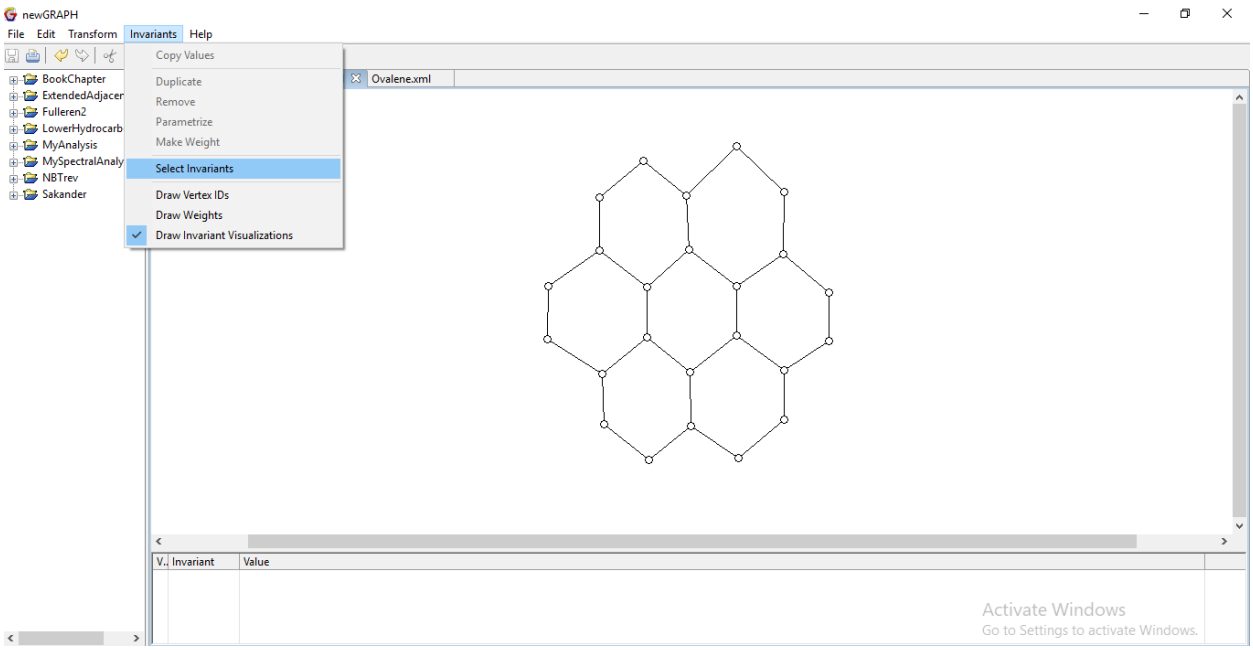
Workflow of our proposed method with a Minimal Working Example (MWE)

