ACS Publications
MOST TRUSTED. MOST CITED. MOST READ.

NMR Guidelines for ACS Journals

Updated December 2013

1. NMR Text (Experimental Section)

1.1 The compound must be clearly identified, for example in a header at the beginning of a) the synthetic procedure or b) the summary of spectroscopic data.

1.2 List the nucleus being measured, any nucleus being broad-band decoupled, the solvent used (formula preferred, e.g. C_6D_6 over benzene-d_6), the standard used, and the field strength.

1.2.1 Field strength should be noted for each spectrum, not as a comment in the general experimental section.

1.2.2 The standard(s) may be specified in the general experimental section; as an example, ^{1}H NMR data recorded in C_6D_6 listed as "residual internal C_6D_5H (δ 7.15)".

1.2.3 Indicate solvent or peak suppression protocols used in collecting data.

1.3 List the probe temperature when it is accurately known; ambient probe temperature is otherwise understood.

1.4 Give ^{1}H NMR chemical shifts to two digits after the decimal point. Include the number of protons represented by the signal, peak multiplicity, and coupling constants as needed (*J* italicized, reported with up to one digit after the decimal).

1.4.1 The number of bonds through which the coupling is operative, ^xJ, may be specified by the author if known with a high degree of certainty.

1.4.2 Accepted abbreviations for multiplicities and descriptors are:

s = singlet	dd = doublet of doublets
d = doublet	dt = doublet of triplets
t = triplet	td = triplet of doublets
q = quartet	br = broad signal
quint = quintet	
m = multiplet (denotes complex pattern)	

1.5 Chemical shifts should be listed consistently in a single article, starting either from downfield to upfield or vice-versa. Please consult the Author Guidelines for preferred formatting for each journal.

1.6 Assign peak identities under the following circumstances:

1.6.1 Non-decoupled or equivalent spectra have been collected (^{13}C, ^{31}P, etc.).

1.6.1 2-D experiments have been performed.

1.6.2 Unambiguous assignment is possible without additional experiments, such as in the case of an organometallic metal-hydride ^{1}H signal, PF_6 vs. $MPPh_3$ ^{31}P signal, etc.

1.7 Give ^{13}C chemical shifts to one digit after the decimal point, unless an additional digit will help distinguish overlapping peaks.

1.7.1 Include peak multiplicities for ^{1}H-coupled ^{13}C NMR spectra, or for signals in ^{1}H-decoupled spectra that are coupled to other magnetically active nuclei.

1.7.2 A ^{13}C NMR signal will be considered a singlet if the multiplicity is not assigned.

1.7.3 Only rarely is a true multiplet observed in a $^{13}C\{^{1}H\}$ NMR spectrum. However, a certain region may contain a group of unresolved peaks or signals.

1.8 Mention of unobserved resonances is encouraged.

Example 1 (no 2-D data collected):

$(\eta^5\text{-}C_5Me_5Co)_2\text{-}\mu\text{-}(\eta^4\text{:}\eta^4\text{-}C_9H_{10})$ (**1**): ^{1}H NMR (C_6D_6, 400 MHz): δ -0.53 (s, 1H), 0.72 (d, 1H, *J* = 4.0 Hz), 0.98 (s, 1H), 1.58 (s, 15H), 1.62 (s, 3H), 1.73 (s, 15H), 1.95 (d, 1H, *J* = 4.0 Hz), 5.62 (t, 1H, *J* = 4.0 Hz), 6.00 (t, 1H, *J* = 4.0 Hz). $^{13}C\{^{1}H\}$ NMR (C_6D_6, 125 MHz): δ 10.2, 10.6, 17.4, 38.3, 51.5, 54.2, 60.6, 80.8, 81.0, 88.0, 88.7.

Example 2 (2-D data collected):

