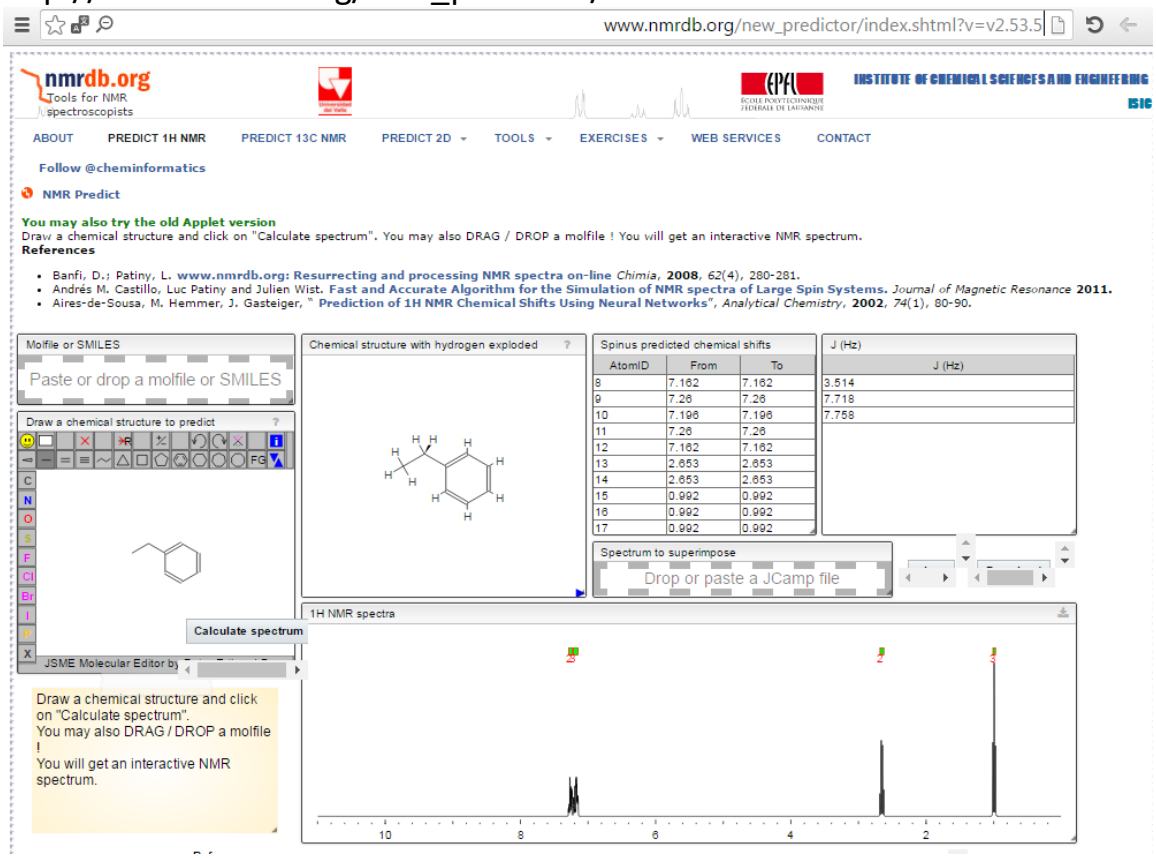
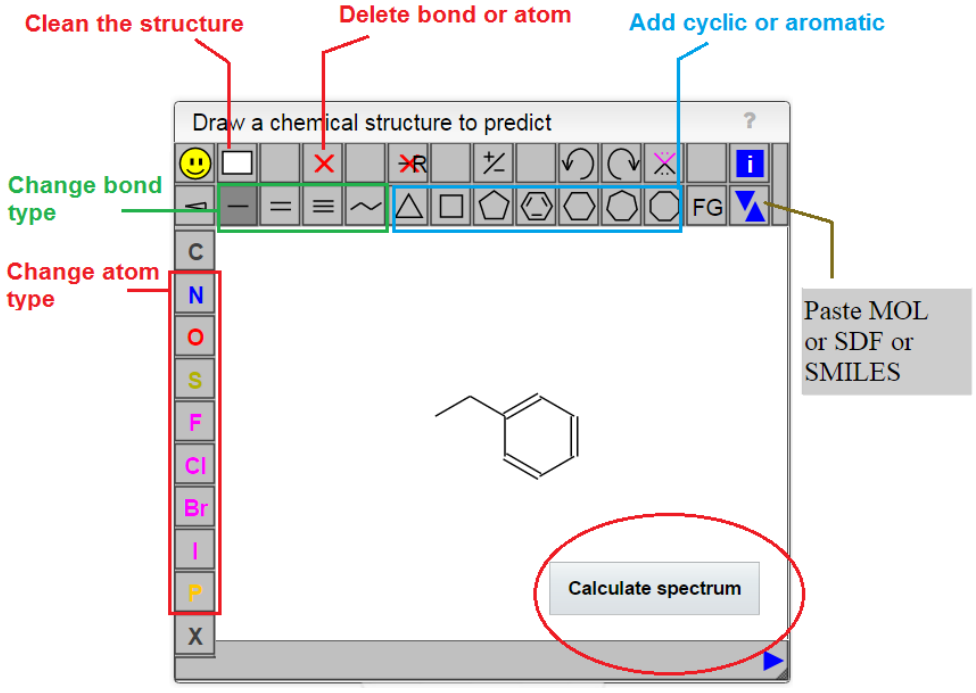
Home Work (II): ^{1}H NMR Spectroscopy

