language queries paired with corresponding function names.

[User Prompt]
Generate 20 realistic but fictional API service names for the domain: {category_description}.
Rules:
- Names should sound like real API products (e.g., 'DataStream Pro', 'MarketPulse API')
- Do NOT use famous brand names (e.g., Bloomberg, Amazon, Google, Apple, Netflix)
- Names should be concise (1-3 words) and professional
- Use formats like: '[Word] [Word]', '[Word][Word] API', '[Word] Data', '[Word] Hub'
- Return only a JSON array of 20 strings, nothing else

Table 7. **Prompt template for the synthetic API name generation.** We provide a category description and prompt GPT-5 to generate synthetic API names.

[User Prompt]
You are naming API functions for a {category_description} platform.
The original function name is: '{function_name}'
Here are real user queries that this function handles:
{query_examples}

Based on the function name AND the actual queries above, generate exactly:
1. 5 alternative function names (snake_case, concise, clearly reflect what the function actually does)
2. 5 alternative one-sentence descriptions of what this function does

Return a JSON object with this exact format:
{"names": ["name1", "name2", "name3", "name4", "name5"],
"descriptions": ["desc1", "desc2", "desc3", "desc4", "desc5"]}

Rules:
- Names must be in snake_case
- Names must clearly represent the same functionality inferred from BOTH the original name and the example queries
- Descriptions must accurately describe what the function does based on the example queries
- Descriptions must be distinct paraphrases (1 sentence each)
- Do not include the original name in the 5 alternatives

Table 8. **Prompt template for the synthetic function name and description generation.** We provide a category description, an existing function name, corresponding queries, and prompt GPT-5 to generate synthetic function names.

[System Prompt]
You are a helpful assistant that simulates realistic API tool usage.
Given a user query, API name, function name, and the function's parameter definitions, output:
1. "function_calling": A JSON object of parameter name-value pairs inferred from the query. Use the parameter definitions to determine the correct keys and extract appropriate values from the query (e.g., "Apple" → "symbol": "AAPL", "flights from NYC to LA" → "origin": "JFK", "destination": "LAX").
2. "observation": A realistic JSON API response returned by the function call.
3. "response": A concise natural language response to the user's query based solely on the observation. Do not mention the tool or API. Only include information explicitly present in the observation.

Rules:
- "function_calling" keys must exactly match the parameter names in the provided definitions
- "function_calling" values must be properly inferred from the query (extract symbols, IDs, keywords, etc.)
- "observation" must be realistic and structured like a real API response
- "observation" must contain at most 3 result items (e.g., list entries, records) in any array field
- "response" must not include any information not present in the observation
- Output only valid JSON with keys "function_calling", "observation", and "response"

[User Prompt]
Query: {query}
API: {tool_name}
Function: {function_name}
Parameter definitions: {parameter_definition}
Generate function_calling, observation, and response JSON:

Table 9. **Prompt template for the tool calling results generation.** We provide a query, tool name, function name, and parameter definition, and prompt GPT-5 to generate realistic tool calling results.

