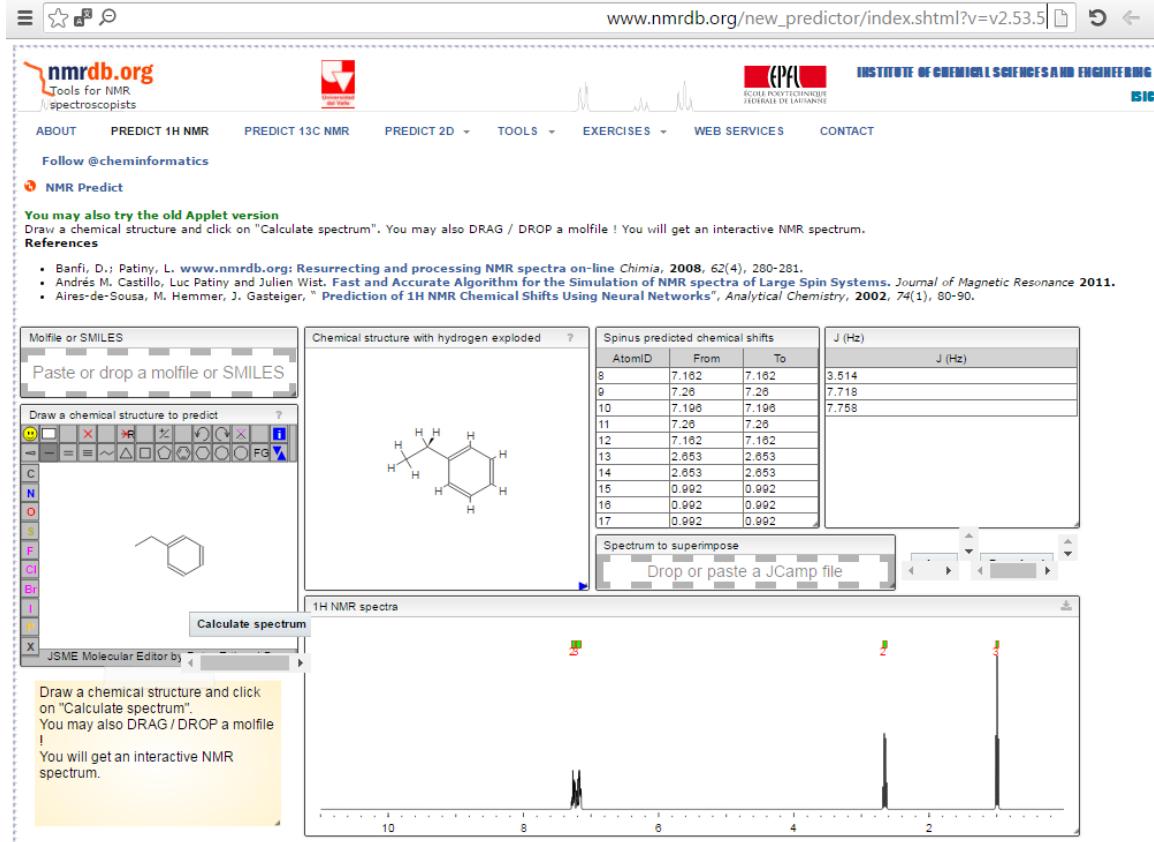
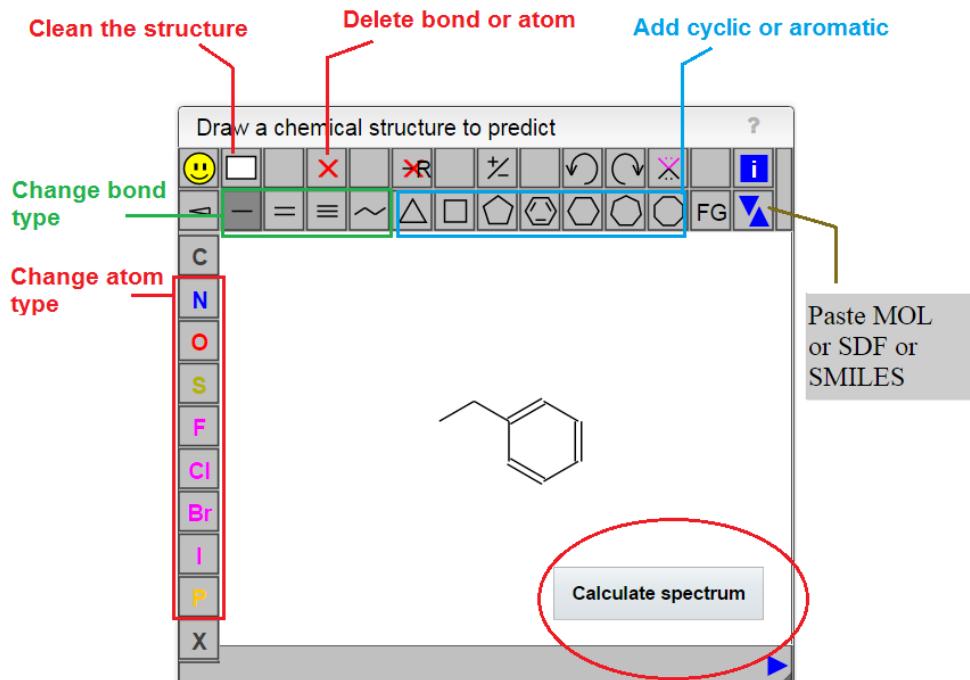


