nature COMMUNICATIONS

Article | OPEN | Published: 01 August 2018

Optimal control theory enables homonuclear decoupling without Bloch–Siegert shifts in NMR spectroscopy

Paul W. Coote, Scott A. Robson, Abhinav Dubey, Andras Boeszoermenyi, Mengxia Zhao, Gerhard Wagner & Haribabu Arthanari ✉

Nature Communications **9**, Article number: 3014 (2018) | Download Citation ↓

INSTRUCTIONS:

You can download following from the website

a) Bruker pulse sequence trhncagp2h3d2_cops

b) the parameter file

c) the four shape pulses pulse GOODCOP (GC), BADCOP1 (BC1), BADCOP2 (BC2), and BADCOP3 (BC3).

Proceed by setting the experiment as Trosy-HNCA with accompanying pulse sequence, parameter file, and following additional parameters.

1. Enter the pulse duration for GC, BC1, BC2, or BC3 in p15 (from table below).
2. Enter the pulse name in sp10. The shape pulses GC, BC1, BC2 and BC3 should be in the folder /lists/wave/user/
3. The shaped pulse power in Decibels can be calculated by

$$20 \log_{10} \frac{TC}{\mathrm{TE}}$$

where TE is the calibrated carbon 90 degrees hard pulse duration, and TC is from the table. TE and TC both have units of microseconds. At different field strengths e.g. (B_0 MHz), TC is scaled by 800/B_0.

4. The shaped pulse duration T is given in the table below. At different field strengths (e.g. B_0 MHz), T is scaled by B_0/800.

Shaped pulse Name	Field strength (MHz)	Shaped pulse duration T (µs)	TC (µs)
GC	800	150	16.67
BC1	800	1000	42.07
BC2	800	1000	51.38
BC3	800	1000	34.61
GC	750	160	17.78
BC1	750	1066.7	44.87
BC2	750	1066.7	54.81
BC3	750	1066.7	36.92
GC	600	200	22.23
BC1	600	1333.3	56.09
BC2	600	1333.3	68.51
BC3	600	1333.3	46.15
GC	n.800	150 /n	16.67/n
BC1	n.800	1000/n	42.07/n
BC2	n.800	1000 /n	51.38/n
BC3	n.800	1000 /n	34.61/n

n scales between 800 MHz and an arbitrary field strength (n = 6/8 for 600 MHz, ⅝ for 500 MHz, etc).