SUPPORTING INFORMATION

AI-Designed RF Pulses Enable Fast Pulsing Heteronuclear Multiple Quantum Coherence NMR Experiment at High and Ultra-High Magnetic Fields

Manu Veliparambil Subrahmanian and Gianluigi Veglia*

Department of Biochemistry, Molecular Biology & Biophysics, and Department of Chemistry, University of Minnesota, Minneapolis, MN, 55455, USA. E-mail: vegli001@umn.edu

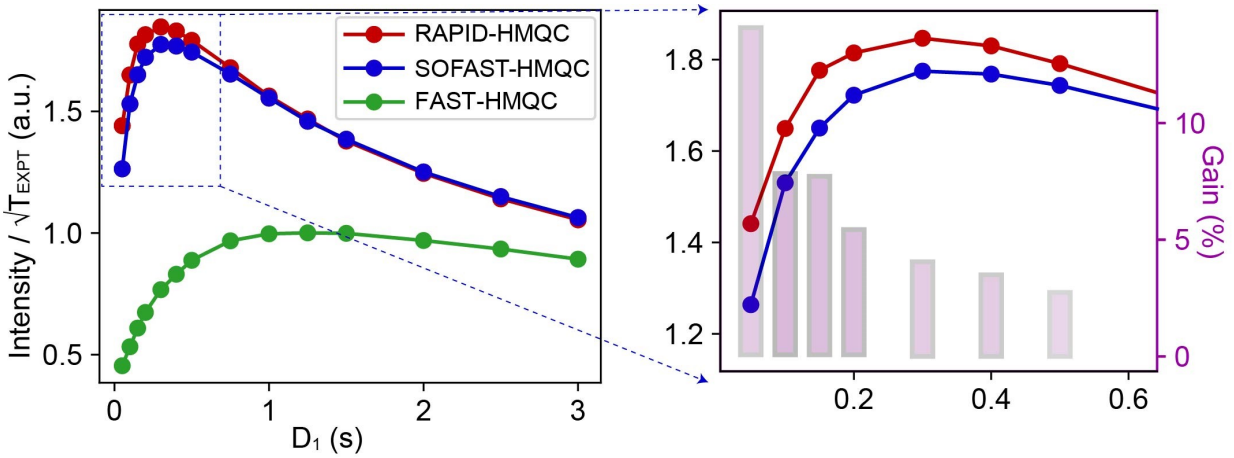

Figure S1. Performance of the RAPID-HMQC, SOFAST-HMQC, and Fast-HMQC experiment using Ernst angle pulses as a function of the interscan delay (D_1). The inset shows the percent gain of the RAPID-HMQC over the SOFAST-HMQC for short D_1 (0.1 – 0.5 sec).