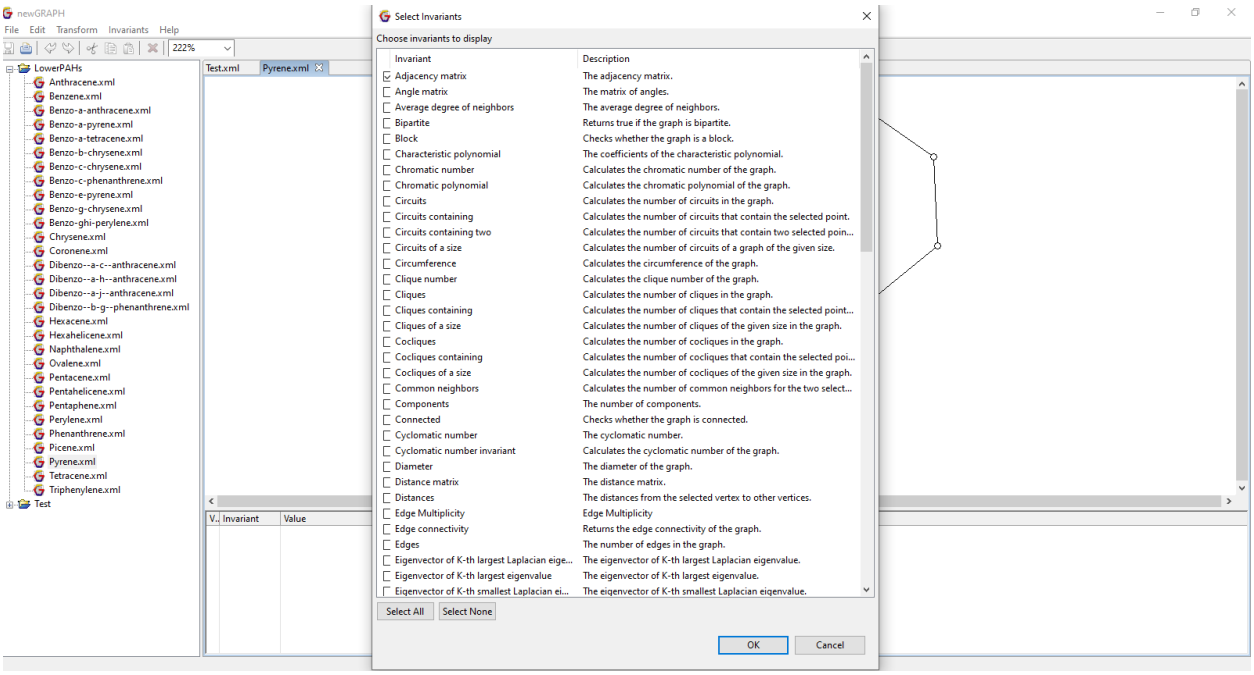
In this document, we will explain the working pattern of our technique to compute certain valency-based descriptors of general graphs.

1. Let *G* be a graph for which you want to compute a distance-based spectral topological index from the following list:
   i. Randic index
   ii. General Randic index
   iii. ABC index
   iv. AZI index
   v. First & second Zagreb indices
   vi. First & second multiplicative Zagreb indices
   vii. GA index
   viii. Sum-connectivity index
   ix. General sum-connectivity index

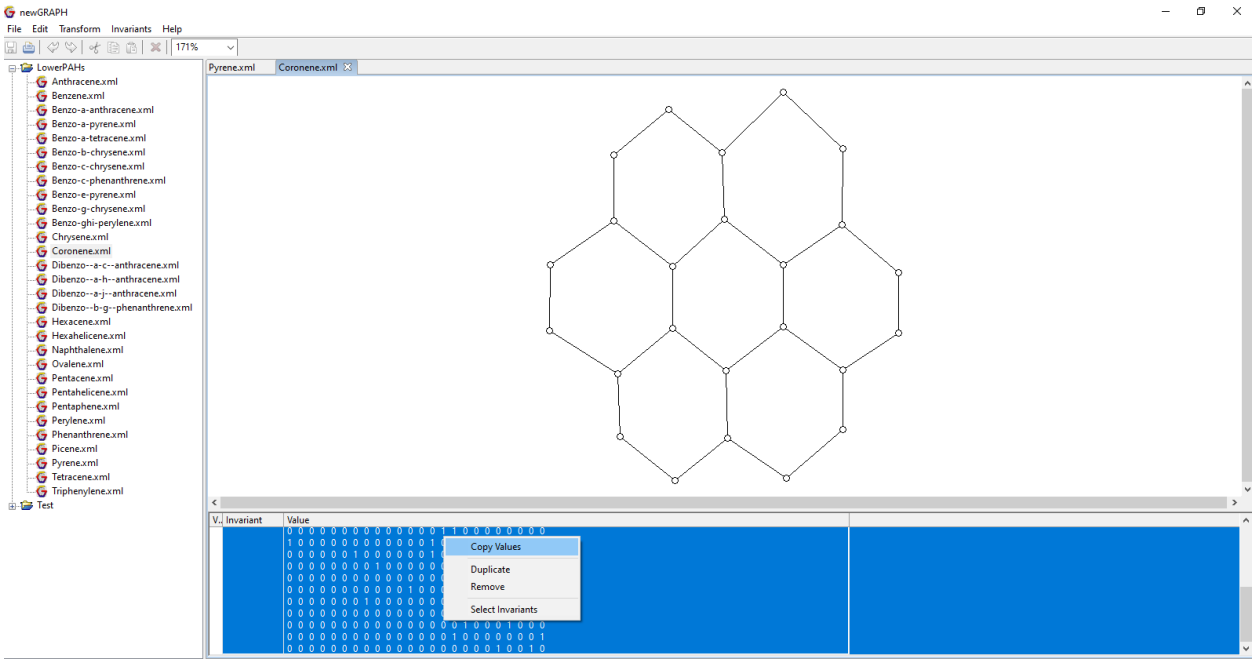
   We would like to set the coronene graph as our MWE.

