Supporting Information
A pH-enhanced resolution in benchtop NMR spectroscopy

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Determining pK_a of the pH indicators

Series of thirty 10 mM samples of each of three pH indicators (2,6-lutidine, L-tyrosine, sodium formate) at pH values from 1.0 to 12.0 have been prepared. We used a digital pH-meter (SevenCompact S210, Mettler Toledo, Switzerland) to check the pH in each sample. The pH measurement has been performed twice, using two different calibration buffers to obtain ΔpK_a, as described by Wallace et al.[1] (half of the difference between the two obtained pK_a values). The position of the D_2O peak was set to 4.75 ppm in all spectra.

To determine pK_a values, we calculated fits using the Equation (1) from the main text. We employed the Non-linear Solver from LibreOffice[2] to minimize the root-mean-square difference between the model and the experimental data. Three parameters have been optimized: pK_a, δ_H, δ_L. The fits for one of the two pH calibration buffers are shown in Figures S1-S3. The results of the calculation are presented in Table S1.

pH indicator	literature pKa	experimental pKa	δ_H/ppm	δ_L/ppm
formate	3.63±0.04[1]	3.34±0.03	8.21	8.39
2,6-lutidine	6.87[1]	6.96±0.03	2.69	2.37
L-tyrosine	9.60[3]	9.71±0.03	3.15	2.80

Table S1 Comparison of literature and experimental pKa values and limiting chemical shifts of NMR pH-indicators present in the test sample.

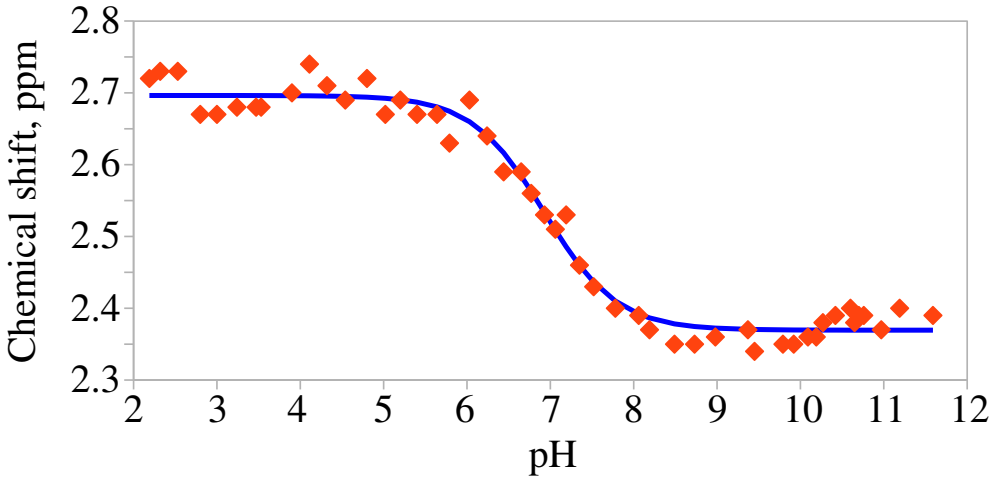

Figure S1 Chemical shift vs pH for the ^{1}H NMR peak of 10mM 2,6-lutidine measured at pH values from 2 to 12. The orange diamond corresponds to experimental values, and the blue line to the fit according to Equation (1) from the main text.