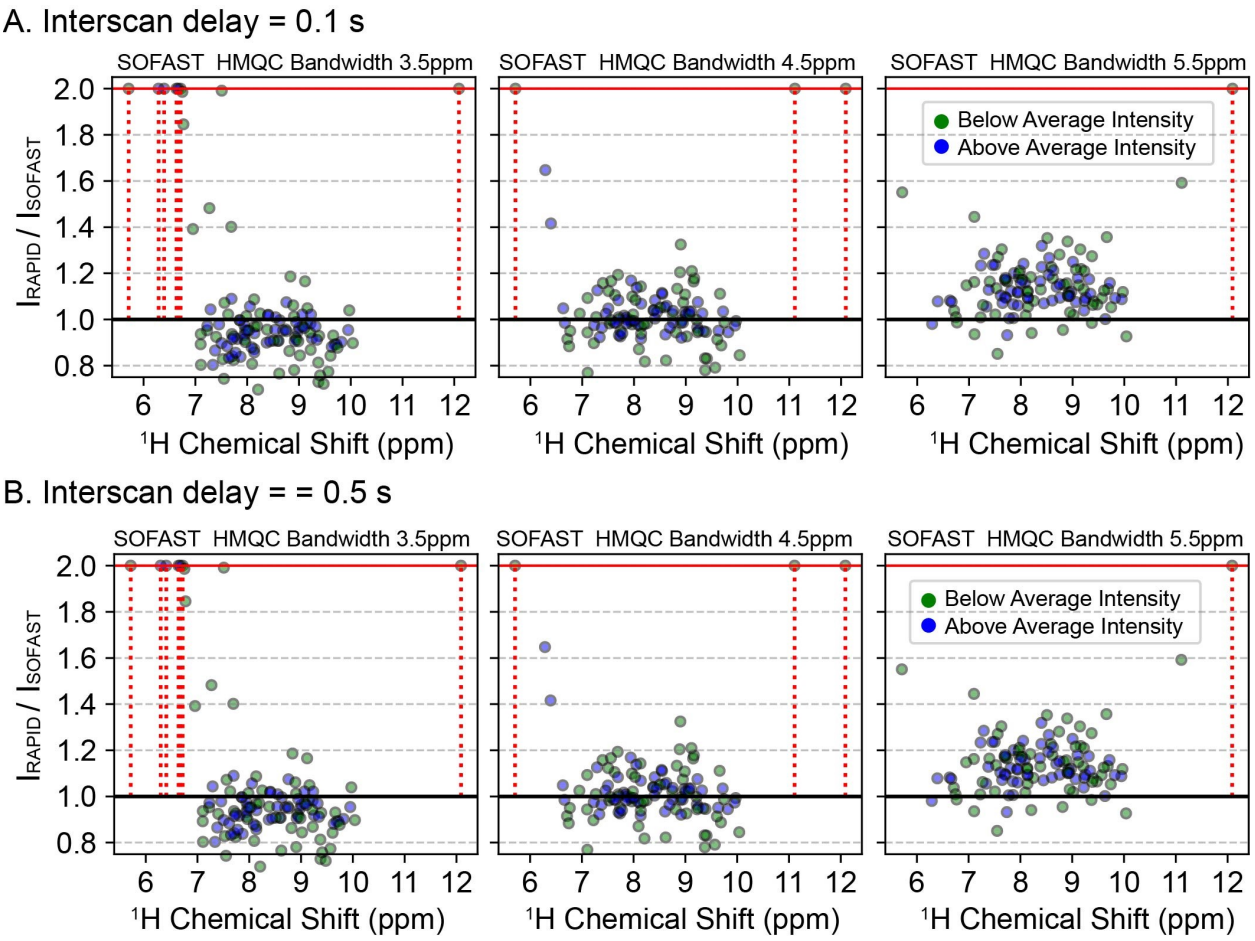

Figure S2: Comparison of the amide resonance intensities of the SOFAST-HMQC and RAPID-HMQC for 0.1 (a) and 0.5 (b) interscan delays (D_1), respectively. The SOFAST-HMQC experiment was run with band-selective pulses covering 3.5, 4.5, and 5.5 ppm bandwidths.

