**Socratic Method Evaluation Form**

In this paper, we apply the Mixed Socratic Prompting Approach to a range of problems in chemistry and materials science, developing a structured methodology to enhance LLM reasoning through Socratic inquiry. This framework is designed to evaluate the performance of the Socratic Prompting Approach by comparing it with regular LLM reasoning. It is structured to help you track and assess LLM performance across different approaches. Please complete the provided sections accordingly.

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Field: Molecular Simulations

Are you the expert on the field of question? Yes No

Does this prompt directly relate with your active research area? Yes No

1. Go to **ARGO** and select **Custom Task Type.**
2. **Write your prompt in a conventional, direct-answer manner.**

Prompt:

What are the free energy barriers governing water permeation into an oil phase?

Add follow up prompts below:

Follow-up 1:

How can simulation techniques quantify the contributions of interfacial tension, hydrogen bonding, and dispersion forces for water permeation into an oil phase?

Follow-up 2:

Click or tap here to enter text.

Follow-up 3:

Click or tap here to enter text.

Do you have more follow-up prompts? Yes No

What is the exported file name? conventional\_water\_oil\_set\_2\_more\_technical\_Abhishek\_Aggarwal.txt

1. **Evaluate the performance of conventional approach.**

|  |  |
| --- | --- |
| Clarity | 3 |
| Depth of reasoning | 3 |
| Hypothesis refinement | 2 |
| Novelty of insights | 2 |
| Consistency | 3 |
| Applicability to real problems | 2 |
| Logical Coherence | 3 |
| Correctness of conclusions | 3 |
| Self-correction & iteration | 3 |
| Overall effectiveness | 2 |

1. **Enter observations and comments about conventional approach.**

The conventional approach gives more general responses, focusing on methodology rather than the exact answer to the question.

1. Start a new chat on ARGO, and switch to Socratic prompting. Develop a reasoning flow for your problem. Refer the page 17*,* ***Socratic Questioning & Chain-of-Thought Prompting*** section in the paper. Use **Figure 2 & Tables 3 & 4** to select Socratic principles.
2. Did you used same prompt at the beginning? Yes No
3. Did you use same follow up prompts? Yes No

If your answer is no, please fill the boxes below.

Follow-up 1:

How can we define the free energy barrier for water permeation into an oil phase in terms of molecular interactions and thermodynamics?

Follow-up 2:

If interfacial tension were the sole determinant of water entry into oil, what experimental or computational evidence might challenge this assumption?

Follow-up 3:

How does the free energy barrier for water permeation compare to ion transport across a lipid bilayer, and what key molecular similarities and differences inform this comparison?

Do you have more follow-up prompts? Yes No

What is the exported file name? socratic\_water\_oil\_set\_2\_more\_technical\_Abhishek\_Aggarwal.txt

1. **Evaluate the performance of Socratic Prompting approach.**

|  |  |
| --- | --- |
| Clarity | 4 |
| Depth of reasoning | 3 |
| Hypothesis refinement | 4 |
| Novelty of insights | 3 |
| Consistency | 3 |
| Applicability to real problems | 3 |
| Logical Coherence | 3 |
| Correctness of conclusions | 4 |
| Self-correction & iteration | 2 |
| Overall effectiveness | 3 |

1. **Enter observations and comments about Socratic Prompting approach.**

I found Socratic prompting approach to be better than direct approach in terms of accuracy, and depth. However, the novelty of answers was not affected in my opinion.

1. **Analysis of results from an expert point of view.**

Both approaches gave accurate answers. The water permeation into oils depends on temperature, pressure, oil composition and so on, which were listed in both approaches. However, the direct approach did not provide a comprehensive guidance on further simulations to set up, as the Socratic method did. The simulations suggested by Socratic approach were based on more scientific approach.

1. **Evaluate the performance of Socratic and non-Socratic responses. Which one provides accurate and reliable responses? Why?**

The Socratic prompting approach should be used in order to get accurate answers. The Socratic approach gave better insights on designing molecular dynamics simulations compared to the general approach. The emphasis was more on scientific quantities like entropy, thermodynamic entities, etc. in socratic approach.

1. **What are the limitations and possible improvements?**

Limitations: Lack of novelty is the main limitation. A possible improvement might be to feed novel ideas to the prompt to generate further novel ideas.