Home Work (II): ^1H NMR Spectroscopy

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:

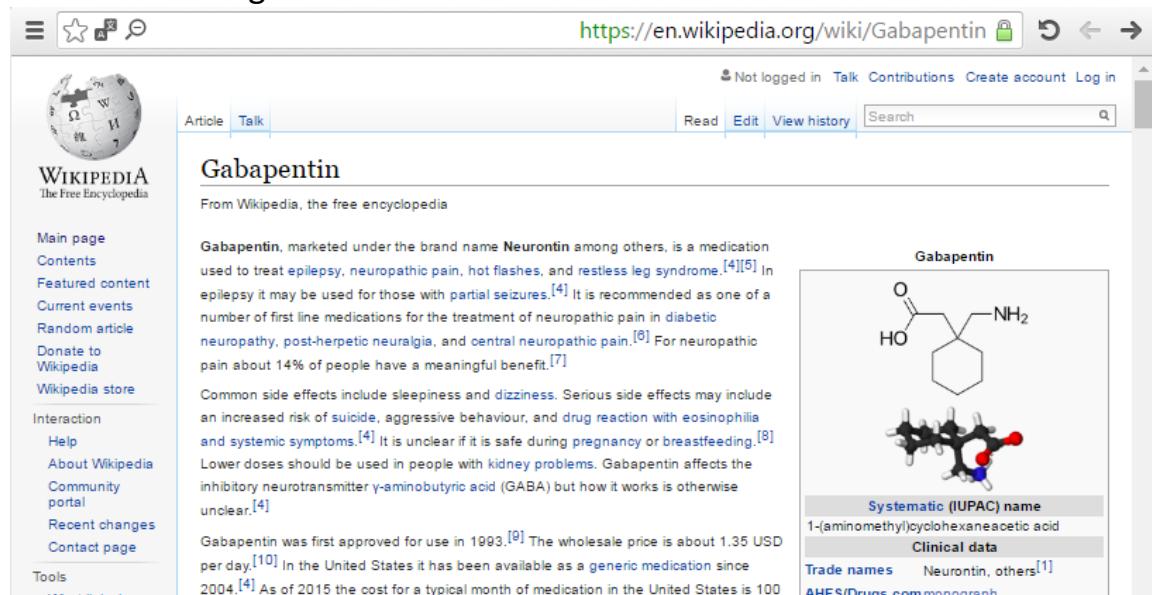
https://en.wikipedia.org/wiki/Main_Page

b- Type your chemical name in the “search” line



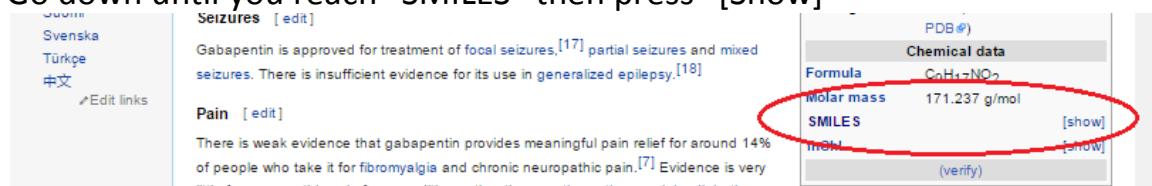
The screenshot shows the main Wikipedia page. At the top, there is a navigation bar with links for "Main Page", "Talk", "Read", "View source", and "View history". To the right of these is a search bar with a magnifying glass icon, which is circled in red. Below the search bar, the text "Welcome to Wikipedia, the free encyclopedia that anyone can edit. 5,153,611 articles in English" is displayed. To the right of this text are two columns of links: "Arts", "History", "Biography", "Mathematics", "Geography", and "Science". On the left side of the page, there is a sidebar with links for "Main page", "WIKIPEDIA The Free Encyclopedia", and various interaction and tools links.

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



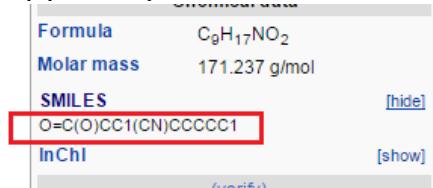
The screenshot shows the Wikipedia page for "Gabapentin". The page title is "Gabapentin" and it is described as "From Wikipedia, the free encyclopedia". The text on the page discusses Gabapentin's use in epilepsy, neuropathic pain, hot flashes, and restless leg syndrome. It also mentions its side effects and history of approval. On the right side of the page, there is a chemical structure of Gabapentin and its SMILES string: CC1(CNC)CCC1C(=O)O. Below the structure, the systematic (IUPAC) name is given as "1-(aminomethyl)cyclohexaneacetic acid". There is also a "Clinical data" section with trade names like "Neurontin, others".