Category	Data Type	Examples
E-commerce	Query	”Look up deals on Samsung 65-inch TVs.”
	Tool Name	ShopSync API
	Function Name	search_deals_by_keywords
	Tool Call	{”ItemName”: ”Samsung 65-inch TV”}
	Observation	{”query”: ”Samsung 65-inch TV”, ..., ”deals”: [{ ”id”: ”D001”, ”title”: ”Samsung 65-inch Class QLED Q60C (2023) 4K Smart TV”, ”price”: 699.99, ”original_price”: 899.99, ”discount_percent”: 22, ”seller”: ”BestBuy” ...
	Response	Found 3 deals for ”Samsung 65-inch TV”:\n\n- Samsung 65-inch Class QLED Q60C (2023) 4K Smart TV — $699.99 (was $899.99, 22% off). Seller: BestBuy. Availability: In Stock. Shipping: Free 2-day shipping ...
Finance	Query	”Show me the live price for Tesla shares right now.”
	Tool Name	StockWave Data
	Function Name	fetch_current_price
	Tool Call	{”symbol”: ”TSLA”}
	Observation	{”status”: ”ok”, ”symbol”: ”TSLA”, ”price”: ”193.45”, ”bid”: ”193.40”, ”ask”: ”193.50”, ”previous_close”: ”190.12”, ”exchange”: ”NASDAQ”, ”currency”: ”USD”, ”timestamp”: ”2026-03-29T14:32:10Z”, ”datetime”: ”2026-03-29 14:32:10”}
	Response	TSLA (NASDAQ) — Last price: USD 193.45. Bid: 193.40 / Ask: 193.50. Previous close: 190.12. Timestamp: 2026-03-29T14:32:10Z (2026-03-29 14:32:10).
Music	Query	”Search for the electronic producer Fred again..”
	Tool Name	MelodySync
	Function Name	find_artist_by_name
	Tool Call	{”q”: ”Fred again”}
	Observation	{”status”: ”ok”, ”query”: ”Fred again”, ”results”: [{”id”: ”ss_art_001”, ”name”: ”Fred again”, ”slug”: ”fred-again”, ”artist_url”: ”https://songstats.com/artist/fred-again”, ”spotify_id”: ”6fredAg12345”, ”genres”: [”Electronic”, ”Dance”], ”followers”: 1450000, ”image_url”: ”https://images.songstats.com/artists/fred_again.jpg”} ...
	Response	Found 2 results for ”Fred again”\n\n1) Fred again\n- slug: fred-again\n- artist page: https://songstats.com/artist/fred-again\n- spotify_id: 6fredAg12345\n- genres: Electronic, Dance\n- followers: 1,450,000\n- image: https://images.songstats.com/artists/fred_again.jpg\n\n ...
Movies	Query	”Can you find the documentary Free Solo?”
	Tool Name	SceneTrack Hub
	Function Name	top_trending_anime
	Tool Call	{”type”: ”adventure”, ”q”: ”Free Solo”}
	Observation	{”results”: [{”id”: 98765, ”title”: ”Free Solo”, ”type”: ”adventure”, ”year”: 2018, ”runtime_minutes”: 100, ”imdb_id”: ”tt7775622”, ”tmdb_id”: 511, ”overview”: ”Documentary following rock climber Alex Honnold’s attempt to free-solo climb El Capitan in Yosemite National Park.”, ”rating”: 8.2}]}
	Response	Yes. Free Solo (2018) is a documentary film. Runtime: 100 minutes. Overview: ”Documentary following rock climber Alex Honnold’s attempt to free-solo climb El Capitan in Yosemite National Park.R̈ating: 8.2 ...
Travel	Query	”Show direct flight deals from Istanbul to Antalya leaving 2026-06-25 and returning 2026-07-02.”
	Tool Name	TripCast Data
	Function Name	search_nonstop_flights
	Tool Call	{”destination”: ”AYT”, ”origin”: ”IST”, ”return_date”: ”2026-07-02”, ”depart_date”: ”2026-06-25”}
	Observation	{”request”: {”origin”: ”IST”, ”destination”: ”AYT”, ”depart_date”: ”2026-06-25”, ”return_date”: ”2026-07-02”, ”non_stop_only”: true}, ”currency”: ”EUR”, ”results”: [... {”airline”: ”Pegasus Airlines”, ”flight_outbound”: { ”flight_number”: ”PC452”, ”departure_airport”: ”IST”, ”arrival_airport”: ”AYT”, ”departure_datetime”: ”2026-06-25T12:30”, ”arrival_datetime”: ”2026-06-25T13:55”, ”duration”: ”1h25”}, ”flight_return”: ...
	Response	1) Pegasus Airlines — €149\n - Outbound: PC452 IST → AYT, 2026-06-25 12:30 → 13:55 (1h25)\n - Return: PC453 AYT → IST, 2026-07-02 09:45 → 11:10 (1h25)\n - Fare class: Economy (Light)\n - Baggage: Cabin bag only (checked bags extra)\n - Refundable: No\n - Seats left: 3\n\n2) Turkish Airlines — €185\n ...

Table 10. **Examples of Generated Queries, Tool Names, Function Names, Tool Calls, Observations, and Responses.**

[EVALUATION CRITERIA]
[tool_calling] - Success if ALL of:
- All keys exactly match parameter names from the provided definitions
- Values are correctly extracted or inferred from the user query
- No extra keys beyond the defined parameters
Fail if: wrong/extra keys, values unrelated to the query, or values are null/empty when the query implies a value.
Exception: empty dict {} is Success if the function has no parameters.