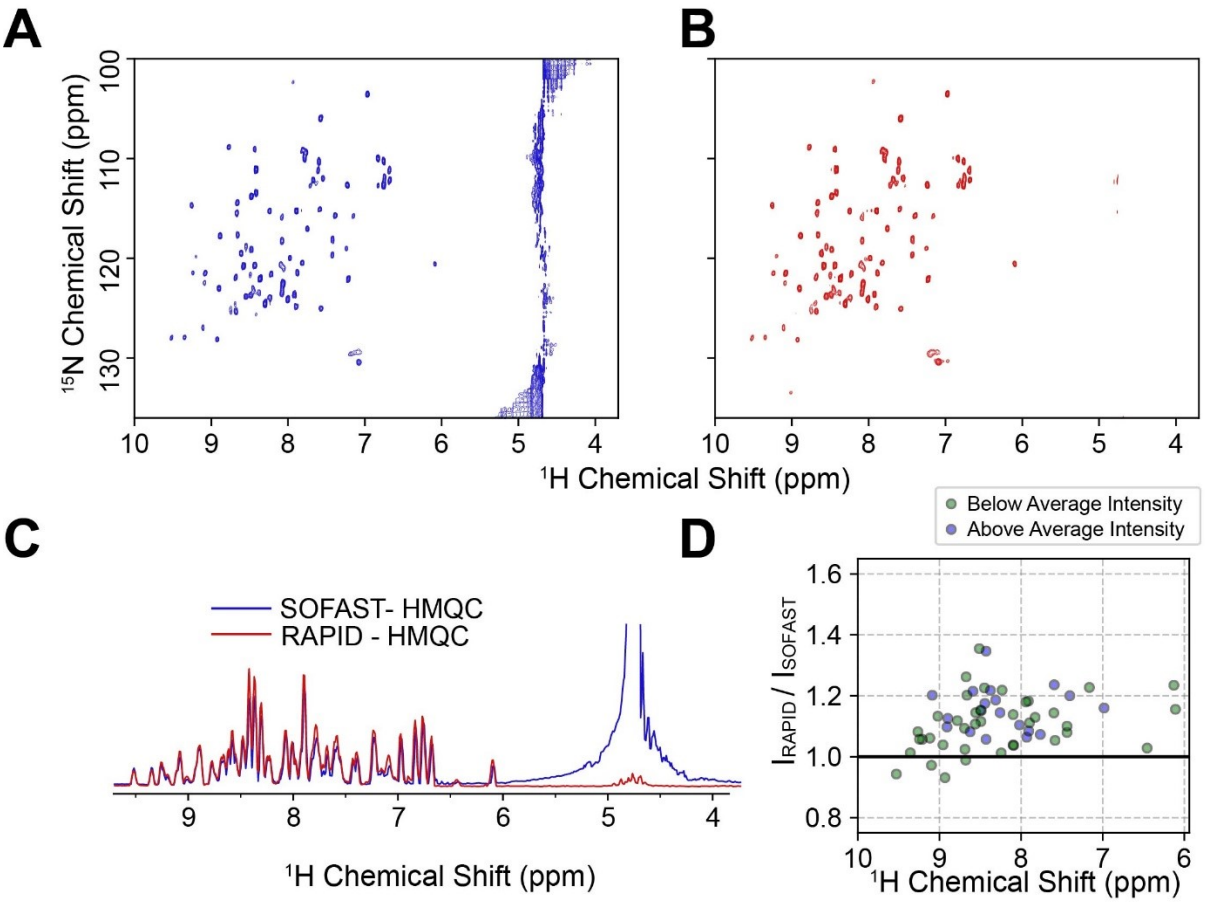

Figure S3: Comparison of the SOFAST-HMQC versus RAPID-HMQC experiments using a U-^{15}N labeled Ubiquitin (K48C mutant) sample of 0.5 mM. (a) 2D SOFAST-HMQC spectrum. (b) RAPID-HMQC spectrum, (c) comparison of the 1D ^{15}N-edited spectrum showing the quality of the water suppression. (d) Sensitivity gain expressed as intensity ratio of the resonances in the two experiments. Both experiments were acquired on a 900 MHz spectrometer with D_1 = 0.1 sec and a total experimental time of 15 sec. Eight dummy scans were used with 256 x 48 complex points in the direct and indirect dimensions, respectively. A sine-bell function with an offset of 0.1 was used to process the FIDs. The 2D matrices were zero filled to a final size of 512 x 256 complex points.

