

checkHNMR (beta): PDF input template

Characterization data in the ACS style, one block per compound

How to fill in

- Write one block per compound, up to 20 compounds per file.
- Put the compound label on its own line (for example **3a**), then the name.
- Add a line “SMILES: ...” for each compound. It is optional but strongly recommended: without a structure the proton count (item 1) is compared only with the HRMS formula, and the checks that need a structure are not run.
- Write the ¹H NMR description in one paragraph: “¹H NMR (frequency, solvent) δ shift (multiplicity, *J* = ... Hz, number of protons, assignment if you wish), ...” The order of the parts inside the brackets may differ.
- Report signals of non-first-order spin systems (e.g., the AA'XX' systems of para-disubstituted benzenes and of X–CH₂–CH₂–Y fragments such as BrCH₂CH₂I, including CH₂–CH₂ fragments of saturated rings, and monosubstituted phenyl groups) as multiplets without coupling constants, giving the range: “6.82–6.76 (m, 2H)”. Alternatively, mark the signal as non-first-order and give the splitting as an apparent value: “7.76 (nfod, *J*_{app} = 8.3 Hz, 2H)”, where nfod (nfot, nfom) is a non-first-order doublet (triplet, multiplet) and *J*_{app} is the observed spacing (for an AA'XX' system, *J*_o + *J*_p), as defined by Tang, Xu and Hoyer (*Molecules* **2025**, *30*, 2610). Coupling constants may be given for a multiplet only if they were obtained by total lineshape analysis or spectral simulation; state the method (and the program) in the experimental section.
- ¹³C NMR, ¹⁹F NMR, ³¹P NMR and HRMS lines are optional. The molecular formula is taken from the HRMS line. For H–F and H–P couplings, give the proton-coupled ¹⁹F or ³¹P description: the splitting is looked for there (a {¹H}-decoupled spectrum cannot show it).
- Save the file from Word as PDF (File → Save As → PDF). Scans and pictures of text cannot be read: the text in the PDF must be selectable.
- Before the report, checkHNMR shows how each description was read. Check this table first.

The file is read in your browser and is not uploaded or stored.

Example*

**All values below are invented to illustrate the format. They are not measured data for these compounds.*

1

Ethyl (*E*)-but-2-enoate

SMILES: CCOC(=O)/C=C/C

Colorless liquid (98 mg, 86%).

¹H NMR (400 MHz, CDCl₃) δ 6.97 (dq, *J* = 15.6, 6.9 Hz, 1H), 5.84 (dq, *J* = 15.6, 1.7 Hz, 1H), 4.18 (q, *J* = 7.1 Hz, 2H), 1.88 (dd, *J* = 6.9, 1.7 Hz, 3H), 1.28 (t, *J* = 7.1 Hz, 3H).

¹³C{¹H} NMR (101 MHz, CDCl₃) δ 166.6, 144.6, 122.8, 60.1, 18.0, 14.3.

HRMS (ESI) *m/z*: [M + H]⁺ calcd for C₆H₁₁O₂ 115.0754; found 115.0756.

2

N-Benzyl-4-methoxyaniline

SMILES: COc1ccc(NCc2ccccc2)cc1

Yellow oil (171 mg, 80%).

¹H NMR (400 MHz, CDCl₃) δ 7.38–7.25 (m, 5H), 6.82–6.76 (m, 2H), 6.64–6.58 (m, 2H), 4.29 (s, 2H), 3.80 (br s, 1H, NH), 3.75 (s, 3H).

¹³C{¹H} NMR (101 MHz, CDCl₃) δ 152.2, 142.5, 139.7, 128.6, 127.6, 127.2, 114.9, 114.2, 55.8, 49.3.

HRMS (ESI) *m/z*: [M + H]⁺ calcd for C₁₄H₁₆NO 214.1226; found 214.1229.

3

Ethyl 2-fluoroacetate

SMILES: CCOC(=O)CF

Colorless liquid (87 mg, 82%).

¹H NMR (400 MHz, CDCl₃) δ 4.83 (d, *J* = 47.1 Hz, 2H), 4.28 (q, *J* = 7.1 Hz, 2H), 1.31 (t, *J* = 7.1 Hz, 3H).

¹³C{¹H} NMR (101 MHz, CDCl₃) δ 167.8 (d, *J* = 22.0 Hz), 77.6 (d, *J* = 180.2 Hz), 61.6, 14.1.

¹⁹F NMR (376 MHz, CDCl₃) δ -230.6 (t, *J* = 47.1 Hz).

HRMS (ESI) *m/z*: [M + H]⁺ calcd for C₄H₈FO₂ 107.0503; found 107.0505.

4

Dimethyl methylphosphonate

SMILES: COP(C)(=O)OC

Colorless liquid (105 mg, 85%).

¹H NMR (400 MHz, CDCl₃) δ 3.74 (d, *J* = 11.0 Hz, 6H), 1.48 (d, *J* = 17.6 Hz, 3H).

¹³C{¹H} NMR (101 MHz, CDCl₃) δ 52.4 (d, *J* = 6.2 Hz), 10.0 (d, *J* = 144.6 Hz).

³¹P NMR (162 MHz, CDCl₃) δ 32.9 (qsept, *J* = 17.6, 11.0 Hz).

HRMS (ESI) *m/z*: [M + H]⁺ calcd for C₃H₁₀O₃P 125.0362; found 125.0360.