[observation] - Success if ALL of:
- Structured as a realistic API response for the given function
- Content is relevant to both the query and the function's purpose
- Contains reasonable data (no inconsistent values)
- Exact alignment with real-world information is not required (e.g., timezone information or stock price).
Fail if: empty, irrelevant to the query, or completely unrealistic.

[response] - Success if ALL of:
- Directly answers the user's query
- Based solely on information present in the observation
- No hallucinated information beyond what the observation contains
Fail if: ignores observation content, contradicts observation, or adds information not in observation.

Table 11. **Evaluation Criteria for Human Evaluation.**

Category	Data Type	Error Type	Error Examples
E-commerce	Observation	Data Inconsistency	**Query:** "I want to browse premium deals first." **Results:** "{'sorted_by': 'deal_price_desc', ..., 'deals': [{'id': 'D1003', 'title': 'Sony WH-1000XM5 Headphones', 'original_price': 249.99, 'deal_price': 299.99, ..."
E-commerce	Response	Over Specification	**Query:** "Find shops that specialize in yoga and fitness accessories like resistance bands and foam rollers." **Results:** "Here are nearby shops that specialize in yoga and fitness accessories (resistance bands, foam rollers):\n\n1) ZenFit Supplies ..."
Finance	Observation	Factual Mismatches	**Query:** "What's the current exchange rate for BTC/USD?" **Results:** "{'meta': { 'symbol': 'BTC/USD', ..., 'provider': 'COINBASE', 'exchange': 'COINBASE'}, 'rate': '67245.12', ..., 'datetime': '2026-03-29T00:00:00Z', ..."
Movies	Observation	Factual Mismatches	**Query:** "Search for anime results related to Demon Slayer." **Results:** "{'season_name': 'spring', ..., 'title': 'Demon Slayer: Kimetsu no Yaiba', 'type': 'TV', 'episodes': 26, 'aired': {'from': '2019-04-06', 'to': '2019-09-28'}, ..."
Music	Observation	Invalid URL	**Query:** "Find the song Water by Tyla." **Results:** "{'query': 'Water Tyla', 'results': [{ 'id': 'st_trk_987654', 'title': 'Water', 'artist': 'Tyla', ..., 'urls': {'spotify': 'https://open.spotify.com/track/4Example', ..."
Travel	Observation	Data Inconsistency	**Query:** "Show all records for QR701 from May 1, 2026 to May 3, 2026." **Results:** "{'flight': 'QR701', ..., 'actual_departure': '2026-05-01T08:45:00+03:00', ..., 'actual_arrival': '2026-05-01T15:10:00-04:00', ..., 'flight_duration': '13:20', ..."

Table 12. **Error Examples in Generated Tool Calling Observations and Responses.** Although GPT-5 occasionally produces errors such as data inconsistencies, over-specification, factual mismatches, and invalid URLs, it still generates realistic data that does not significantly affect our analysis. Red-colored text indicates the parts where errors occur.

Category	Data Type
E-commerce	**Turn 1:** "I need to search for products or deals. {tool_name1} is an online shopping and product search platform, so I'll use it." **Turn 2:** "I need to search for products or deals. I should select an API that is an online shopping and product search platform."
Finance	**Turn 1:** "I need to retrieve the financial data for this query. {tool_name1} is a financial data and market information provider, so I'll use it." **Turn 2:** "I need to retrieve the financial data for this query. I should select an API that provides financial data and market information."
Movies	**Turn 1:** "I need to look up movie or entertainment content. {tool_name1} is a movie and entertainment content provider, so I'll use it." **Turn 2:** "I need to look up movie or entertainment content. I should select an API that handles movie and entertainment content."
Music	**Turn 1:** "I need to search for music or artist information. {tool_name1} is a music data and streaming information provider, so I'll use it." **Turn 2:** "I need to search for music or artist information. I should select an API that provides music data and streaming information."
Travel	**Turn 1:** "I need to find flight or travel information. {tool_name1} is a flight and travel data provider, so I'll use it." **Turn 2:** "I need to find flight or travel information. I should select an API that provides flight and travel data."

Table 13. **Reasoning Texts Used for Each Category.**

[System Prompt]
You are a helpful tool-usage agent that can use multiple tools (functions) to solve a given task.
You will be given a task description. Your goal is to complete the task step by step.
At each step, you need to give your reasoning to analyze the status now and what to do next, with a function call to actually execute your step.
After the call, you will get the call result.
Task description: You should use API functions to help handle the real time user queries.