1. Go to “NMR Predict - Predict 1H proton NMR spectra” in nmrdb.org web site by typing the following address: http://www.nmrdb.org/new_predictor/index.shtml?v=v2.53.5



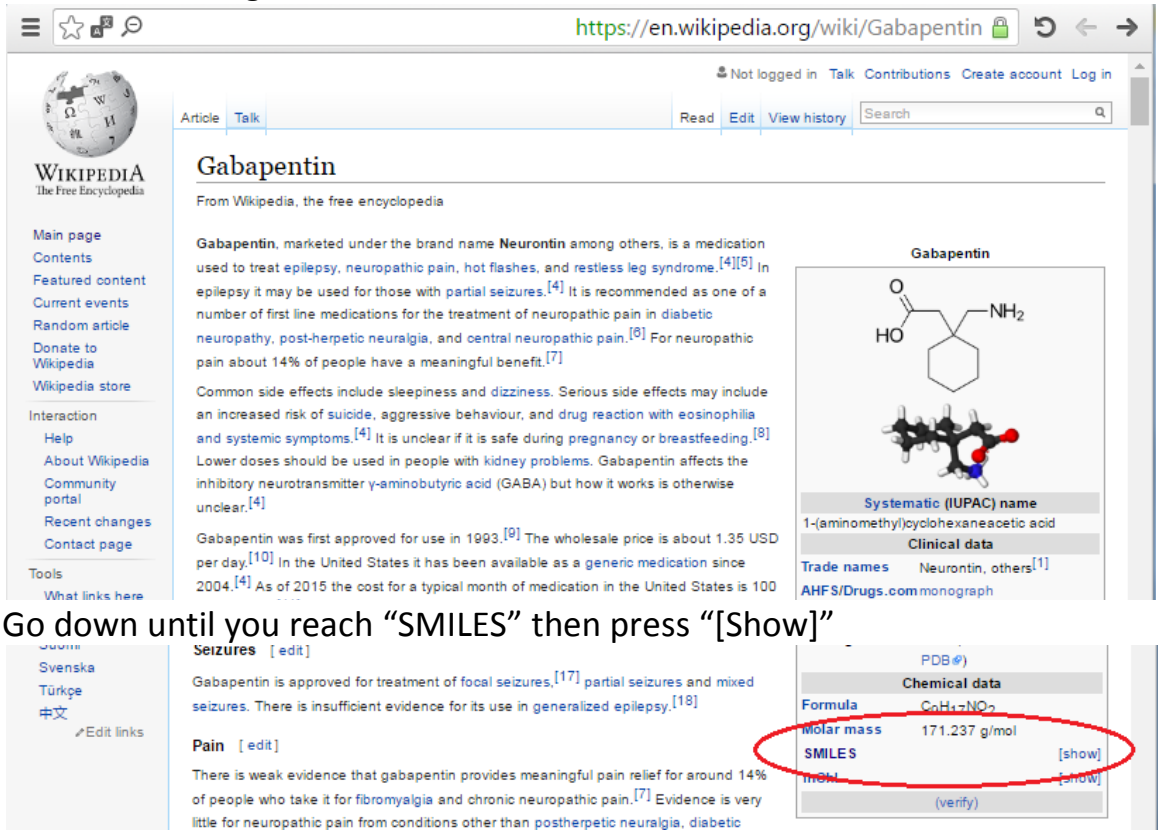
2. Now go to “Draw a chemical structure to predict” window



Start drawing the desired chemical structure, examine the icons to edit and/or delete atoms and bonds in the chemical structure and also to clean the structure and draw new one.