Silvestrol (**2**): ^{1}H NMR ($CDCl_3$ with 0.05% v/v TMS, 400 MHz): δ_H 7.10 (2H, d, *J* = 8.9 Hz, H2′ and H6′), 7.03-7.07 (3H, m, H3′′, H4′′ and H5′′), 6.83-6.85 (2H, m, H2′′ and H6′′), 6.66 (2H, d, *J* = 8.9 Hz, H3′ and H5′), 6.42 (1H, d, *J* = 1.8 Hz, H5), 6.26 (1H, d, *J* = 1.7 Hz, H7), 5.18 (1H, s, H1′′′), 5.01 (1H, d, *J* = 6.6 Hz, H1), 4.52 (1H, s, H2′′′), 4.27 (1H, d, *J* = 14.2 Hz, H3), 4.15 (1H, br d, *J* = 11.2 Hz, H4′′′), 4.05 (1H, t, *J* = 11.2 Hz, $H3_b$′′′), 3.88 (1H, *J* = 14.3, 6.8 Hz, H2), 3.86 (3H, s, $OCH_3$8), 3.69 (3H, s, $OCH_3$4′), 3.64 (3H, s, $COOCH_3$2), 3.49 (3H, br s, H5′′′ and H6′′′), 3.43-3.47 (1H, overlapped, $H3_a$′′′), 3.45 (3H, s, $OCH_3$2′′′). ^{13}C NMR ($CDCl_3$, 125 MHz): δ_C 170.6 (s, $\underline{CO}CH_3$2), 160.6 (s, C4a), 160.0 (s, C6), 158.8 (s, C4′), 157.1 (s, C8), 136.7 (s, C1′′), 129.0 (d, C2′ and C6′), 127.8 (d, C2′′, C3′′, C5′′ and C6′′), 126.6 (d, C4′′), 126.3 (s, C1′), 112.7 (d, C3′ and C5′), 109.6 (s, C8a), 101.9 (s, C3a), 95.2 (d, C2′′′), 94.0 (d, C1′′′), 93.9 (d, C7), 93.4 (s, C8b), 92.9 (d, C5), 79.7 (d, C1), 70.7 (d, C5′′′), 68.3 (d, C4′′′), 63.3 (t, C6′′′), 59.0 (t, C3′′′), 55.9 (q, $OCH_3$8), 55.1 (q, $OCH_3$4′), 55.0 (d, C3; q, $OCH_3$2′′′), 52.1 (q, $CO\underline{CH_3}$2), 50.3 (d, C2).

Note

Broad peaks between δ_H 1.5 to 3.0 ppm and at δ_H 3.79 ppm correspond to the protons of the OH groups on C-1, C-8, C-5′′′ and C-6′′′, which disappeared after D_2O exchange.

Example 3:

(*E,E*)-3,7,11-Trimethyl-2,6,10-dodecatrien-I-yl diphosphate (Farnesyl diphosphate, FPP, **3**): ^{1}H NMR (D_2O, 300 MHz): δ 1.61 (s, 6H), 1.68 (s, 3H), 1.72 (s, 3H), 2.17-1.99 (m, 8H), 4.45 (d of d, 2H, $J_{H,H}$ = 6 Hz, $J_{P,H}$ = 6 Hz), 5.23-5.15 (m, 2H), 5.46 (t, 1H, *J* = 6 Hz). ^{13}C NMR (D_2O, 75

MHz): δ 16.3, 16.6, 17.9, 25.9, 27.0, 27.2, 40.1, 40.2, 63.2, 120.5, 124.8, 125.1, 131.6, 135.9, 142.8. ^{31}P NMR (D_2O, 121.5 MHz): δ −6.56 (d, 1P, $J_{P,P}$ = 21.9 Hz), −9.89 (d, 1P, $J_{P,P}$ = 21.9 Hz).

2. NMR Spectra (Supporting Information)

Submission of spectra (.doc, .docx, .txt, .pdf, .tif) is strongly recommended for all new and/or key compounds. When submitting spectra, please consider the following guidelines:

2.1 A caption should be included on the spectrum, noting the nucleus being measured, the solvent (formula preferred, e.g. C_6D_6 over benzene-d_6) and the field strength.

2.2 A representation of the compound should be included on the spectrum – please use ChemDraw or a related program. The compound identifier used in the manuscript should be included.

2.3 The largest peak in the ^{1}H NMR spectrum should normally arise from the compound, not the solvent.

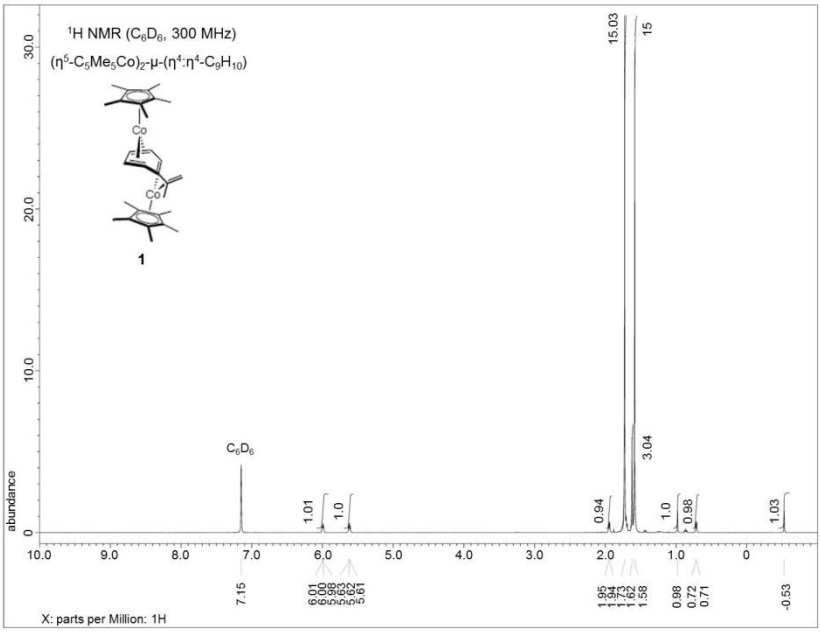
2.4 All peaks in the ^{1}H NMR spectrum should be integrated. Chemical shift values should be included.