Your output should follow this format:
Reasoning: ¡your reasoning¿
Action: {"api_name": ¡api name¿, "function_name": ¡function name¿}
Action Input: ¡input parameters as JSON¿

[User Prompt]
{query1}

[Assistant Response]
I have access of the following tools:
{tool_descriptions1}

I MUST select one tool from the list above and fill in api_name, function_name, and all required parameters with values appropriate to the user query. Specifically, I have access to the following APIs: {tool_list1}
Reasoning: {reasoning1}
Action: {tool_name1}
Action Input: {tool_arguments1}
Observation: {tool_observation1}
Response: {agent_response1}

[User Prompt]
{query2}

[Assistant Response]
I have access of the following tools:
{tool_descriptions2}

I MUST select one tool from the list above and fill in api_name, function_name, and all required parameters with values appropriate to the user query. Specifically, I have access to the following APIs: {tool_list2}
Reasoning: {reasoning2}
Action:

Table 14. **Prompt template for experiments.** We construct the prompt following a ReAct-style interaction format (Yao et al., 2022), where the agent iteratively performs reasoning and tool use. The system prompt defines the agent as a tool-usage assistant and enforces a structured output consisting of reasoning, action (API and function name), and input arguments.

Model	Method	E-commerce		Finance		Music		Movies		Travel	
		ANCHOR	VALID	ANCHOR	VALID	ANCHOR	VALID	ANCHOR	VALID	ANCHOR	VALID
Qwen3-4B	DEFAULT	0.89	1.0	0.73	1.0	0.78	1.0	0.61	1.0	0.61	1.0
	PERSONA	0.88 (-0.01)	1.0	0.72 (-0.01)	1.0	0.76 (-0.02)	1.0	0.59 (-0.02)	1.0	0.61 (+0.00)	1.0
	INSTRUCT	0.88 (-0.01)	1.0	0.72 (-0.01)	1.0	0.77 (-0.01)	1.0	0.57 (-0.04)	1.0	0.63 (+0.02)	1.0
	DIRECT	0.83 (-0.06)	1.0	0.69 (-0.04)	1.0	0.69 (-0.09)	1.0	**0.46** (-0.15)	1.0	0.50 (-0.11)	1.0
	TBFAIR	**0.11** (-0.78)	1.0	**0.56** (-0.17)	1.0	**0.62** (-0.16)	1.0	0.56 (-0.05)	1.0	**0.34** (-0.27)	1.0
Qwen3-30B	DEFAULT	0.76	1.0	0.59	1.0	0.72	1.0	0.54	1.0	0.57	1.0
	PERSONA	0.77 (+0.01)	1.0	0.60 (+0.01)	1.0	0.72 (+0.00)	1.0	0.53 (-0.01)	1.0	0.55 (-0.01)	1.0
	INSTRUCT	0.75 (-0.01)	1.0	0.61 (+0.02)	1.0	0.72 (+0.00)	1.0	0.53 (-0.01)	1.0	0.55 (-0.02)	1.0
	DIRECT	0.63 (-0.13)	1.0	**0.21** (-0.38)	1.0	0.53 (-0.19)	1.0	0.31 (-0.21)	1.0	0.31 (-0.26)	1.0
	TBFAIR	**0.07** (-0.69)	1.0	0.11 (-0.48)	1.0	**0.27** (-0.45)	1.0	**0.13** (-0.41)	1.0	**0.27** (-0.30)	1.0
Gemma3-27B	DEFAULT	0.78	1.0	0.86	1.0	0.84	1.0	0.63	1.0	0.73	1.0
	PERSONA	0.80 (+0.02)	1.0	0.87 (+0.01)	1.0	0.83 (-0.01)	1.0	0.63 (+0.00)	1.0	0.74 (+0.01)	1.0
	INSTRUCT	0.77 (-0.01)	1.0	0.87 (+0.01)	1.0	0.83 (-0.01)	1.0	0.63 (+0.00)	1.0	0.73 (+0.00)	1.0
	DIRECT	0.59 (-0.19)	1.0	0.71 (-0.15)	1.0	0.73 (-0.11)	1.0	0.52 (-0.11)	1.0	0.69 (-0.04)	1.0
	TBFAIR	**0.19** (-0.59)	1.0	**0.24** (-0.62)	1.0	**0.21** (-0.63)	1.0	**0.21** (-0.42)	1.0	**0.26** (-0.47)	1.0

Table 15. **Tool Selection Bias Mitigation Results for the SAME dataset.** Values in parentheses indicate the change in bias relative to the default score, where negative and positive values denote decreases and increases, respectively.