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

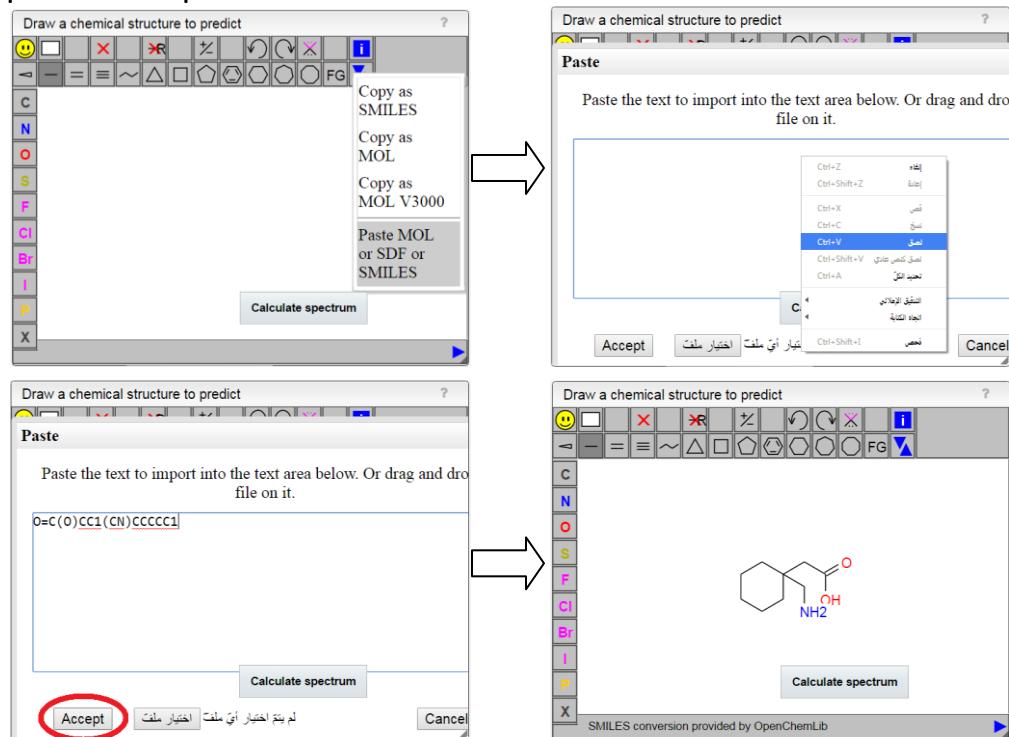


The screenshot shows the "Chemical data" section of the Gabapentin page. It includes the SMILES string CC1(CNC)CCC1C(=O)O, its formula C9H13NO2, and its molar mass (171.237 g/mol). There are "Show" and "Verify" buttons next to the SMILES string. The entire "Chemical data" section is circled in red.

