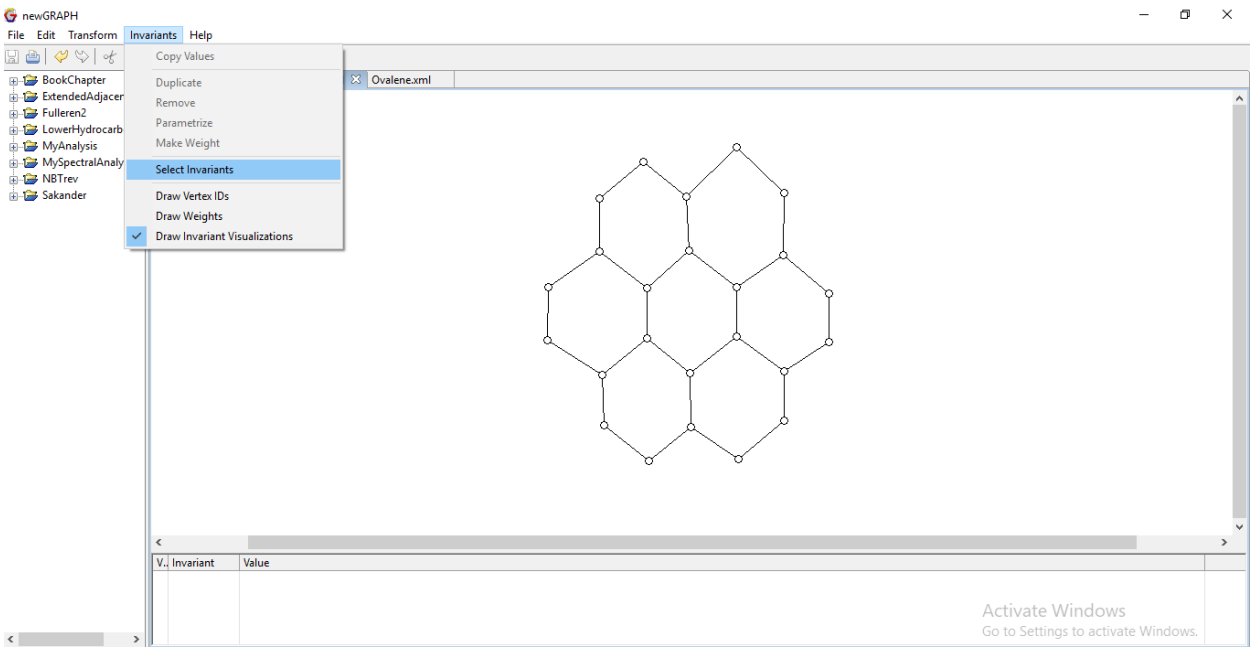
Workflow of our proposed method with a Minimal Working Example (MWE)