2.5 The solvent peak should be clearly labeled on the spectrum.

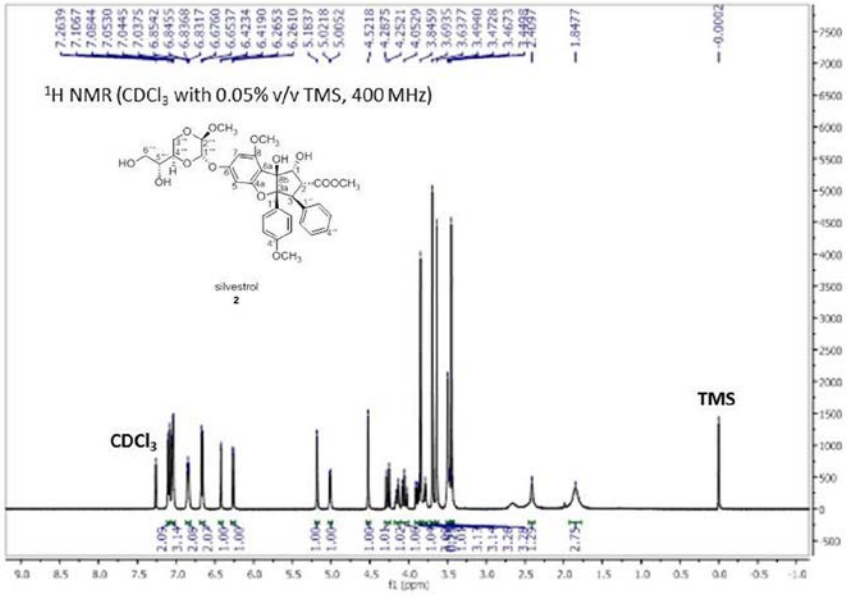
2.6 All peaks should be visible on the spectrum. Insets are encouraged to show expanded regions. At minimum, the spectral window should be -1 ppm to 9 ppm for ^{1}H NMR and -10 ppm to 180 ppm for ^{13}C NMR.

2.7 Font should be clear and large enough to read (minimum of 10 point). Horizontal orientation is preferred for spectra.

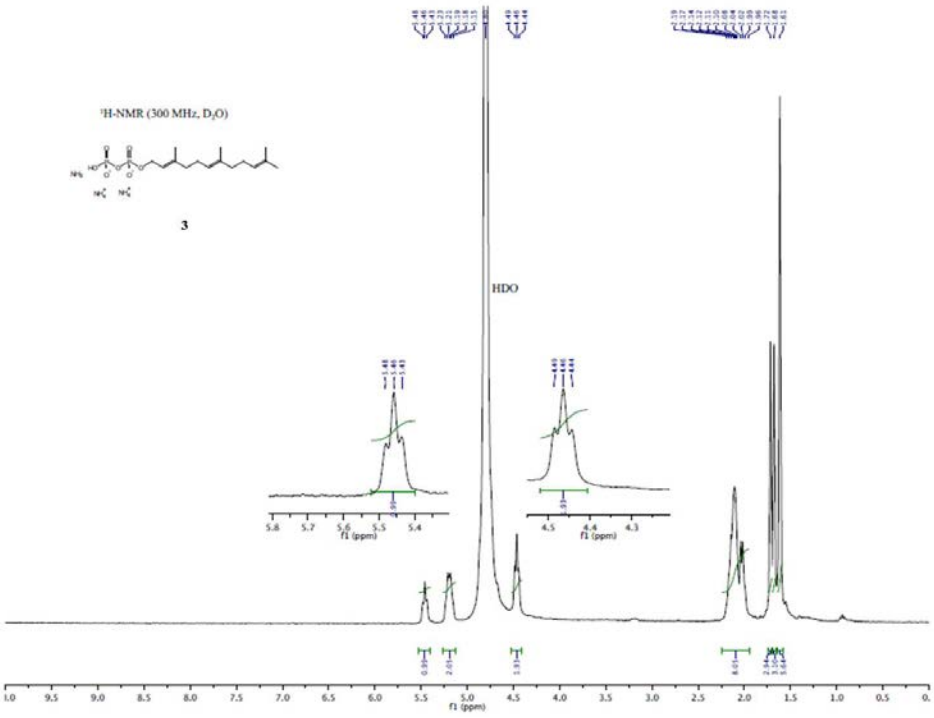
Example 1:

