

## Home Work (II): $^1\text{H}$ NMR Spectroscopy

1. Go to “NMR Predict - Predict  $^1\text{H}$  proton NMR spectra” in nmrd.org web site by typing the following address:

[http://www.nmrd.org/new\\_predictor/index.shtml?v=v2.53.5](http://www.nmrd.org/new_predictor/index.shtml?v=v2.53.5)

nmrd.org  
Tools for NMR spectroscopists

ABOUT PREDICT 1H NMR PREDICT 13C NMR PREDICT 2D TOOLS EXERCISES WEB SERVICES CONTACT

Follow @cheminformatics

NMR Predict

You may also try the old Applet version

Draw a chemical structure and click on "Calculate spectrum". You may also DRAG / DROP a molfile ! You will get an interactive NMR spectrum.

References

- Banfi, D.; Patiny, L. *www.nmrd.org: Resurrecting and processing NMR spectra on-line* *Chimia*, **2008**, 62(4), 280-281.
- Andrés M. Castillo, Luc Patiny and Julien Wist. *Fast and Accurate Algorithm for the Simulation of NMR spectra of Large Spin Systems*. *Journal of Magnetic Resonance* **2011**.
- Aires-de-Sousa, M. Hemmer, J. Gasteiger, " *Prediction of  $^1\text{H}$  NMR Chemical Shifts Using Neural Networks*", *Analytical Chemistry*, **2002**, 74(1), 80-90.

Molfile or SMILES

Paste or drop a molfile or SMILES

Draw a chemical structure to predict

Chemical structure with hydrogen exploded

Spinus predicted chemical shifts

AtomID	From	To
8	7.182	7.182
9	7.28	7.28
10	7.198	7.198
11	7.28	7.28
12	7.182	7.182
13	2.853	2.853
14	2.853	2.853
15	0.992	0.992
16	0.992	0.992
17	0.992	0.992

J (Hz)

J (Hz)
3.514
7.718
7.758

Spectrum to superimpose

Drop or paste a JCamp file

1H NMR spectra

Calculate spectrum

JSME Molecular Editor by

Draw a chemical structure and click on "Calculate spectrum". You may also DRAG / DROP a molfile ! You will get an interactive NMR spectrum.

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

Clean the structure

Delete bond or atom

Add cyclic or aromatic


Change bond type

Change atom type

Paste MOL or SDF or SMILES

Calculate spectrum

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”

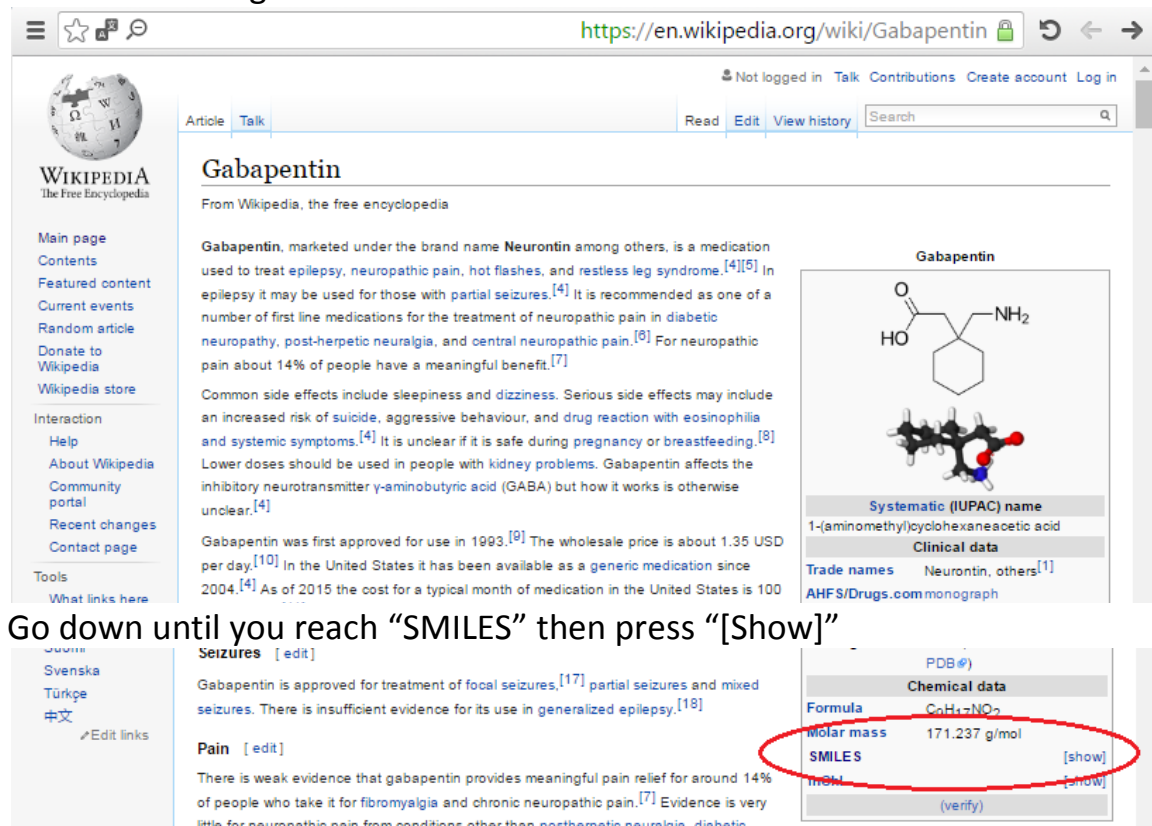
a- Go to “Wikipedia” by typing:

