Assessment Overview

- Objective: Assess proficiency in AI skills specific to the chemical domain.
- Duration: 2 weeks from the date of issue.
- Submission: Working code files should be uploaded to your public GitHub repository and share the repository link with anandu.balachandran@accenture.com

Part 1: Coding Skills

1. Graph Neural Networks (GNN)

- Task: Implement a GNN to predict the Heat Capacity (cal/(mol K)) using dataset - QM9 Dataset. (You don't need to use the entire dataset for training the model (take sample data); we are more interested in your approach rather than the model's accuracy.)
- Requirements: Use Python and any preferred GNN library. The model should include detailed comments explaining each step.
- Deliverable: A Jupyter notebook containing the implemented model, your analysis, and a brief discussion on the chosen architecture's effectiveness.

2. RDKit

- Task: Write a script using RDKit to convert a dataset of molecular structures from SMILES to 3D conformations.
- Requirements: Your script should handle errors gracefully and optimize the geometry of the generated conformers.
- Deliverable: A Python script and a short report summarizing the methodologies used.

3. Density Functional Theory (DFT)

- Task: Use Python to perform a basic DFT calculation on a simple molecule (e.g., water) and analyze its electronic structure.
- Requirements: Include explanations for each step and parameter in your code.
- Deliverable: Python script and a document explaining your findings and the implications of the results.

Submission Instructions

- All code must be well-documented and presented in a clean, readable format.

Timeline to submit Part 1 Assessment

- Issued Date: 16th July
- Due Date: 30th July (2 weeks from the issued date).

Shortlist Candidates based on the Part1 Assessment

- Shortlisted candidates will be invited to the Part 2 session two days after the submission deadline.

Part 2: 1-1 Interactions with Shortlisted Candidates

- Prepare a presentation detailing your approach and solutions to the tasks outlined in Part 1.