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:

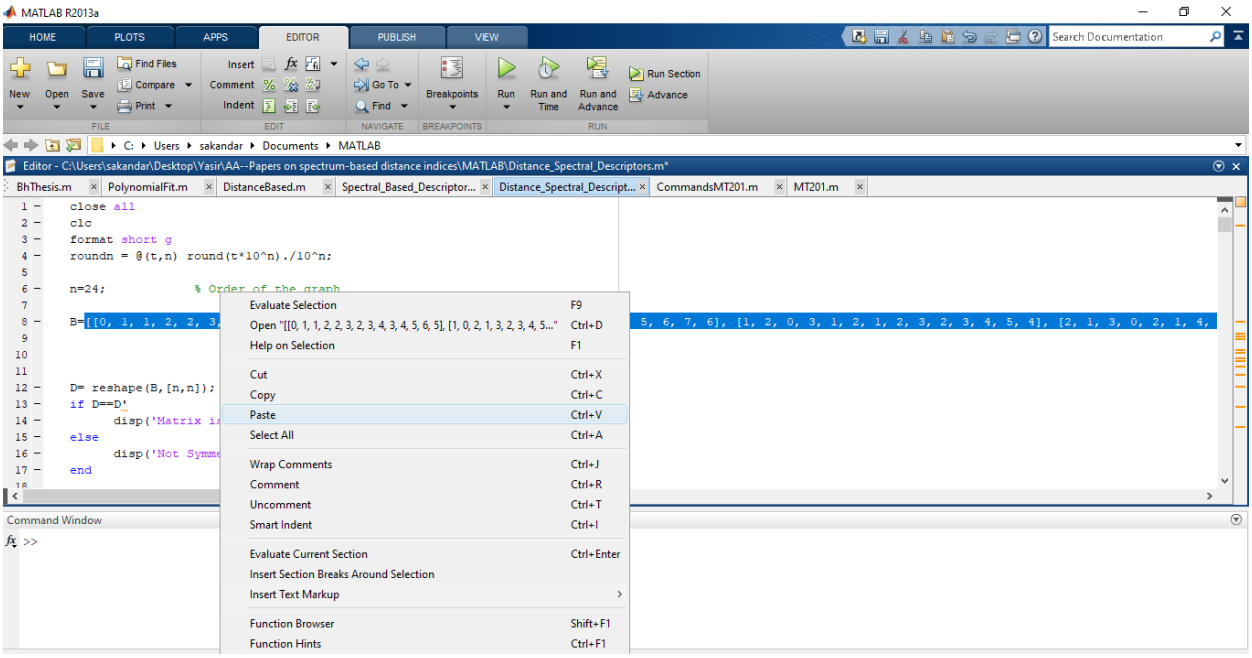




3. By right clicking on the matrix values, select “Copy Values” as follows:



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



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