Model	Method	E-commerce		Finance		Music		Movies		Travel	
		ANCHOR	VALID	ANCHOR	VALID	ANCHOR	VALID	ANCHOR	VALID	ANCHOR	VALID
Qwen3-4B	DEFAULT	0.91	1.0	0.62	1.0	0.72	1.0	0.58	1.0	0.46	1.0
	PERSONA	0.91 (+0.00)	1.0	0.62 (+0.00)	1.0	0.73 (+0.01)	1.0	0.59 (+0.01)	1.0	0.46 (+0.00)	1.0
	INSTRUCT	0.91 (+0.00)	1.0	0.61 (-0.01)	1.0	0.72 (+0.00)	1.0	0.57 (-0.01)	1.0	0.45 (-0.01)	1.0
	DIRECT	0.86 (-0.05)	1.0	0.57 (-0.05)	1.0	0.71 (-0.01)	1.0	0.52 (-0.06)	1.0	0.41 (-0.05)	1.0
	TBFAIR	**0.26** (-0.65)	1.0	**0.29** (-0.33)	0.99	**0.49** (-0.23)	1.0	**0.44** (-0.14)	1.0	**0.30** (-0.16)	1.0
Qwen3-30B	DEFAULT	0.89	1.0	0.57	1.0	0.65	1.0	0.54	1.0	0.54	1.0
	PERSONA	0.87 (-0.02)	1.0	0.58 (+0.01)	1.0	0.65 (+0.00)	1.0	0.52 (-0.02)	1.0	0.54 (+0.00)	1.0
	INSTRUCT	0.85 (-0.04)	1.0	0.59 (+0.02)	1.0	0.62 (-0.03)	1.0	0.54 (+0.00)	1.0	0.53 (-0.01)	1.0
	DIRECT	0.86 (-0.03)	1.0	0.57 (+0.00)	1.0	0.71 (-0.06)	1.0	0.52 (-0.02)	1.0	0.41 (-0.13)	1.0
	TBFAIR	**0.26** (-0.63)	1.0	**0.20** (-0.37)	1.0	**0.22** (-0.43)	1.0	**0.26** (-0.28)	1.0	**0.35** (-0.19)	1.0
Gemma3-27B	DEFAULT	0.98	1.0	0.78	1.0	0.85	1.0	0.83	1.0	0.77	1.0
	PERSONA	0.98 (+0.00)	1.0	0.79 (+0.01)	1.0	0.86 (+0.01)	1.0	0.83 (+0.00)	1.0	0.78 (+0.01)	1.0
	INSTRUCT	0.98 (+0.00)	1.0	0.79 (+0.01)	1.0	0.87 (+0.02)	1.0	0.83 (+0.00)	1.0	0.76 (-0.01)	1.0
	DIRECT	0.97 (-0.01)	1.0	0.73 (-0.05)	1.0	0.83 (-0.02)	1.0	0.78 (-0.05)	1.0	0.73 (-0.04)	1.0
	TBFAIR	**0.25** (-0.73)	1.0	**0.37** (-0.41)	1.0	**0.26** (-0.59)	1.0	**0.20** (-0.63)	1.0	**0.31** (-0.46)	1.0

Table 16. **Tool Selection Bias Mitigation Results for the DIFF dataset.** Values in parentheses indicate the change in bias relative to the default score, where negative and positive values denote decreases and increases, respectively.