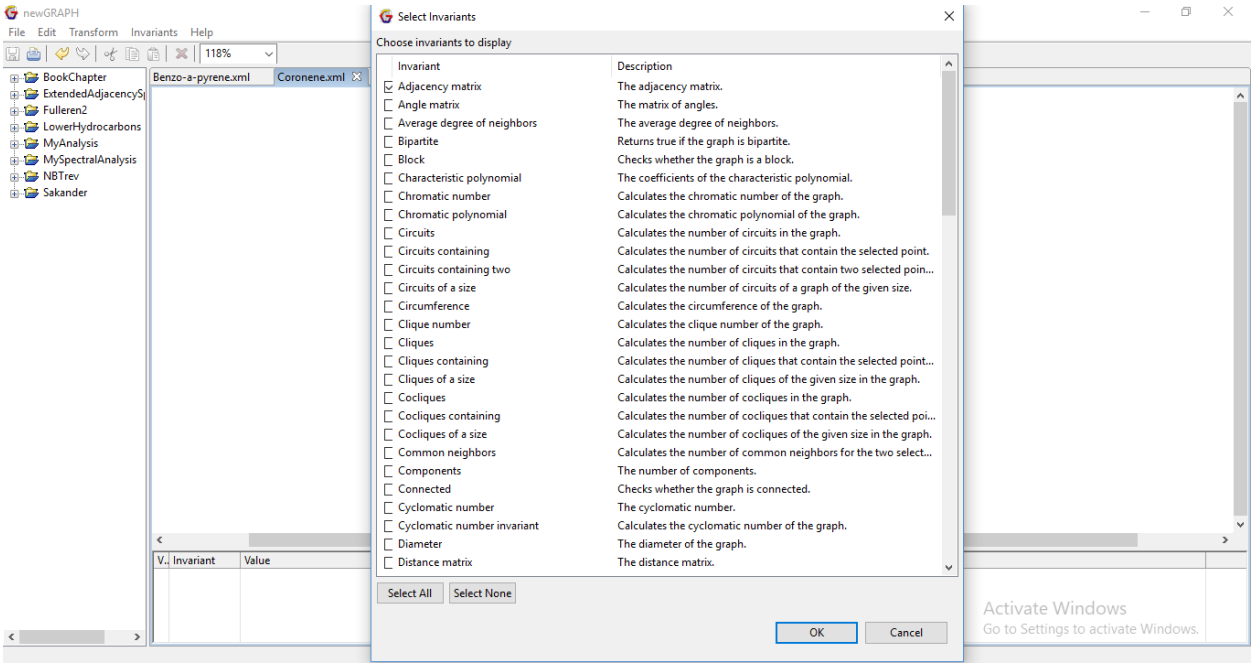
In this document, we will explain the working pattern of our technique to compute certain spectrum-based topological descriptors of graphs.

1. Let *G* be a graph for which you want to compute a spectrum-based topological index from the following list of indices:
   i. Energy
   ii. Estrada index
   iii. Positive inertia index
   iv. Negative inertia index
   v. Nullity
   vi. Signature

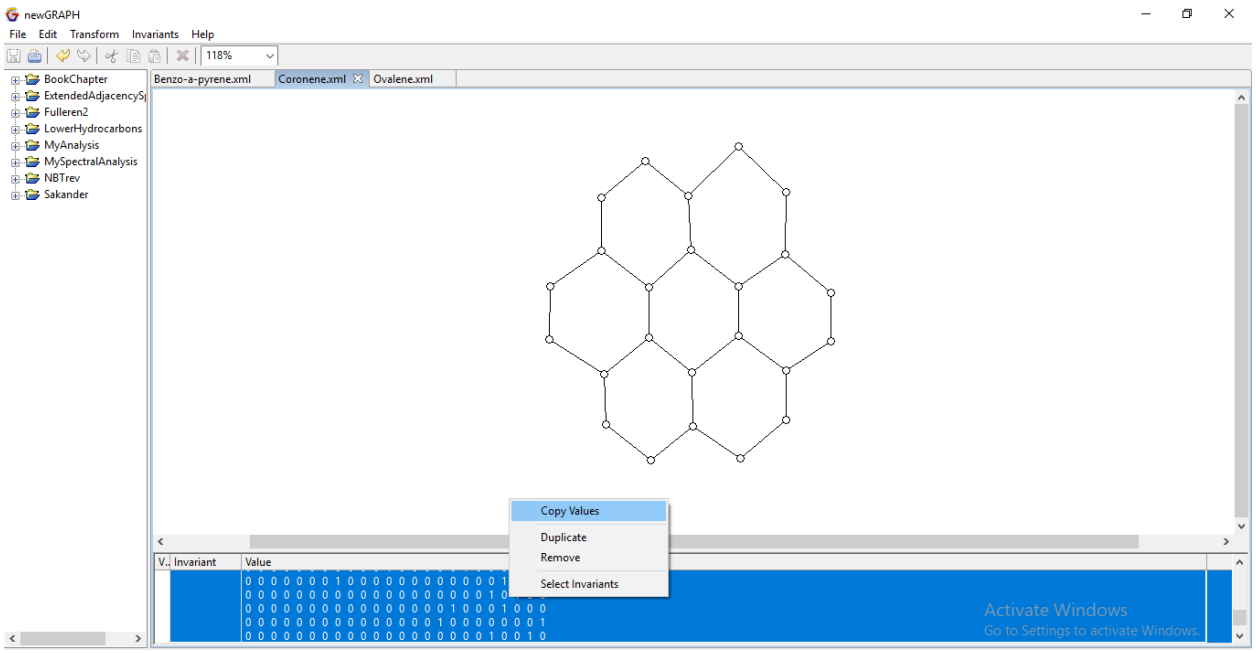
   We would like to set the coronene graph as our MWE.