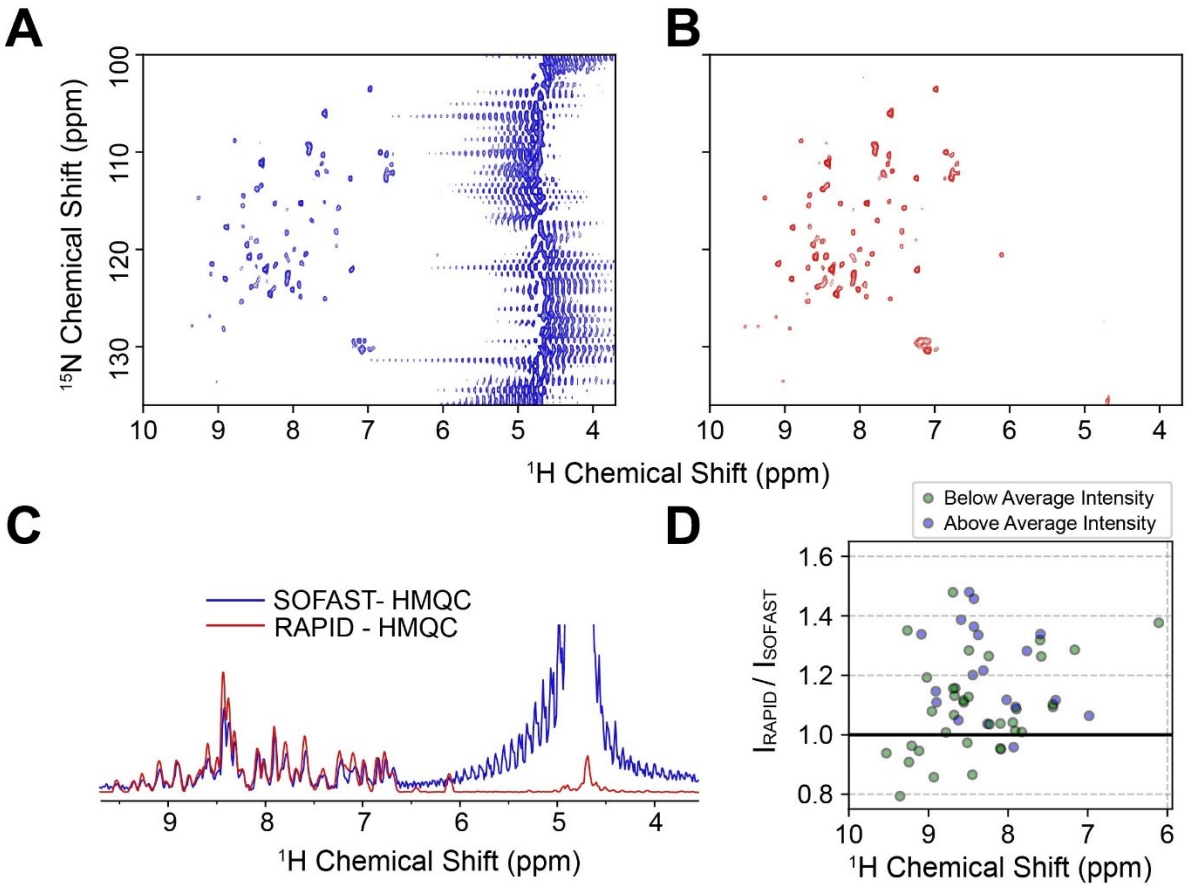

Figure S4: Comparison the SOFAST-HMQC versus RAPID-HMQC experiment tested on a U-^{15}N labeled Ubiquitin (K48C mutant) sample of 0.5 mM. Both experiments were acquired on a 900 MHz Bruker spectrometer with D_1 = 0.1 sec and a total experimental time of 6 sec. (a) 2D SOFAST-HMQC spectrum, (b) RAPID-HMQC spectrum, (c) comparison of the 1D ^{15}N edited spectrum showing the quality of the water suppression. (d) Sensitivity gain expressed as intensity ratio of the resonances in the two experiments. Eight dummy scans were used with 256 x 48 complex points in the direct and indirect dimensions, respectively. A sine-bell function with an offset of 0.1 was used to process the FIDs. The 2D matrices were zero filled for a final size of 512 x 256 complex points.

