1D descriptors

1. Fill the Table 1:

Table 1	Pubchem ID	Summary formula	Molecular weight	Dissociation constant (pKa)
2,4,6-trinitrophenol				
2,3-dinitrophenol				
3-hydroxybenzaldehyde				
2,4,6-trimethylphenol				

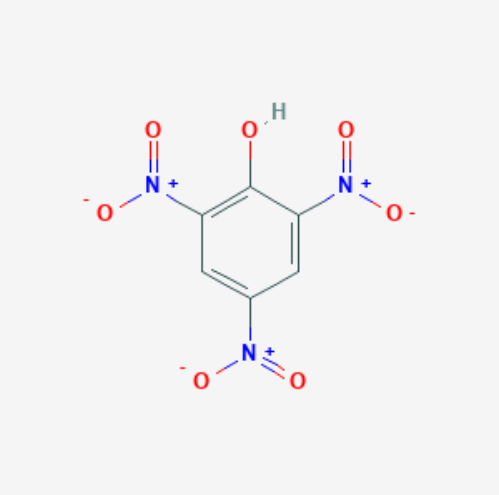
Note: If you can't find something in PubChem, look elsewhere on the Internet.

2. What other 1D descriptors are you able to find in PubChem? Write them here:
What others can you find in DrugBank and LigandExpo? Write them here:

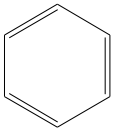
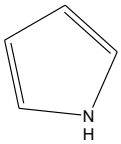
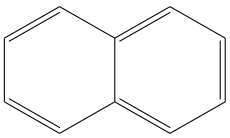
2D descriptors

3. Fill Table 2 with 2D structures:

Table 2:

2,4,6-trinitrophenol	2,3-dinitrophenol
	
3-hydroxybenzaldehyde	**2,4,6-trimethylphenol**

4. Fill Table 3 with fingerprints:

Table 3				-OH	-Cl	-NO_2	-CH_3	-COOH
2,4,6-trinitrophenol	1	0						
2,3-dinitrophenol								
3-hydroxybenzaldehyde								
2,4,6-trimethylphenol								

5. Fill Table 4, for each pair of atoms in the glycine molecule (see picture), write the smallest number of bonds separating them.

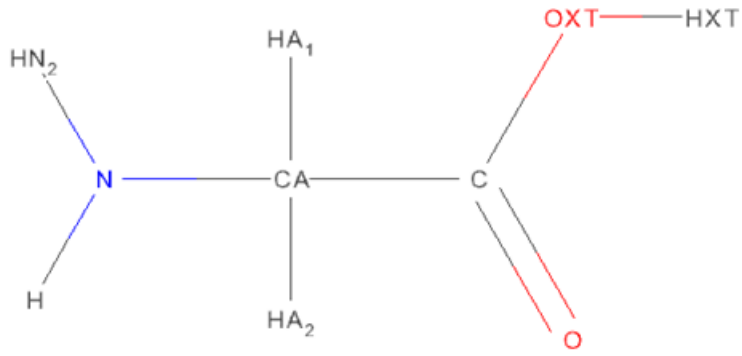


Table 4	HN2	H	N	HA1	CA	HA2	C	O	OXT	HXT
HN2	0	2	1							
H										
N										
HA1										
CA										
HA2										
C										
O										
OXT										
HXT										

6. Count the Wiener index for the glycine molecule. Use the formula:

$$\frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} D_{ij}$$

where N is the number of atoms and Dij is the distance between atoms i and j.

3D descriptors

7. Use MolView (molview.org) to view the molecules from Table 1 one by one. (It is best to trace them using the English name.) Add the column "Distance between O and H atoms" in Table 5 - measure this distance using (in MolView it is the Jmol tab and the "Distance" command, you have to click on the pair of atoms where you measure the distance).

Table 5	Dissociation constant (pKa)	Distance between atoms O and H	Charge on O (from OH group)	Charge on H (from OH group)
2,4,6-trinitrophenol				
2,3-dinitrophenol				
3-hydroxybenzaldehyde				
2,4,6-trimethylphenol				

8. In what unit are the measured distances?
9. In the first column of the table, copy the values from Table 1 then. Is there any relationship between the bond lengths O and H and the value of pKa? If so, what is it?

10. Download the 3D structures of the molecules listed in Table 1 from PubChem. Use the Atomic Charge calculator II tool (https://acc2.ncbr.muni.cz/) to calculate the charges on them and fill in the table.
11. Is there any relationship between the charges on O and H and the value of pKa? If so, what is it?