Model	Method	E-commerce		Finance		Music		Movies		Travel	
		ANCHOR	VALID	ANCHOR	VALID	ANCHOR	VALID	ANCHOR	VALID	ANCHOR	VALID
Qwen3-4B	DEFAULT	0.89	1.0	0.73	1.0	0.78	1.0	0.61	1.0	0.61	1.0
	TBFAIR(Ecommerce)	0.11 (-0.78)	1.0	0.12 (-0.61)	1.0	0.22 (-0.56)	1.0	0.20 (-0.41)	1.0	0.29 (-0.32)	1.0
	TBFAIR(Travel)	0.72 (-0.17)	1.0	0.35 (-0.38)	0.99	0.61 (-0.17)	0.99	0.39 (-0.22)	0.99	0.34 (-0.27)	1.0
Qwen3-30B	DEFAULT	0.76	1.0	0.59	1.0	0.72	1.0	0.54	1.0	0.57	1.0
	TBFAIR(Ecommerce)	0.07 (-0.69)	1.0	0.25 (-0.34)	1.0	0.24 (-0.48)	1.0	0.13 (-0.41)	1.0	0.10 (-0.47)	1.0
	TBFAIR(Travel)	0.33 (-0.43)	1.0	0.27 (-0.32)	1.0	0.29 (-0.43)	1.0	0.15 (-0.39)	1.0	0.27 (-0.30)	1.0
Gemma3-27B	DEFAULT	0.78	1.0	0.86	1.0	0.84	1.0	0.63	1.0	0.73	1.0
	TBFAIR(Ecommerce)	0.19 (-0.59)	1.0	0.20 (-0.66)	1.0	0.35 (-0.49)	1.0	0.21 (-0.42)	1.0	0.21 (-0.52)	1.0
	TBFAIR(Travel)	0.31 (-0.47)	1.0	0.16 (-0.70)	1.0	0.33 (-0.51)	1.0	0.21 (-0.42)	1.0	0.26 (-0.47)	1.0

Table 17. **Tool Selection Bias Transfer Experiments for the SAME dataset.**

Model	Method	E-commerce		Finance		Music		Movies		Travel	
		ANCHOR	VALID	ANCHOR	VALID	ANCHOR	VALID	ANCHOR	VALID	ANCHOR	VALID
Qwen3-4B	DEFAULT	0.91	1.0	0.62	1.0	0.72	1.0	0.58	1.0	0.46	1.0
	TBFAIR(Ecommerce)	0.26 (-0.65)	1.0	0.28 (-0.34)	0.99	0.24 (-0.48)	1.0	0.22 (-0.36)	1.0	0.37 (-0.09)	1.0
	TBFAIR(Travel)	0.89 (-0.02)	1.0	0.32 (-0.30)	1.0	0.49 (-0.23)	1.0	0.56 (-0.02)	1.0	0.30 (-0.16)	1.0
Qwen3-30B	DEFAULT	0.89	1.0	0.57	1.0	0.65	1.0	0.54	1.0	0.54	1.0
	TBFAIR(Ecommerce)	0.26 (-0.63)	1.0	0.34 (-0.23)	1.0	0.29 (-0.36)	1.0	0.26 (-0.28)	1.0	0.21 (-0.33)	1.0
	TBFAIR(Travel)	0.49 (-0.40)	1.0	0.30 (-0.27)	1.0	0.21 (-0.44)	1.0	0.21 (-0.33)	1.0	0.35 (-0.19)	1.0
Gemma3-27B	DEFAULT	0.98	1.0	0.78	1.0	0.85	1.0	0.83	1.0	0.77	1.0
	TBFAIR(Ecommerce)	0.25 (-0.73)	1.0	0.27 (-0.51)	1.0	0.44 (-0.41)	1.0	0.28 (-0.55)	1.0	0.31 (-0.46)	1.0
	TBFAIR(Travel)	0.49 (-0.49)	1.0	0.37 (-0.41)	1.0	0.49 (-0.36)	1.0	0.38 (-0.45)	1.0	0.31 (-0.46)	1.0

Table 18. **Tool Selection Bias Transfer Experiments for the DIFF dataset.**

Model	Method	E-commerce	Finance	Music	Movies	Travel
Qwen3-4B	**TBFAIR(E-commerce)**	0.79%	0.80%	0.19%	0.06%	0.02%
	TBFAIR(Travel)	1.51%	1.52%	1.54%	0.86%	0.71%
Qwen3-30B	**TBFAIR(E-commerce)**	0.48%	0.14%	0.29%	0.19%	0.31%
	TBFAIR(Travel)	0.92%	1.68%	1.85%	1.85%	0.78%
Gemma3-27B	**TBFAIR(E-commerce)**	0.38%	0.23%	0.23%	0.22%	0.23%
	TBFAIR(Travel)	0.46%	0.46%	0.24%	0.46%	0.23%

Table 19. **The Proportion of Neurons Removed for Table 3.**