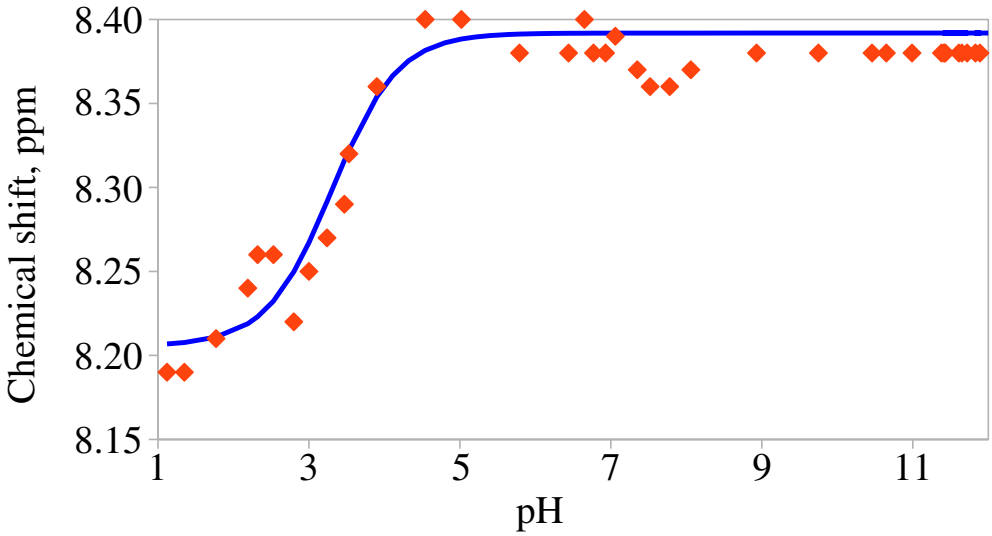

Figure S2 Chemical shift vs pH for the ^{1}H NMR peak of 10mM sodium formate measured at pH values from 1 to 12. The orange diamond corresponds to experimental values, and the blue line to the fit according to Equation (1) from the main text.

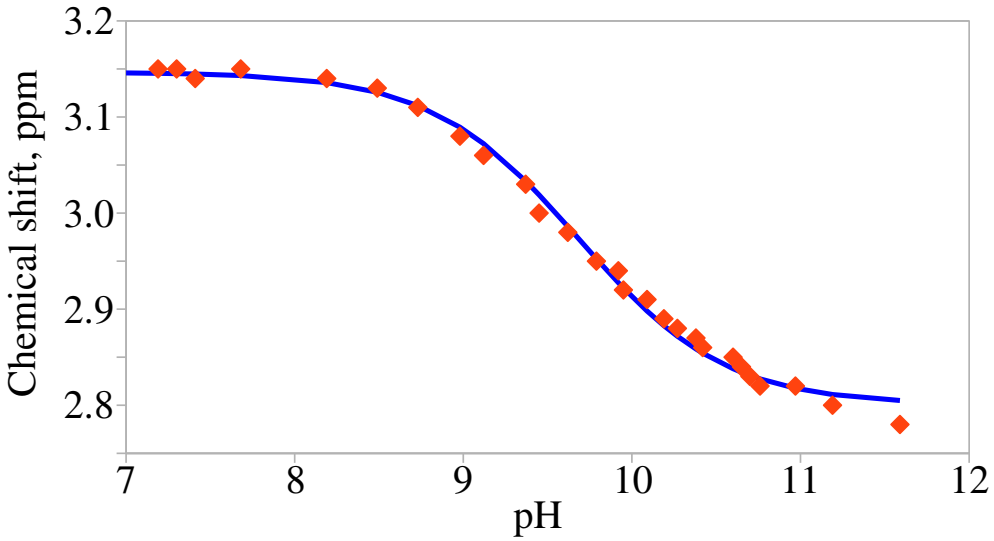

Figure S3 Chemical shift vs pH for the ^{1}H NMR peak of 10mM L-tyrosine measured at pH values from 7 to 12. The orange diamond corresponds to experimental values, and the blue line to the fit according to Equation (1) from the main text.

