Developer Task: Integrating UniProt and Ensembl APIs

Background:

UniProt and Ensembl are public APIs for biological data. This task assesses your ability to integrate APIs, handle both GET and POST requests, and process biological data in Python.

Your Tasks

1. Learn about APIs

Get familiar with the concept of APIs, how to send GET/POST requests, and how to use JSON request bodies:

- Real Python: API Integration in Python: https://realpython.com/api-integration-in-python/
- Real Python: Python Requests Library: https://realpython.com/python-requests/

2. Explore the APIs

- UniProt REST API information: https://www.ebi.ac.uk/proteins/api/doc/#/proteins
- Ensembl REST API: https://rest.ensembl.org/

Step-by-Step Instructions

Use the UniProt API to retrieve information for the following protein accessions:

- P12345, Q8N726, O00255

Step 0:

Setup the project using virtual environment, prepare project structure. One can easily follow all necessary requirements for the project.

You can gain bonus points if you will use Poetry.

Step 1: Get Protein Information

- Write a function 'get_protein_information' to fetch data from the UniProt API for a list of protein accessions.
- Endpoint: https://www.ebi.ac.uk/proteins/api/proteins/{id}
- Extract the following fields for each protein:
- Protein Accession
- Protein Name
- Gene
- Organism (Scientific)
- Organism (Common)
- Molecular Weight

- Return the results as a pandas DataFrame.

Step 2: Get Ensembl Gene IDs

- Write a function `get_ensembl_gene_ids` to fetch Ensembl Gene IDs for the genes retrieved in Step 1.
- Endpoint: https://rest.ensembl.org/xrefs/symbol/{species}/{gene}
- Documentation: https://rest.ensembl.org/
- Replace `{species}` with the organism name (e.g., `homo_sapiens`) from `Organism (Scientific)` and `{gene}` with the gene name.
- Add a new column, `Ensembl Gene ID`, to the DataFrame.

Step 3: Get Gene Details

- Write a function 'get_gene_data' to fetch additional gene details using the Ensembl Gene API.
- Endpoint: https://rest.ensembl.org/lookup/id
- Swagger Documentation: https://rest.ensembl.org/
- Use a list of Ensembl Gene IDs as a request body
- Extract the following details for each Ensembl Gene ID:
- Description
- Seq Region Name
- Return a new pandas DataFrame containing these details.

Step 4: Merge Data

- Combine the data from Steps 1, 2, and 3 into a single DataFrame.

Step 5: Save the Data

- Save the final DataFrame as an Excel file named `protein_gene_analysis.xlsx`.

Additional Requirements

- Logging: Log key steps and errors (e.g., when a request fails).
- Modular Structure: Write reusable, modular functions for each task.
- Error Handling and Exceptions: Ensure the code can handle failed requests gracefully.
- Best Practices:
- Use clear and concise docstrings.
- Follow PEP 8 guidelines for clean, readable code.

Hints

- 1. For species names in `Organism (Scientific)`, ensure the names are lowercase before calling the Ensembl API
- 2. Use the 'merge' function in pandas to combine DataFrames.

Deliverables

- 1. Python script/s containing all functions and implementation.
- 2. The final Excel file `protein_gene_analysis.xlsx`.
- 3. A brief explanation of your approach in comments.
- 4. Upload the script and Excel file to your Github and share the link to the project..