SUPPORTING INFORMATION FOR AGENT-BASED LEARNING OF MATERIALS DATASETS FROM SCIENTIFIC LITERATURE

Mehrad Ansari[1,2] and Seyed Mohamad Moosavi*[1,2]

[1]Acceleration Consortium, University of Toronto, Toronto, Ontario M5S 3E5, Canada
[2] Department of Chemical Engineering & Applied Chemistry, University of Toronto, Toronto, Ontario M5S 3E5, Canada
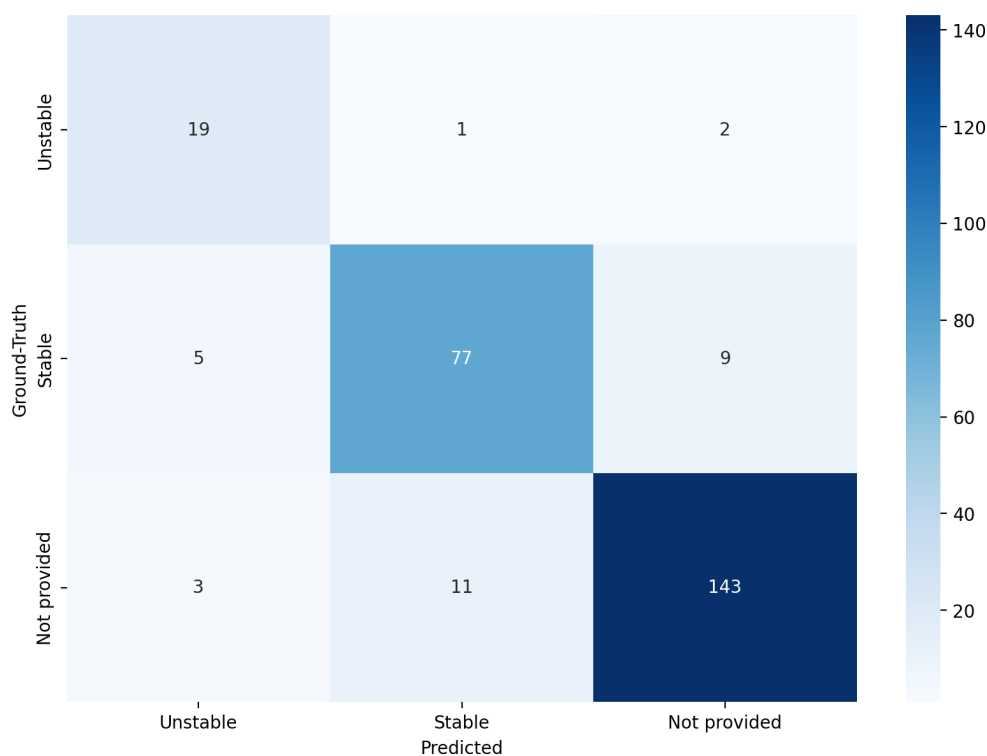
1 Supporting Figures

Figure S1: Confusion matrix for ternary classification of water stability property in Case Study 3 using Cohere embed-english-v3.0 embeddings. It is apparent that our agent exercises cautious in its judgments. Specifically, the abundance of "Not provided" predictions, when matched against their actual ground-truth categories, suggests that the agent prefers to concede some uncertainty in instances where making an accurate prediction is not feasible, rather than incorrectly assigning samples to the "Stable" or "Unstable" categories. The ternary accuracy is found to be 0.88 with a yield of 72.96%, which is lower than performance coming from OpenAI's text-ada-002 embeddings (see Figure 4b in the main article).

*Corresponding author: mohamad.moosavi@utoronto.ca

2 Supporting Tables

Table S1: Performance comparison between LLM-NERRE, Eunomia, and Eunomia + CoV on hosts and dopants relation extraction (Case Study 1). Eunomia embeddings are generated using Cohere embed-english-v3.0.