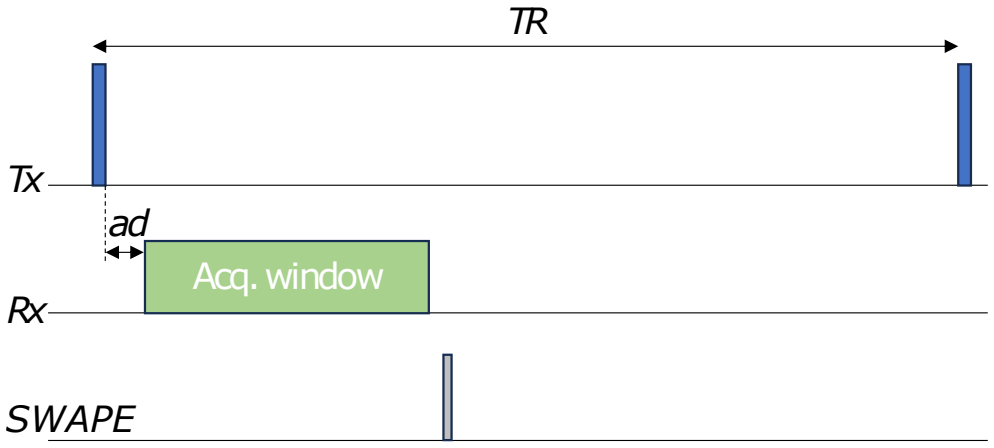

Figure S4 Schematic diagram of the acquisition sequence, showing the synchronization between transmitter (Tx), receiver (Rx), and SWAPE apparatus. The RF sequence consisted of a single 11.5 μs hard-pulse, with a repetition time (TR) of 3.5 s. The acquisition window was 1638.4 ms in length, with an acquisition delay (ad) of 20 μs. The trigger pulse for SWAPE to shift the sample vertically was set to 10 ms after the acquisition window, and the shuttle time was approximately 300 ms. Synchronization was achieved by writing a macro in the Spinsolve Expert software (see below).

Experimental setup for Magritek 43 MHz with SWAPE device

The code below performs a serial ^{1}H NMR experiment according to scheme from Fig. S4 and using a standard `1Pulse-H` pulse program with 8192 time-domain points, 64 scans, and pulse length of 11.5 μs. The sample is shifted between experiments in a series using a `move_tube_down` program, which sends the command to the step motor of SWAPE.

```
########################################################################
# This code should be in all scripts just change the procedure name
########################################################################

procedure(simpleScript)

   cd("$appdir$\\Macros\\Spinsolve-Expert\\Script Macros")
   win = InitScript(getmacropath(),getmacroname())
   th = thread(":runScript")
   threadwait(th)
   EndScript(win)

endproc()

########################################################################
# This code provides F1 help for special function commands
########################################################################

procedure(showHelp, command)

   help("Macros\\Spinsolve-Expert","ScriptEditor.htm#$command$")

endproc()

########################################################################
# User defined script goes here
########################################################################
# move_tube_down - a program sending command to SWAPE motor to move by one step

procedure(runScript)

   PATH = "pH_gradient_data"
   M1 = 1
   Nscans = 64
   time(0)
   for(k = 0 to M1-1)

      #1st volume
      NewDataFolder("C:\\$PATH$\\sub_sample_1\\$k$")
      r = RunExpt("1Pulse-H",
                  ["nrPnts = 8192",
                   "repTime = 3500",
                   "acqDelay = 20",
                   "nrScans = $Nscans$",
                   "zf = 1",
                   "dwellTime = 200",
                   "pulseLength1H = 11.5",
                   "tdPhaseCorr = \"none\"",
                   "fdPhaseCorr = \"autophase\"",
                   "saveData=\"true\""])
```

```
␣␣␣␣␣␣r␣=␣RunExpt("move_tube_down",
␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣["nrPnts␣=␣8192",
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␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣"tdPhaseCorr␣=␣\"none\"",
␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣"fdPhaseCorr␣=␣\"autophase\"",
␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣"saveData=\"false\""])

␣␣␣␣␣␣#␣2d␣volume
␣␣␣␣␣␣NewDataFolder("C:\\$PATH$\\sub_sample_2\\$k$")
␣␣␣␣␣␣r␣=␣RunExpt("1Pulse-H",
␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣["nrPnts␣=␣8192",
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␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣"tdPhaseCorr␣=␣\"none\"",
␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣"fdPhaseCorr␣=␣\"autophase\"",
␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣"saveData=\"true\""])

␣␣␣␣␣␣r␣=␣RunExpt("move_tube_down",
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␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣"fdPhaseCorr␣=␣\"autophase\"",
␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣"saveData=\"false\""])

␣␣␣␣␣␣#␣3th␣volume
␣␣␣␣␣␣NewDataFolder("C:\\$PATH$\\sub_sample_3\\$k$")
␣␣␣␣␣␣r␣=␣RunExpt("1Pulse-H",
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␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣"fdPhaseCorr␣=␣\"autophase\"",
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```

```
                    "dwellTime = 200",
                    "tdPhaseCorr = \"none\"",
                    "fdPhaseCorr = \"autophase\"",
                    "saveData=\"false\""])