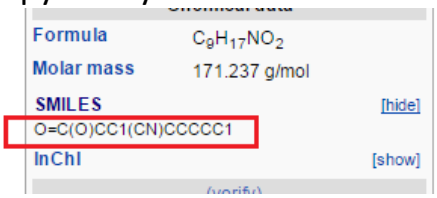
3. If the chemical structure is complicated then you could use the "Paste SMILES" option by pressing on  icon.
   By using this icon you have to write or paste SMILES symbols for your chemical compound. You can find it many database web sites, especially "Wikipedia"
   a- Go to "Wikipedia" by typing:
      https://en.wikipedia.org/wiki/Main_Page
   b- Type your chemical name in the "search" line

   c- For example type "Gabapentin" then Enter. You will get a page like the following

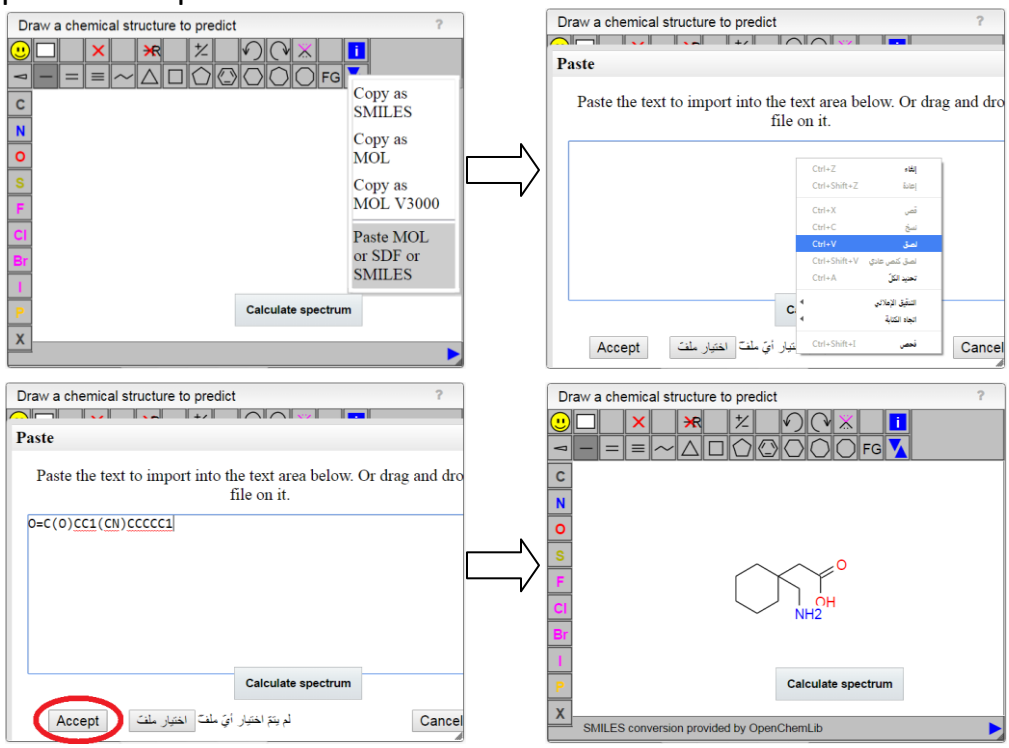


   d- Go down until you reach "SMILES" then press "[Show]"

e- Copy the symbols



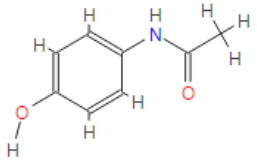
f- Go to “Paste SMILES” icon in “Draw a chemical structure to predict” window, press on it and Paste the symbols there then press “Accept”.



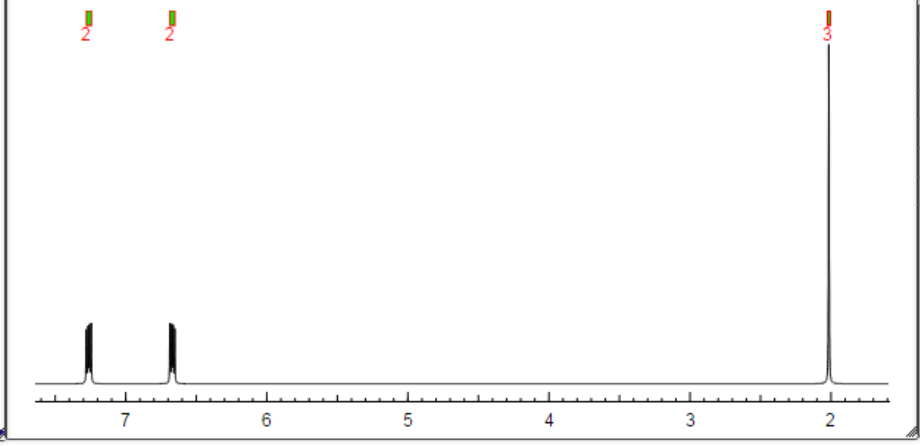
4. Once you draw the chemical structure, press on “Calculate spectrum”
5. Now copy spectrum and chemical shift data to word document
6. Go back to the chemical structure and make some modification then re-calculate the spectrum and copy it on the document file.
7. Repeat step 6 to make another modification.
8. Print the document file. You can draw the spectrum, structure and chemical shifts table by hand and deliver it. (see example below)