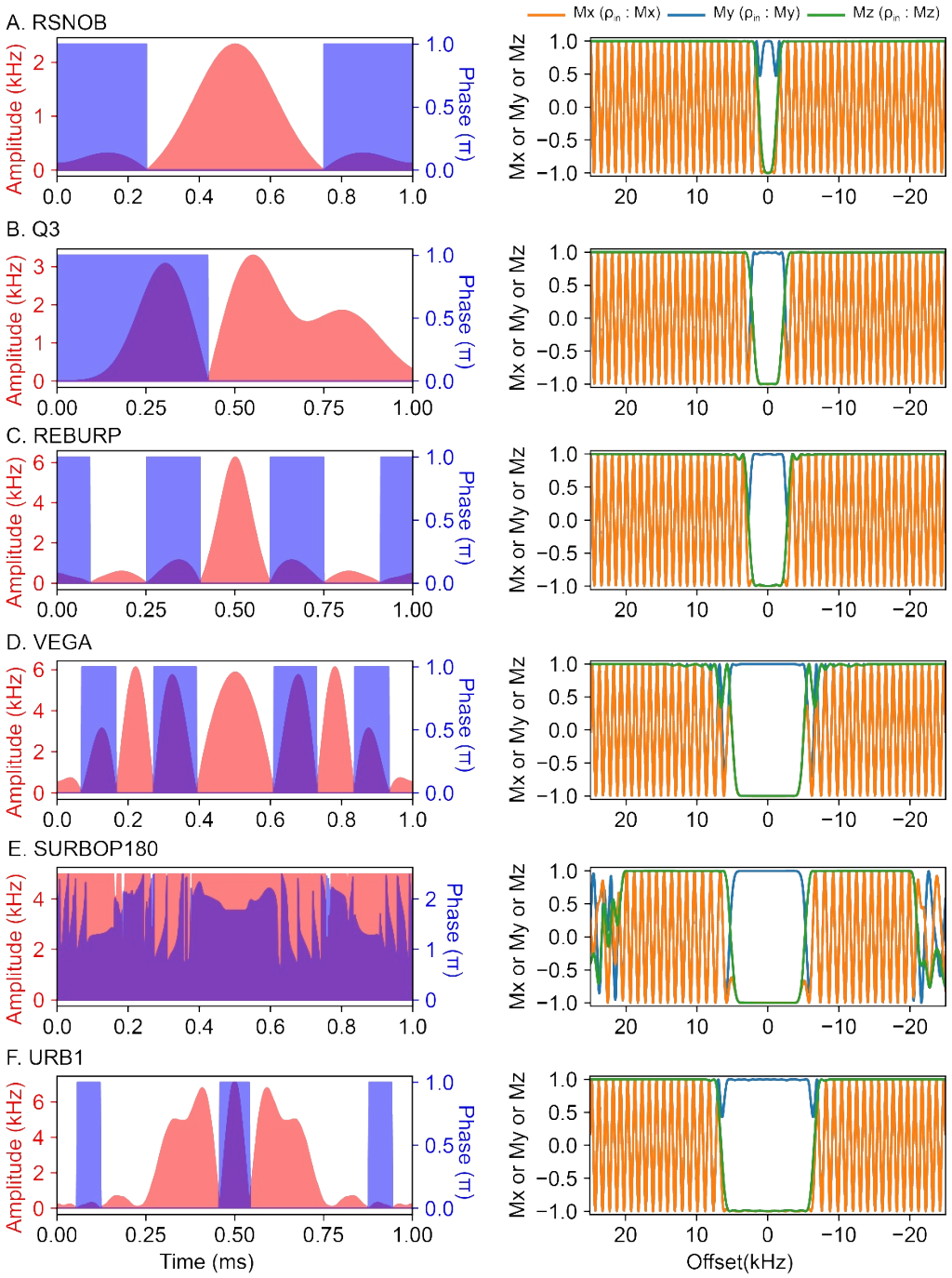

Figure S5. Numerical simulations of the most common band-selective refocusing pulses used in solution NMR spectroscopy (RSNOB, Q3, REBURP, VEGA, and SURBOP180) and our newly developed URB1 pulse. All pulse shapes were simulated with 1 ms pulse length. The pulses are organized based on increasing value of bandwidth covered. RSNOB covers a bandwidth of 1.1 kHz, Q3 2.8 kHz, REBURP 4.1 kHz, VEGA 8.5 kHz, SURBOP180 8.7 kHz, and URB1 11.4 kHz. Unlike, URB1, the VEGA response plot shows RF modulations at the edges of the bandwidth irradiated, and the SURBOP180 plot shows random RF modulations outside the irradiation bandwidth.