    #4th volume
    NewDataFolder("C:\\$PATH$\\sub_sample_4\\$k$")
    r = RunExpt("1Pulse-H",
                    ["nrPnts = 8192",
                    "repTime = 3500",
                    "acqDelay = 20",
                    "nrScans = $Nscans$",
                    "zf = 1",
                    "dwellTime = 200",
                    "pulseLength1H = 11.5",
                    "tdPhaseCorr = \"none\"",
                    "fdPhaseCorr = \"autophase\"",
                    "saveData=\"true\""])

    r = RunExpt("move_tube_down",
                    ["nrPnts = 8192",
                    "repTime = 2500",
                    "acqDelay = 327000",
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                    "zf = 1",
                    "dwellTime = 200",
                    "tdPhaseCorr = \"none\"",
                    "fdPhaseCorr = \"autophase\"",
                    "saveData=\"false\""])

    #5th volume
    NewDataFolder("C:\\$PATH$\\sub_sample_5\\$k$")
    r = RunExpt("1Pulse-H",
                    ["nrPnts = 8192",
                    "repTime = 3500",
                    "acqDelay = 20",
                    "nrScans = $Nscans$",
                    "zf = 1",
                    "dwellTime = 200",
                    "pulseLength1H = 11.5",
                    "tdPhaseCorr = \"none\"",
                    "fdPhaseCorr = \"autophase\"",
                    "saveData=\"true\""])


    r = RunExpt("move_tube_down",
                    ["nrPnts = 8192",
                    "repTime = 2500",
                    "acqDelay = 327000",
                    "nrScans = 1",
                    "zf = 1",
                    "dwellTime = 200",
                    "tdPhaseCorr = \"none\"",
                    "fdPhaseCorr = \"autophase\"",
                    "saveData=\"false\""])
```

```
      # 6th volume
      NewDataFolder("C:\\$PATH$\\sub_sample_6\\$k$")
      r = RunExpt("1Pulse-H",
                  ["nrPnts = 8192",
                   "repTime = 3500",
                   "acqDelay = 20",
                   "nrScans = $Nscans$",
                   "zf = 1",
                   "dwellTime = 200",
                   "pulseLength1H = 11.5",
                   "tdPhaseCorr = \"none\"",
                   "fdPhaseCorr = \"autophase\"",
                   "saveData=\"true\""])

      r = RunExpt("move_tube_down",
                  ["nrPnts = 8192",
                   "repTime = 2500",
                   "acqDelay = 327000",
                   "nrScans = 1",
                   "zf = 1",
                   "dwellTime = 200",
                   "tdPhaseCorr = \"none\"",
                   "fdPhaseCorr = \"autophase\"",
                   "saveData=\"false\""])

      # 7th volume
      NewDataFolder("C:\\$PATH$\\sub_sample_7\\$k$")
      r = RunExpt("1Pulse-H",
                  ["nrPnts = 8192",
                   "repTime = 3500",
                   "acqDelay = 20",
                   "nrScans = $Nscans$",
                   "zf = 1",
                   "dwellTime = 200",
                   "pulseLength1H = 11.5",
                   "tdPhaseCorr = \"none\"",
                   "fdPhaseCorr = \"autophase\"",
                   "saveData=\"true\""])

      r = RunExpt("move_tube_down",
                  ["nrPnts = 8192",
                   "repTime = 2500",
                   "acqDelay = 327000",
                   "nrScans = 1",
                   "zf = 1",
                   "dwellTime = 200",
                   "tdPhaseCorr = \"none\"",
                   "fdPhaseCorr = \"autophase\"",
                   "saveData=\"false\""])


      # 8th volume
      NewDataFolder("C:\\$PATH$\\sub_sample_8\\$k$")
      r = RunExpt("1Pulse-H",
                  ["nrPnts = 8192",
                   "repTime = 3500",
                   "acqDelay = 20",
```

```
                    "nrScans = $Nscans$",
                    "zf = 1",
                    "dwellTime = 200",
                    "pulseLength1H = 11.5",
                    "tdPhaseCorr = \"none\"",
                    "fdPhaseCorr = \"autophase\"",
                    "saveData=\"true\""])

    r = RunExpt("move_tube_down",
                    ["nrPnts = 8192",
                    "repTime = 2500",
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                    "zf = 1",
                    "dwellTime = 200",
                    "tdPhaseCorr = \"none\"",
                    "fdPhaseCorr = \"autophase\"",
                    "saveData=\"false\""])

