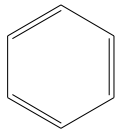
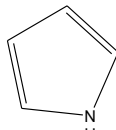
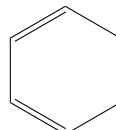


From the previous exercise, take the following table:

Table 1 with fingerprints:

Table 1				-OH	-Cl	-NO <sub>2</sub>	-CH <sub>3</sub>	-COOH
2,4,6-trinitrophenol	1	0	0	1	0	1	0	0
2,3-dinitrophenol	1	0	0	1	0	1	0	0
3-hydroxybenzaldehyd	1	0	0	1	0	0	0	0
2,4,6-trimethylphenol	1	0	0	1	0	0	1	0

a) Count Tanimoto coefficient for pairs:

- 2,4,6-trinitrofenol and 2,3-dinitrofenol:
- 2,4,6-trinitrofenol and 3-hydroxybenzaldehyd:

b) Fill values of Tanimoto coefficient into the table:

Table 2	2,4,6-trinitrophenol	2,3-dinitrophenol	3-hydroxybenzaldehyd	2,4,6-trimethylphenol
2,4,6-trinitrophenol				
2,3-dinitrophenol				
3-hydroxybenzaldehyd				
2,4,6-trimethylphenol				

c) Which pair(s) have the Tanimoto coefficient the lowest and the highest?

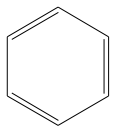
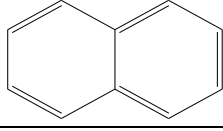
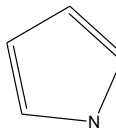
d) Count the Cosine coefficient for the pairs:

- 2,4,6-trimethylphenol and 2,3-dinitrophenol:
- 2,4,6-trimethylphenol and 3-hydroxybenzaldehyd:

e) Count (binary) Euclid distance for pairs:

- 2,4,6-trinitrophenol and 2,3-dinitrophenol:
- 2,4,6-trinitrophenol and 3-hydroxybenzaldehyd:

1. Do consensus fingerprints for fingerprints from Table 1 (use OR):

Table 1	 	 -NO <sub>2</sub>	-OH -COOH	-Cl -CH <sub>3</sub>
2,4,6-trinitrophenol				
2,3-dinitrophenol				
3-hydroxybenzaldehyd				
2,4,6-trimethylphenol				

2. Use the charges on atoms O and H from the previous exercise:

Table with charges:

Table 3	Charge on O (from OH skupiny)	Charge from H (from OH skupiny)
2,4,6-trinitrophenol	-0,5690	0,5670
2,3-dinitrophenol	-0,6110	0,4640
3-hydroxybenzaldehyd	-0,6910	0,4060
2,4,6-trimethylphenol	-0,7140	0,3670

a) Create a descriptor space graph in Excel, specifically: Put a charge on the x-axis at O, a charge on the y-axis at H. Show a graph that shows the X and Y points.

Note: If you are not familiar with Excel, do the following: Copy the above table into Excel. Label the values of the hubs. Put "Insert" and select "Charts" and select the X,Y chart.

b) Count the Euclid distance:

- 2,4,6-trinitrophenol and 2,3-dinitrophenol:
- 2,4,6-trinitrophenol and 3-hydroxybenzaldehyd:

b) Which pair has the biggest Euclid distance?

c) Which pair has the lowest Euclid distance?

d) Which Euclid distance is more informative? Binary or with real numbers?