Model	Entity	Precision (Exact Match)	Recall (Exact Match)	F1 Score (Exact Match)
LLM-NERRE	hosts	0.892	0.874	0.883
Eunomia	hosts	0.710	0.747	0.728
Eunomia + CoV	hosts	0.793	0.726	0.758
LLM-NERRE	dopants	0.831	0.812	0.821
Eunomia	dopants	0.782	0.800	0.791
Eunomia + CoV	dopants	0.863	0.812	0.836

Table S2: Performance comparison between LLM-NERRE and Eunomia on MOF formula and guest species relation extraction (Case study 2). Eunomia embeddings are generated using Cohere embed-english-v3.0.

Model	Entity	Precision (Exact Match)	Recall (Exact Match)	F1 Score (Exact Match)
LLM-NERRE	mof formula	0.409	0.455	0.424
Eunomia	mof formula	**0.615**	**0.571**	**0.593**
LLM-NERRE	guest species	**0.588**	0.665	**0.606**
Eunomia	guest species	0.213	**0.769**	0.333

3 Details on Used Prompts

The following prompt is used in case study 3:

```
You are an expert chemist. The document describes the water stability properties of a few materials
including materials, crystal structures
Metal-Organic Frameworks(MOF) or coordination polymers, coordination networks or ZIF compounds.
Find the exact full name or chemical formula for
materials (crystal structures), and their stability in water.
As an example, sentence "UiO-66-X compounds with X = NO2,
NH2, OH, CH3 and (CH3)2 show enhanced CO2 uptake", contains the five following MOFS:
[UiO-66-NO2, UiO-66-NH2, UiO-66-OH, UiO-66-CH3, UiO-66-(CH3)2], but does not provide any
information their water stability.
Use this example to guide yourself better on finding
other MOFs in the document.

There are only 3 options for water stability:
1. Stable: No change in properties after exposure to moisture or steam, soaking or boiling in
water or an aqueous solution.
Retaining its porous structure in solution.
No loss of crystallinity.
insoluble in water or an aqueous solution.
Water adsorption isotherm should have a steep uptake.
Good cycling performance.

2. Unstable
The MOF will decompose or change properties or has a change in its crystal structure after
exposure/soak to a humid environment, steam or if it partially dissolves in water.
Soluble or partially soluble in water or an aqueous solution.

3. Not provided,
If you don't know or cannot justify 1 or 2

Read paper, find all the mentioned materials
(crystal structures), their full names (or chemical formula) and their
water stability with a reasoning of your answers.
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Evaluate each reasoning. Find the paper DOI. Do not make up answers.
If the reasoning is not valid, recheck for a better reasoning and then evaluate it,
if the rechecked reasoning is still not valid change "Predicted Stability" and
"reasoning" to "Not provided" in your final answer.
If the paper does not talk about water stability, list the full MOF names you find
and set their "water stability" to "Not provided".
If don't know any of the items, just say "Not provided" for that one.

Your final answer should be in a Python parsable JSON format containing the following:
 - The water stability of each MOF.
 - item The exact sentences without any changes from the document that justifies your decision.
   Try to find more than one sentence. Do not summarize. Do not make up a reasoning
   that does not exist in the document. This should be "Not provided" if you cannot
   find water stability.
 - item Paper's DOI.

Each observation should contain information about a single MOF. Do not summarize them altogether
in one item. You MUST report the answer for each MOF individually. Find the paper DOI.

"MOF-15":
    - Predicted Stability: "Stable"
    - reasoning: "Sentence ..."
    - DOI: "DOI"

"MOF-20":
    - Predicted Stability: "Unstable"
    - reasoning: "Sentence ..."
    - DOI: "DOI"

"MOF-25":
    - Predicted Stability: "Not provided"
    - reasoning: "Not provided"
    - DOI: "DOI"

If you do not know the answer, use this output format:

"Not provided":
    - Predicted Stability: "Not provided"
    - reasoning: "Not provided"
    - DOI: "Not provided"

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