    # 9th volume
    NewDataFolder("C:\\$PATH$\\sub_sample_9\\$k$")
    r = RunExpt("1Pulse-H",
                    ["nrPnts = 8192",
                    "repTime = 3500",
                    "acqDelay = 20",
                    "nrScans = $Nscans$",
                    "zf = 1",
                    "dwellTime = 200",
                    "pulseLength1H = 11.5",
                    "tdPhaseCorr = \"none\"",
                    "fdPhaseCorr = \"autophase\"",
                    "saveData=\"true\""])


    r = RunExpt("move_tube_down",
                    ["nrPnts = 8192",
                    "repTime = 2500",
                    "acqDelay = 327000",
                    "nrScans = 1",
                    "zf = 1",
                    "dwellTime = 200",
                    "tdPhaseCorr = \"none\"",
                    "fdPhaseCorr = \"autophase\"",
                    "saveData=\"false\""])

    # 10th volume
    NewDataFolder("C:\\$PATH$\\sub_sample_10\\$k$")
    r = RunExpt("1Pulse-H",
                    ["nrPnts = 8192",
                    "repTime = 3500",
                    "acqDelay = 20",
                    "nrScans = $Nscans$",
                    "zf = 1",
                    "dwellTime = 200",
                    "pulseLength1H = 11.5",
                    "tdPhaseCorr = \"none\"",
                    "fdPhaseCorr = \"autophase\"",
```

```
␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣"saveData=\"true\""])

␣␣␣␣␣␣r␣=␣RunExpt("move_tube_down",
␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣["nrPnts␣=␣8192",
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␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣"dwellTime␣=␣200",
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␣␣␣␣␣␣#␣11th␣volume
␣␣␣␣␣␣NewDataFolder("C:\\$PATH$\\sub_sample_11\\$k$")
␣␣␣␣␣␣r␣=␣RunExpt("1Pulse-H",
␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣["nrPnts␣=␣8192",
␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣"repTime␣=␣3500",
␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣"acqDelay␣=␣20",
␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣"nrScans␣=␣$Nscans$",
␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣"zf␣=␣1",
␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣"dwellTime␣=␣200",
␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣"pulseLength1H␣=␣11.5",
␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣"tdPhaseCorr␣=␣\"none\"",
␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣"fdPhaseCorr␣=␣\"autophase\"",
␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣"saveData=\"true\""])

␣␣␣␣␣␣r␣=␣RunExpt("move_tube_down",
␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣["nrPnts␣=␣8192",
␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣"repTime␣=␣2500",
␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣"acqDelay␣=␣327000",
␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣"nrScans␣=␣1",
␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣"zf␣=␣1",
␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣"dwellTime␣=␣200",
␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣"tdPhaseCorr␣=␣\"none\"",
␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣"fdPhaseCorr␣=␣\"autophase\"",
␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣"saveData=\"false\""])

␣␣␣␣␣␣#␣12th␣volume
␣␣␣␣␣␣NewDataFolder("C:\\$PATH$\\sub_sample_12\\$k$")
␣␣␣␣␣␣r␣=␣RunExpt("1Pulse-H",
␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣["nrPnts␣=␣8192",
␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣"repTime␣=␣3500",
␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣"acqDelay␣=␣20",
␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣"nrScans␣=␣$Nscans$",
␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣"zf␣=␣1",
␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣"dwellTime␣=␣200",
␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣"pulseLength1H␣=␣11.5",
␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣"tdPhaseCorr␣=␣\"none\"",
␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣"fdPhaseCorr␣=␣\"autophase\"",
␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣"saveData=\"true\""])

␣␣␣␣␣␣r␣=␣RunExpt("move_tube_down",
␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣["nrPnts␣=␣8192",
␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣"repTime␣=␣2500",
␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣"acqDelay␣=␣327000",
␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣"nrScans␣=␣1",
```

