Coding Project – Topological Indices

The goal of this assignment is to write a python script that computes three topological indices for a given molecular structure:

- Edge Density
- Wiener Index
- PetitJean Index

I have uploaded the original paper of the PetitJean Index on Blackboard for extra resources.

This is a team project of two students per team.

The deadline for this project is **April 14, 2025,** by midnight and it must be respected. A student failing to meet the deadline will get 20% of the grade deducted per day late.

Students must upload on Blackboard an archive containing the python script or a Jupyter Notebook and the test cases used to validate the code (mol or sdf files of a minimum of 5 and a maximum of 20 molecular structures). Ensure that both students' names are mentioned at the top of the script or notebook.

The script should start by asking the user whether to compute one of the three indices or all three, and it should support the following input formats:

- A single `.mol` file containing a molecular structure.
- A folder containing multiple `.mol` files.
- An `.sdf` file containing multiple chemical structures.

The input can be provided interactively or as a command-line argument.

Code Structure:

Define separate functions for each index calculation and use appropriate Python libraries (e.g. `networkx` library for handling graphs). Ensure the code is well-documented with comments and function docstrings.

The output should display the names of the molecules along with the computed values of the selected indices. Adding a graphical user interface (GUI) and implementing a graph visualization using `matplotlib` or `networkx.draw` (**LINK**) are valuable enhancements.

Important Restriction: Students are not allowed to use any library or built-in functions that directly compute these topological indices. They must implement the calculations from scratch using fundamental graph operations.

You will be grades according to the criteria below *(with 2 extra bonus points)*:

Category	Criteria	Points
Correctness (7 pts)	Correctly implements Edge Density, Wiener Index, and PetitJean Index from scratch without using pre-built functions.	**3**
	Handles input formats correctly (.mol, .sdf, folder of .mol files).	**2**
	Produces correct output with molecule names and computed indices.	**2**
Code Structure & Documentation (5 pts)	Use modular, well-structured code with functions for each calculation.	**1.5**
	Includes meaningful comments and docstrings explaining the implementation. Easy to read and understand (commented, variables with useful names)	**1.5**
	The script is user-friendly and allows interactive or command-line input.	**2**
Testing & Validation (2 pts)	Provides at least 5 valid test cases with .mol and .sdf files.	**1**
	Includes clear evidence (in the report or script) that results were validated.	**1**
Visualization & Extras (3 pts)	Implements optional visualization using matplotlib or networkx.draw.	**1**
	Well-designed GUI for user interaction	**1**
	Extends functionality beyond basic requirements (e.g., additional topological indices, enhanced visualization)	**1**