Paracetamol: N-(4-hydroxyphenyl)acetamide

Chemical structure with h...



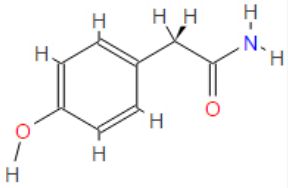
1H NMR spectra



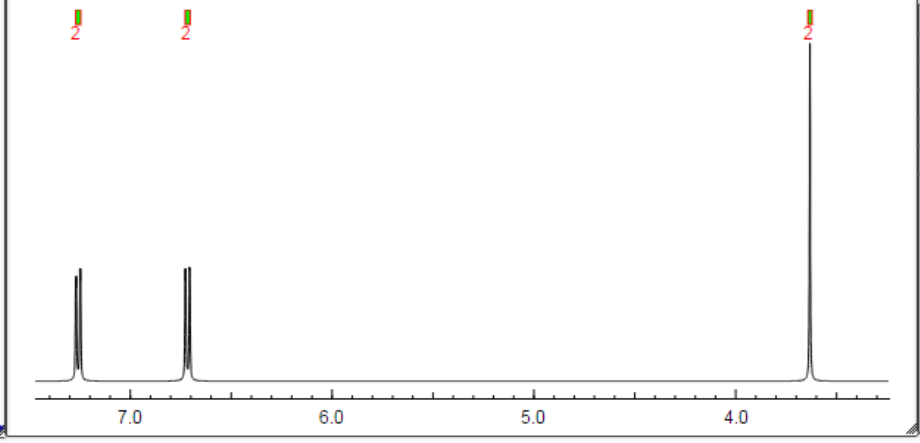
Spinus pred...

Atoml	From	To
11	2.015	2.015
12	2.015	2.015
13	2.015	2.015
15	7.261	7.261
16	6.669	6.669
18	6.669	6.669
19	7.261	7.261

Chemical structure with h...



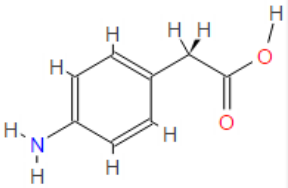
1H NMR spectra



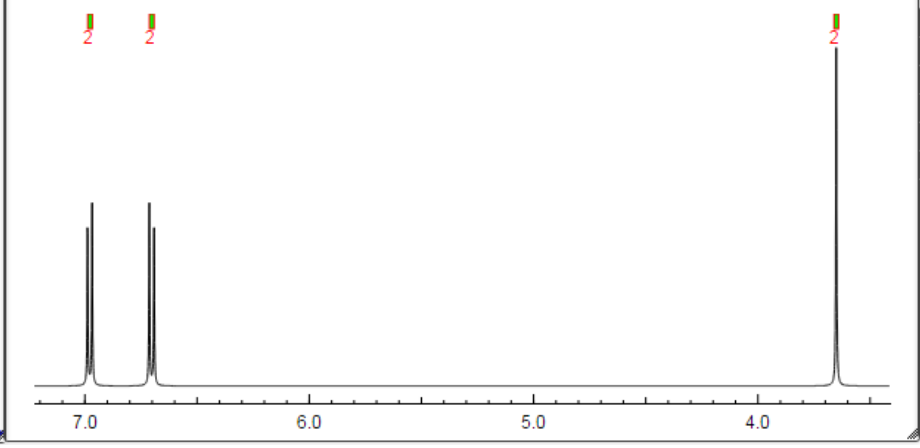
Spinus pred...

Atoml	From	To
13	3.632	3.632
14	3.632	3.632
15	7.258	7.258
16	6.716	6.716
18	6.716	6.716
19	7.258	7.258

Chemical structure with h...



1H NMR spectra



Spinus pred...

Atoml	From	To
12	3.651	3.651
13	3.651	3.651
14	6.977	6.977
15	6.702	6.702
16	6.702	6.702
17	6.977	6.977

Name:_____ Registration No.:_____