[https://en.wikipedia.org/wiki/Main\\_Page](https://en.wikipedia.org/wiki/Main_Page)

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



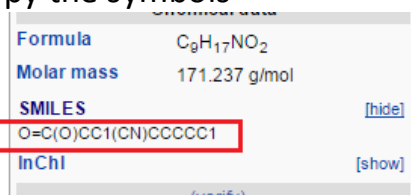
c- For example type “Gabapentin” then Enter. You will get a page like the following


A screenshot of the Wikipedia page for Gabapentin. The page shows the article title, a brief description, and a chemical structure. Below the structure is a table with chemical data. The 'SMILES' field in this table is circled in red. The table also includes fields for 'Molar mass', 'Formula', and 'PDB #'.

Chemical data	
Formula	C <sub>9</sub> H <sub>11</sub> NO <sub>2</sub>
Molar mass	171.237 g/mol
SMILES	<a href="#">[show]</a>
mol	<a href="#">[show]</a>
<a href="#">(verify)</a>	

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”.

Draw a chemical structure to predict

Paste

Paste the text to import into the text area below. Or drag and drop file on it.

Ctrl+Z Undo  
Ctrl+Shift+Z Redo  
Ctrl+X Cut  
Ctrl+C Copy  
Ctrl+V Paste  
Ctrl+Shift+V Paste as text  
Ctrl+A Select all  
Ctrl+Shift+I Select all and copy

Accept

لم يتم اختيار أي ملف اختيار ملف Cancel

Draw a chemical structure to predict

Paste

Paste the text to import into the text area below. Or drag and drop file on it.

O=C(O)CC1(CN)CCCCC1

Calculate spectrum

Accept

لم يتم اختيار أي ملف اختيار ملف Cancel

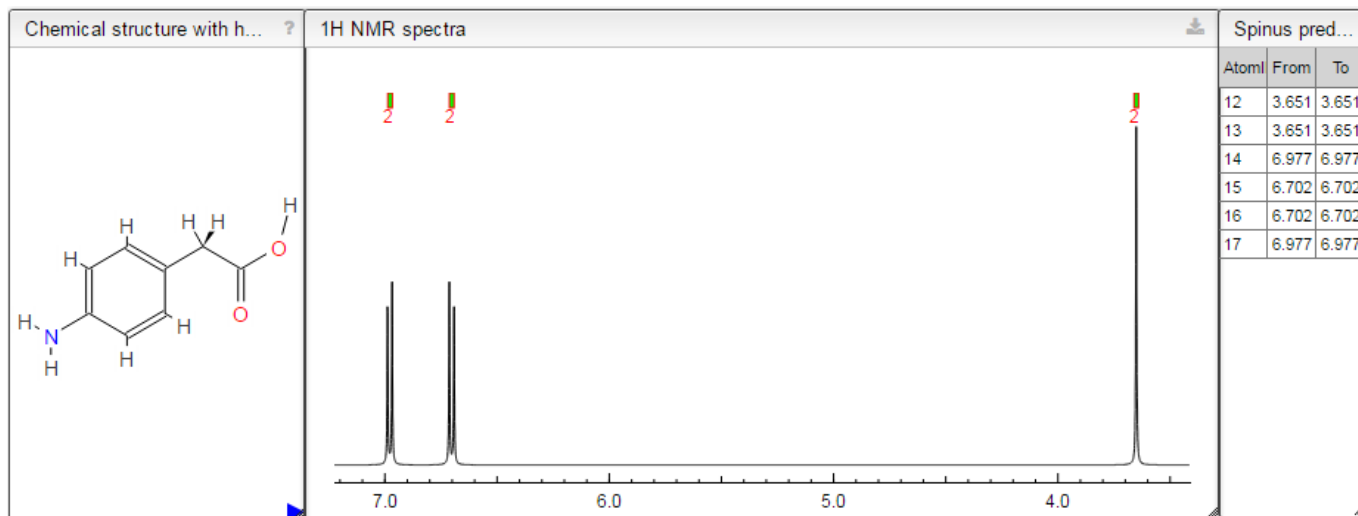
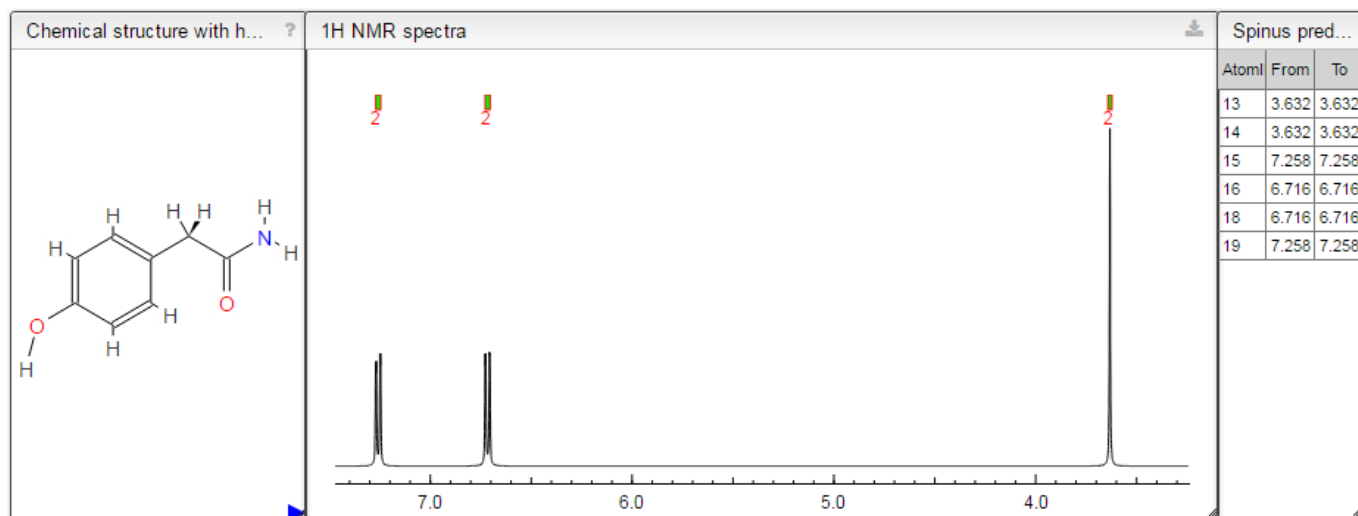
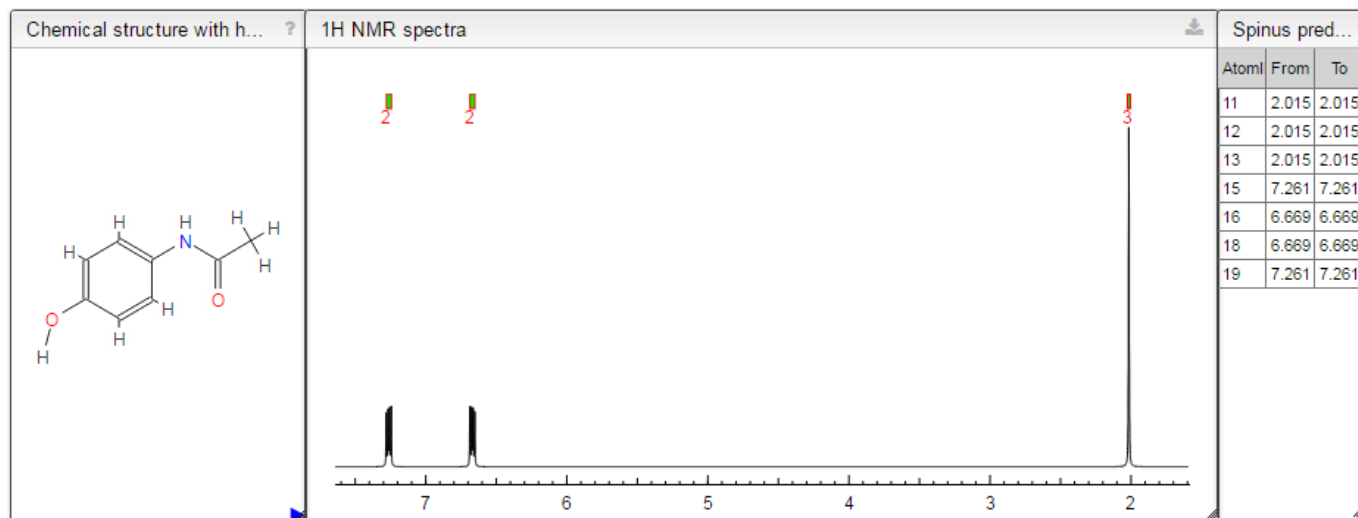
Draw a chemical structure to predict

Calculate spectrum

SMILES conversion provided by OpenChemLib

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



Name: \_\_\_\_\_

Registration No.: \_\_\_\_\_