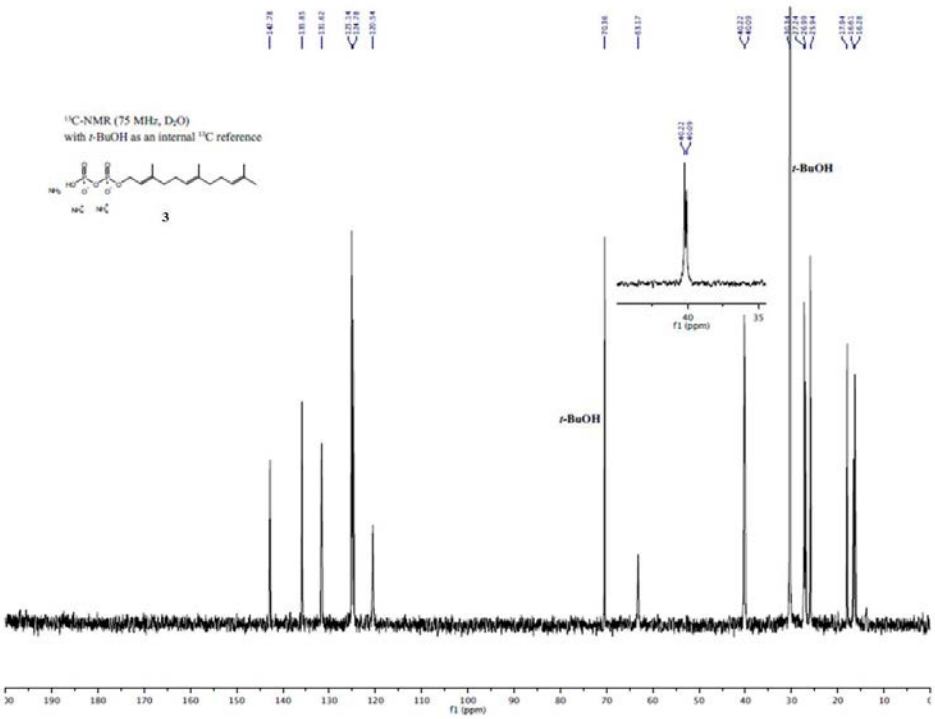


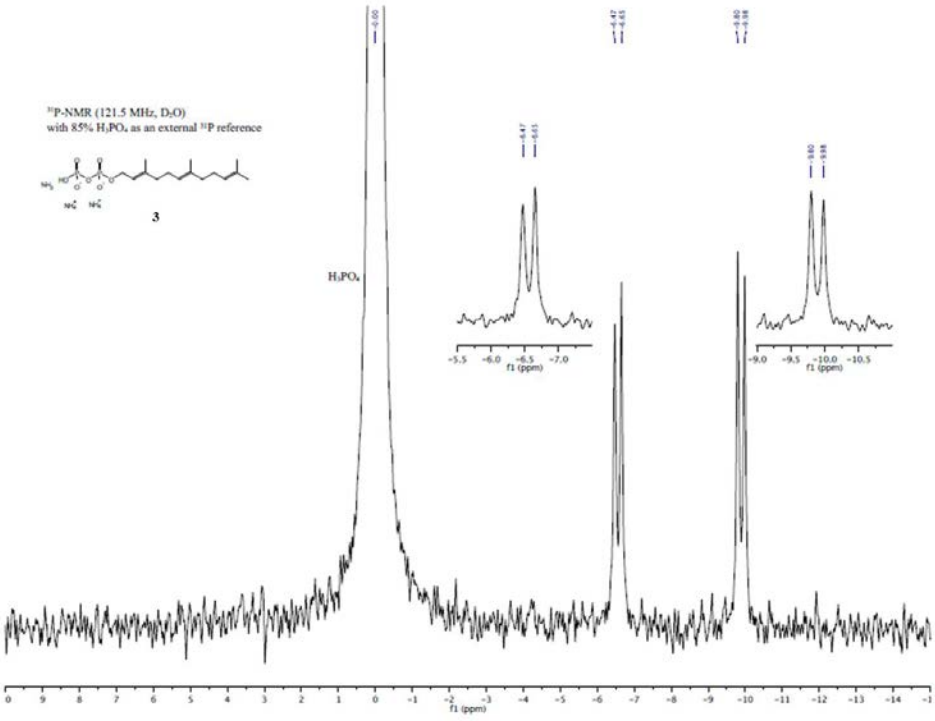
Example 2:



Example 3:




^{13}C-NMR (75 MHz, D_2O)
with *t*-BuOH as an internal ^{13}C reference
3
t-BuOH
t-BuOH
f1 (ppm)


^{31}P-NMR (121.5 MHz, D_2O)
with 85% H_3PO_4 as an external ^{31}P reference
3
H_3PO_4
f1 (ppm)