```
                    "zf = 1",
                    "dwellTime = 200",
                    "tdPhaseCorr = \"none\"",
                    "fdPhaseCorr = \"autophase\"",
                    "saveData=\"false\""])

      #13th volume
      NewDataFolder("C:\\$PATH$\\sub_sample_13\\$k$")
      r = RunExpt("1Pulse-H",
                    ["nrPnts = 8192",
                    "repTime = 3500",
                    "acqDelay = 20",
                    "nrScans = $Nscans$",
                    "zf = 1",
                    "dwellTime = 200",
                    "pulseLength1H = 11.5",
                    "tdPhaseCorr = \"none\"",
                    "fdPhaseCorr = \"autophase\"",
                    "saveData=\"true\""])


      r = RunExpt("move_tube_down",
                    ["nrPnts = 8192",
                    "repTime = 2500",
                    "acqDelay = 327000",
                    "nrScans = 1",
                    "zf = 1",
                    "dwellTime = 200",
                    "tdPhaseCorr = \"none\"",
                    "fdPhaseCorr = \"autophase\"",
                    "saveData=\"false\""])


      #14th volume
      NewDataFolder("C:\\$PATH$\\sub_sample_14\\$k$")
      r = RunExpt("1Pulse-H",
                    ["nrPnts = 8192",
                    "repTime = 3500",
                    "acqDelay = 20",
                    "nrScans = $Nscans$",
                    "zf = 1",
                    "dwellTime = 200",
                    "pulseLength1H = 11.5",
                    "tdPhaseCorr = \"none\"",
                    "fdPhaseCorr = \"autophase\"",
                    "saveData=\"true\""])

      r = RunExpt("move_tube_down",
                    ["nrPnts = 8192",
                    "repTime = 2500",
                    "acqDelay = 327000",
                    "nrScans = 1",
                    "zf = 1",
                    "dwellTime = 200",
                    "tdPhaseCorr = \"none\"",
                    "fdPhaseCorr = \"autophase\"",
                    "saveData=\"false\""])
```

```
      # 15th volume
      NewDataFolder("C:\\$PATH$\\sub_sample_15\\$k$")
      r = RunExpt("1Pulse-H",
                  ["nrPnts = 8192",
                   "repTime = 3500",
                   "acqDelay = 20",
                   "nrScans = $Nscans$",
                   "zf = 1",
                   "dwellTime = 200",
                   "pulseLength1H = 11.5",
                   "tdPhaseCorr = \"none\"",
                   "fdPhaseCorr = \"autophase\"",
                   "saveData=\"true\""])

      r = RunExpt("move_tube_down",
                  ["nrPnts = 8192",
                   "repTime = 2500",
                   "acqDelay = 327000",
                   "nrScans = 1",
                   "zf = 1",
                   "dwellTime = 200",
                   "tdPhaseCorr = \"none\"",
                   "fdPhaseCorr = \"autophase\"",
                   "saveData=\"false\""])


      # 16th volume
      NewDataFolder("C:\\$PATH$\\sub_sample_16\\$k$")
      r = RunExpt("1Pulse-H",
                  ["nrPnts = 8192",
                   "repTime = 3500",
                   "acqDelay = 20",
                   "nrScans = $Nscans$",
                   "zf = 1",
                   "dwellTime = 200",
                   "pulseLength1H = 11.5",
                   "tdPhaseCorr = \"none\"",
                   "fdPhaseCorr = \"autophase\"",
                   "saveData=\"true\""])


      r = RunExpt("move_tube_up",
                  ["nrPnts = 8192",
                   "repTime = 2500",
                   "acqDelay = 20",
                   "nrScans = 1",
                   "zf = 1",
                   "dwellTime = 200",
                   "tdPhaseCorr = \"none\"",
                   "fdPhaseCorr = \"autophase\"",
                   "saveData=\"false\""])

      pause(20)

   next(k)
```

```
endproc()
```

Notes and references

[1] M. Wallace, D. J. Adams and J. A. Iggo, *Analytical Chemistry*, 2018, **90**, 4160–4166.

[2] T. D. Foundation, *LibreOffice Calc*, `https://www.libreoffice.org/discover/calc/`.

[3] M. A. Hass and F. A. Mulder, *Annual Review of Biophysics*, 2015, **44**, 53–75.