e- Copy the symbols

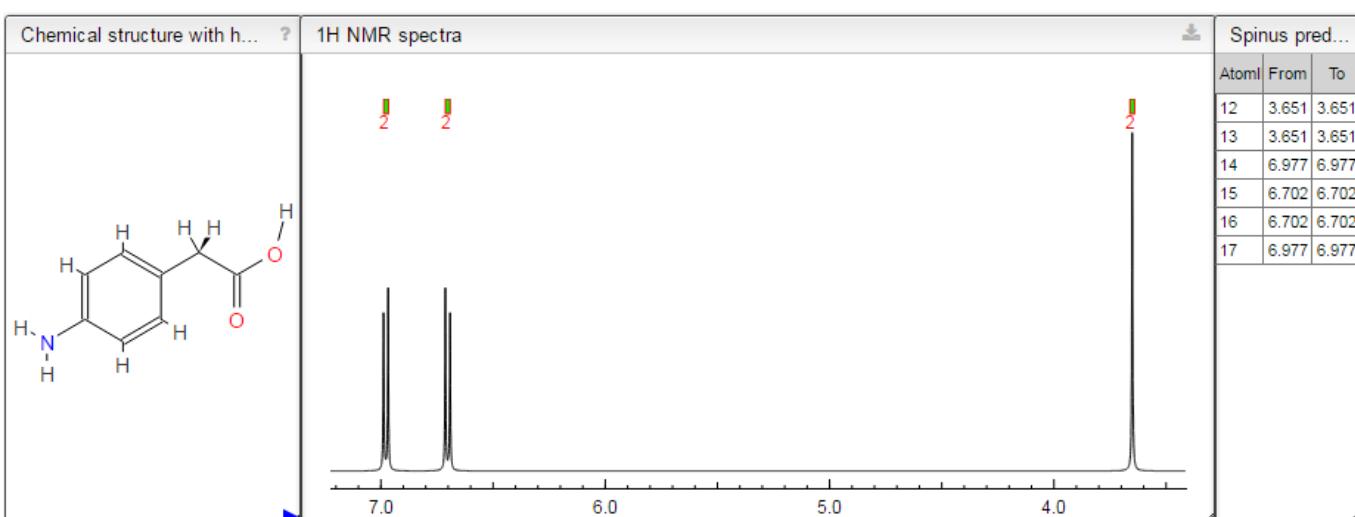
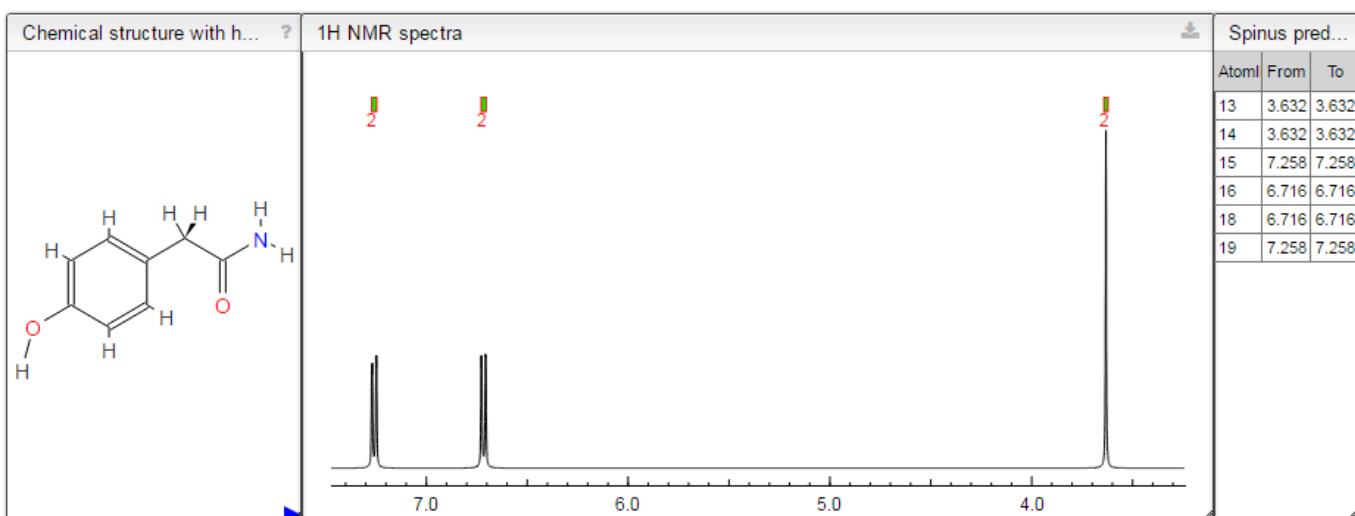
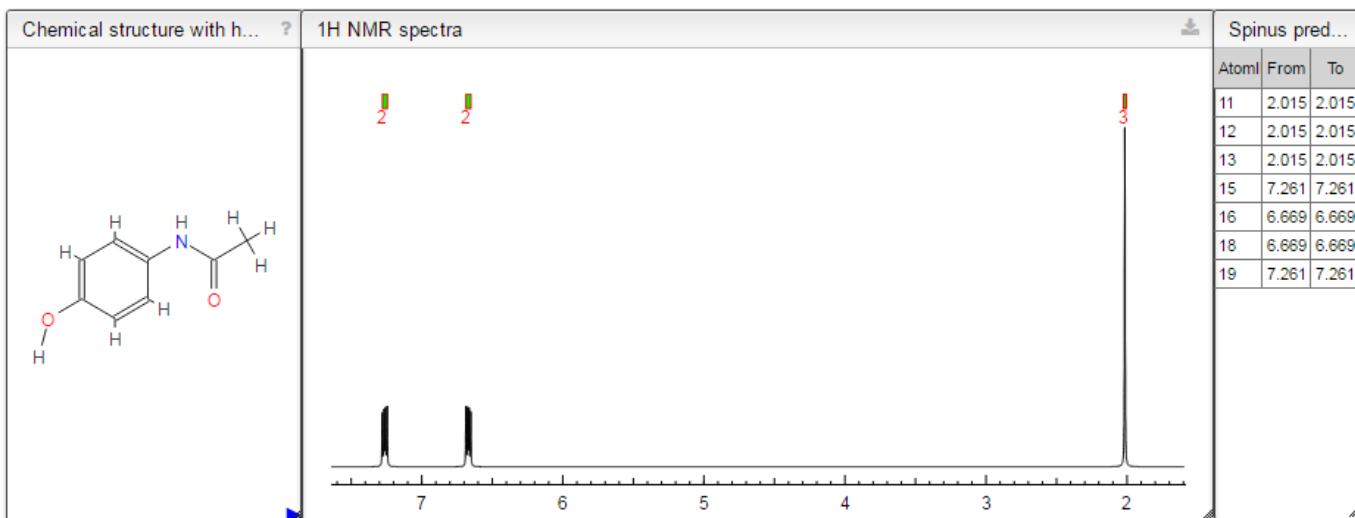


f- Go to “Paste SMILES” icon in “Draw a chemical structure to predict” window, press on it and Paste the symbols there then press “Accept”.



- Once you draw the chemical structure, press on “Calculate spectrum”
- Now copy spectrum and chemical shift data to word document
- Go back to the chemical structure and make some modification then re-calculate the spectrum and copy it on the document file.
- Repeat step 6 to make another modification.
- 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



Name: _____

Registration No.: _____