

Appendix B: Prompts used

XpertAI Prompt for generating final output

```
XPERTAII_PROMPT = """
feature list: {features}
observation: {observation}

Documents: \n
{documents}

- First, list all features identified by the XAI analysis {fe
atures} affecting
the {observation}.
format:
### Features Identified by XAI Analysis
- feature 1
- feature 2
...

```

You are an expert scientist. Your task is to go through the p
rovided documents
and explain the relationship between the features in {feature
s} and the
{observation}.

XAI analysis is used to identify features that are most
impactful to the {observation}.
Are there other impactful features that are correlated with t
he {observation}?

-Next, your task is to describe the relationship of each feat
ure in the
{features} and other features with the {observation} based on
provided

documents.\n

Do the provided documents explicitly explain how each feature
in the {features}

explicitly affects the {observation}? If yes, provide the explanation.

You must critically evaluate your answers, provide reasons and citations.\n

Each claim must be supported by scientific evidence.

In line citations are required. \n eg: <claim (smith et al., 2020)> \n

Important: If the provided documents do not explicitly state the relationship between the feature and the observation, you must say "an explicit relationship

was not found in the given documents".\n

Instead do the documents discuss about synonymous features that are not

identified by the XAI analysis? \n

You can critically evaluate the relationship between such correlated with the

{observation} and generate a hypothesis based on the information provided in

the documents. \n

Important: Each claim/hypothesis must be supported with citations. \n

Format:

<feature>:

****Explanation**:** <relationship of feature to the observation>

****Scientific Evidence**** <provide scientific evidence/citations from the documents>

****Hypothesis**:** <your hypothesis>

- Then, provide a summary of everything you described previously to describe

the relationship between these features and the {observation}.
You must sound like a scientist. Give scientific evidence for these answers and provide citations.

- Finally, provide the list of references only used to answer.

DO NOT make up references.

Use APA style for referencing. \n

Eg: References: \n

1. reference 1 \n

2. reference 2 \n

...

"""

```
XPERTAI_PROMPT = """  
feature list: {features}  
observation: {observation}
```

```
Documents: \n  
{documents}
```

- First, list all features identified by the XAI analysis {features} affecting the {observation}.

format:

Features Identified by XAI Analysis

- feature 1

- feature 2

...

You are an expert scientist. Your task is to go through the provided documents

and explain the relationship between the features in {features} and the {observation}.

XAI analysis is used to identify features that are most impactful to the {observation}.

Are there other impactful features that are correlated with the {observation}?

-Next, your task is to describe the relationship of each feature in the {features} and other features with the {observation} based on provided documents.\n

Do the provided documents explicitly explain how each feature in the {features} explicitly affects the {observation}? If yes, provide the explanation.

You must critically evaluate your answers, provide reasons and citations.\n

Each claim must be supported by scientific evidence.

In line citations are required. \n eg: <claim (smith et al., 2020)> \n

Important: If the provided documents do not explicitly state the relationship between the feature and the observation, you must say "an explicit relationship was not found in the given documents".\n

Instead do the documents discuss about synonymous features that are not

identified by the XAI analysis? \n

You can critically evaluate the relationship between such correlated with the

{observation} and generate a hypothesis based on the information provided in the documents. \n

Important: Each claim/hypothesis must be supported with citations. \n

Format:

<feature>:

****Explanation****: <relationship of feature to the observation>

****Scientific Evidence**** <provide scientific evidence/citations from the documents>

****Hypothesis****: <your hypothesis>

- Then, provide a summary of everything you described previously to describe

the relationship between these features and the {observation}.

You must sound like a scientist. Give scientific evidence for these answers and provide citations.

- Finally, provide the list of references only used to answer.

DO NOT make up references.

Use APA style for referencing. \n

Eg: References: \n

1. reference 1 \n

2. reference 2 \n

...

"" ""

GPT-4o prompt for baseline comparison

```

GPT_PROMPT = """
You are an expert scientist. Your task is to explain the relationship
the molecular features and the {observation}.

First, list all molecular features you think affect the {observation}.
list them all.
format:
### Features Identified by ChatGPT
- feature 1
- feature 2
...

-Next, your task is to describe the relationship of each feature
{observation} based on your knowledge.\n
You must critically evaluate your answers and provide reasons.\n
You can critically evaluate the relationship between correlated
the {observation} and generate a hypothesis. \n

Format:
#### <feature>:
**Explanation**: <relationship of feature to the observation>
**Hypothesis**: <your hypothesis>

- Then, provide a summary of everything you described previously
the relationship between these features and the {observation}.
You must sound like a scientist.

Finally, you must also provide a list of references to support your
Use APA style for referencing.\n
Eg: References: \n
    1. reference 1 \n
    2. reference 2 \n
    ...

```

||||