Exercise 1:

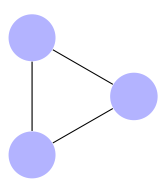
1. Draw the graphs G_A and G_B for which the following 2 adjacency matrices A and B are given.

$$A = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix} B = \begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix}$$

2. Are the two graphs isomorphic?
3. How many different representations (in terms of adjacency matrices) of G_A are there?
4. How many different representations (in terms of adjacency matrices) of G_B are there?
5. Is there a permutation matrix P such that $A = P\,(PB)^T$ holds?
6. If so, give all matrices P, such that $A = P\,(PB)^T$ holds.

Exercise 2:

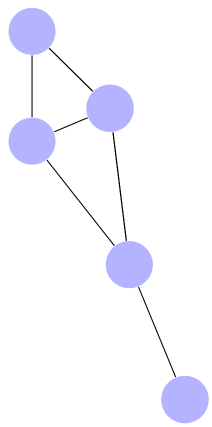
Given the following graph:



1. Give an adjacency matrix A for the graph. (How many different are there?)
2. For your chosen adjacency matrix, how many permutation matrices P are there, such that $A = P\,(PA)^T$ holds? (Remark: this number corresponds to the size of the so-called “automorphism group” of the graph).

Exercise 3:

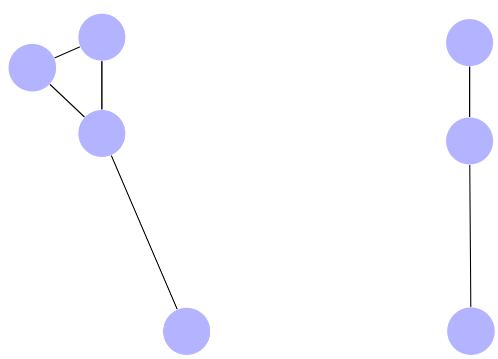
Given the following graph:



1. Give an adjacency matrix A for the graph.
2. For your chosen adjacency matrix, how many permutation matrices P are there, such that $A = P\,(PA)^T$ holds?

Exercise 4*:

Given the following two graphs G_A (left) and G_B (right):



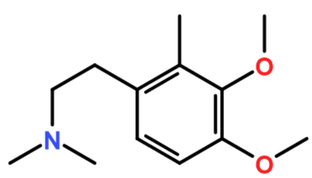
1. Give adjacency matrices for G_A and G_B.
2. Is G_B a subgraph of G_A?
3. How many different ways are there to find G_B as a subgraph in G_A? (i.e., assuming as adjacency matrix A and B for graphs G_A and G_B, how many leaf-nodes would the search the of the Ullmann algorithm have?)

4. How many different ways are there to find G_B as an induced subgraph in G_A?

Exercise 5:
The following is from the unit-testing of the graph theory assignment. Explain the expected result 10.

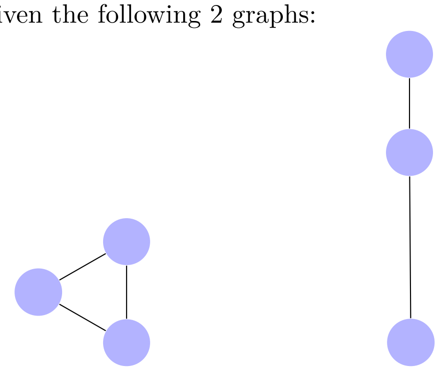
```
>>> A = np.array([[ 0,  1,  0,  0,  1],  \
                  [ 1,  0,  1,  0,  0], \
                  [ 0,  1,  0,  1,  0], \
                  [ 0,  0,  1,  0,  1], \
                  [ 1,  0,  0,  1,  0]])
>>> numIsomorphisms(A, A)
10
```

Exercise 6*:
Use sigma aldrich `https://www.sigmaaldrich.com/catalog/search/substructure/SubstructureSearchPage`to look for chemical structures. How many structures can you find which have the following as a substructure?



Can you find the price for the compounds you found? Any guesses why not?

Exercise 7: (representations and graph isomorphisms)
Given the following 2 graphs:



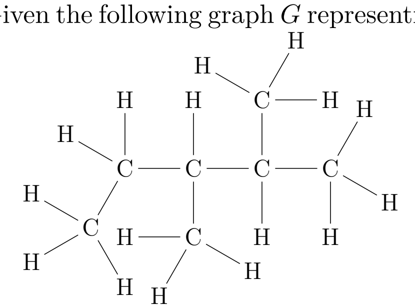
For each of the graphs, in the following called G:

1. How many different representations (adjacency matrices) can you find for graph G? (Let r_G be this number)
2. Chose an adjacency matrix B. How many permutation matrices can you find, such that $B = P(PB)^T$? (Let p_G be this number).

Note: p_G corresponds to the number of isomorphisms from B to itself, which is also called an automorphism. You could chose any pair of representations A and B, and finding the number of different P for which $A = P(PB)^T$ holds, the result will always be p_G.

3. What is the product of the number of representations r_G and the number of isomorphisms p_G?

Exercise 8: (Wiener index and boiling points)
Given the following graph G representing the chemical compound 2,3-dimethylpentan:



1. Determine the edge-weight matrix of the graph of the carbon backbone.
2. Determine the distance matrix.
3. Determine the Wiener-Index.
4. Determine the number of shortest paths of length 3.
5. Determine the value p_0 and w_0 of the formula for predicting the boiling point for this compound.
6. Determine the estimated boiling points and compare it to the real boiling point.
7. What is the asymptotic worst case performance for finding the distance matrix based on repeated squaring?
8. Do you know a method that has a better asymptotic worst case performance?