2. In first step, we draw graph *G* on newGraph and choose “Adjacency matrix” and “Vertices” as “Select Invariants” under the “Invariants” tab as follows:

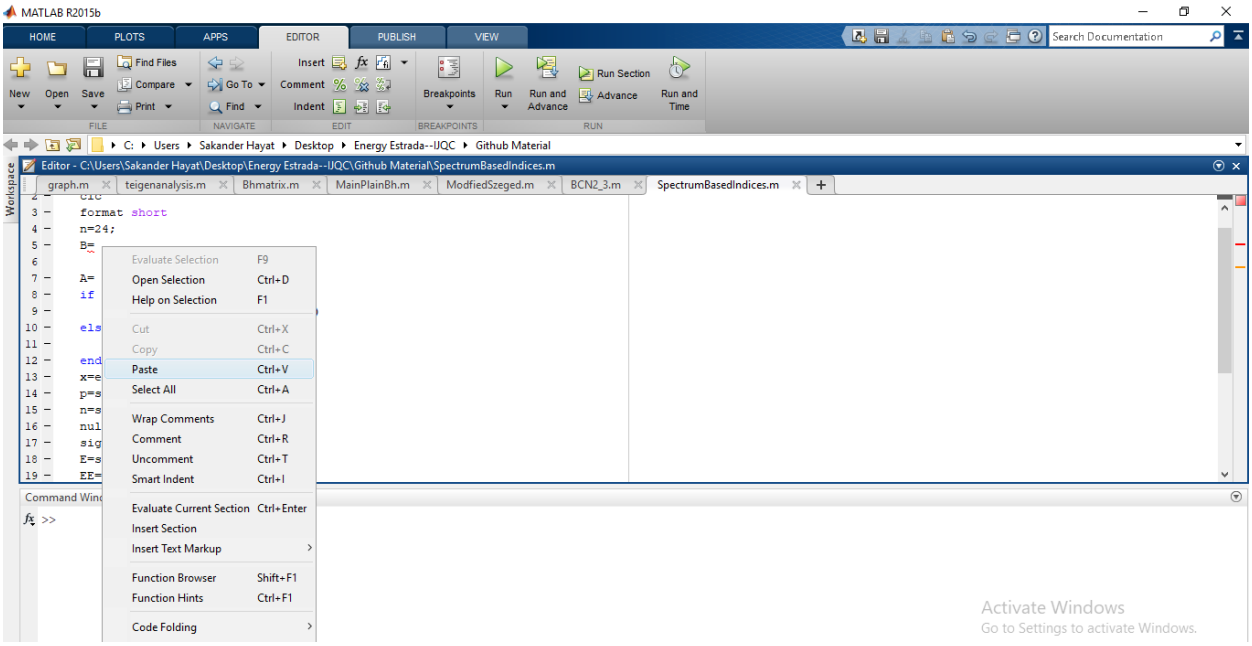




3. By right clicking on the matrix values, select “Copy Values” as follows:



4. Paste the copied matrix values from newGraph to Matlab in SpectrumIndices.m file. Change the value of *n* which 24 in our MWE.



5. Click “run” to obtain the result as follows: