The given set of files 1D_Spectra.pdf and 1D_Spectra_Test_Answers.xlsx provides a helpful guide for students, teachers and anybody interested in the field of NMR spectroscopy. In 1D_Spectra.pdf file, we present ^{1}H and ^{13}C spectra of 90 unique compounds. All structures can be determined using just 1D spectra. Each set of 1D spectra contains also additional information as depicted in Figure 1. Exchangeable hydrogens are highlighted by *.

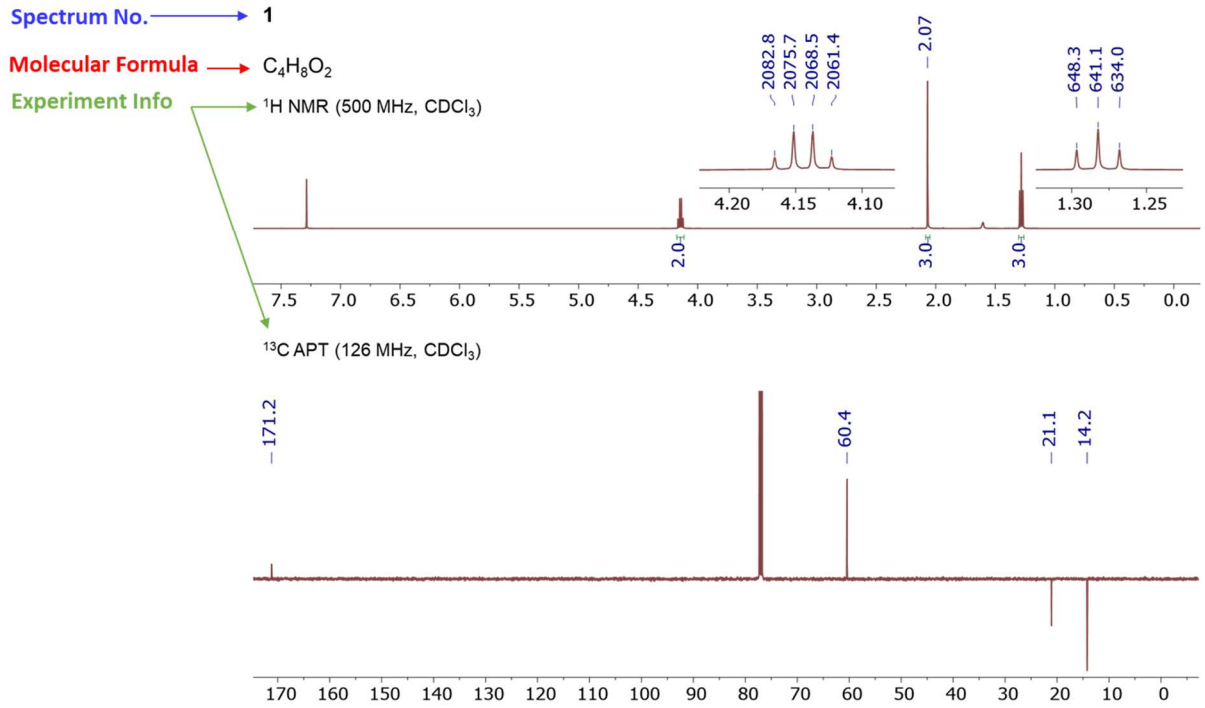

Figure 1 The preview of 1D_Spectra.pdf file. Each set of spectra contains also spectrum number, molecular formula and experiment information.

To encourage users in working out the exercises, we present also fully automized Excel file that is supposed to be used for checking the answers. The users are allowed to edit only the "Compound Name" column. In the case of right answer, the program responds "Correct" and the user gets 1 point. Total points and the success rate are displayed at the bottom of the sheet. The "Level" column provides an estimation of the exercise difficulty (1 – very easy, 5 – very hard).

ÚOCHB AV ČR IOCB PRAGUE NMR SPECTROSCOPY RESEARCH-SERVICE GROUP IOCB PRAGUE

Spectrum No.	Level	Compound Name	Result	Points
1	1	ethyl acetate	Correct	1.00
2	1		No answer	-
3	1		No answer	-
4	3		No answer	-
5	2		No answer	-

Figure 2 The preview of 1D_Spectra_Test.xlsx. The users are allowed to edit Compound Name column only. The checking mechanism is fully automized.

To avoid further problems, we present simple tips for filling in Compound Name column

- The program is not case sensitive
- You can write your answers either in Czech or English language
- Additional to IUPAC name you can also use trivial names of the compound or its canonical SMILES or InChI in "InChI=1S/C4H8O2/c1-3-6-4(2)5/h3H2,1-2H3" form.
- SMILES and InChI can be easily generated from drawn structure using chemical structure drawing software or found in chemical databases.
- A number of equally valid SMILES strings can be written for the same molecule in dependency on the algorithm used. We present SMILES strings generated in ChemDraw 19.0 as "Correct" and it may happen that your valid SMILES string would not be recognised by our algorithm in 1D_Spectra_Test_Answers.xlsx. In this case, try another structure identification e.g. systematic name or InChI.
- While naming acids, the suitable word order is "carboxylic acid" in both languages.
- In case you receive "Incorrect" response although you are quite sure that your answer is correct, check your spelling or try to fill out another compound name, or contact us at zuzana.osifova@uochb.cas.cz or martin.dracinsky@uochb.cas.cz.