Figure S1. Comparison of the selectivity of water suppression by (a) SWET and (b) selective water preirradiation. The curves were simulated using the NMRSIM program in TOPSPIN and present the remaining z-magnetization after the two water suppression schemes. The SWET profile was approximated by a WET profile, simulating the selective pulses as continuous rectangular pulses rather than DANTE pulses and disregarding radiation damping effects. The profile was calculated by selecting the z-component of the magnetization after each of the four selective pulses, applied with flip-angles of 81.4, 101.4, 69.3 and 161.0 degrees and durations of 18.0, 22.4, 15.6 and 35.6 ms, respectively, followed by multiplication of the four profiles. The profile resulting from preirradiation was calculated by averaging ten profiles calculated for pulses of 1 s duration and amplitudes of 75.0, 75.1, 75.2, ..., 75.9 Hz, respectively, in order to simulate the radiofrequency inhomogeneity. 75 Hz was the experimentally determined field-strength required for adequate water suppression with a 100 μM solution of C-peptide in 90% H₂O/10% D₂O. A more accurate simulation of preirradiation would have to take into account the precise frequency distribution of the rf-field (Figure 1), the presence of radiation damping arising from steady-state magnetization after a number of dummy scans, and the $T_1$ and $T_2$ relaxation of the water magnetization during the irradiation. Several of these parameters are dependent on the sample and experimental parameters used. It is unlikely that such a simulation would change the overall conclusion that the selectivity of SWET is at least as good as that achieved by preirradiation. The selectivity of the SWET scheme could further be enhanced by the use of Seduce-shaped rather than rectangular pulse profiles as proposed for WET (Smallcombe et al., (1995) J. Magn. Reson. A, 117, 295-303).
Fig. S1
Figure S2. COSY spectra recorded of a 3.6 mM solution of hen egg-white lysozyme in 90% H₂O/10% D₂O at pH 7.0 and 25 °C. The spectra were recorded under identical conditions on a Bruker 800 MHz NMR spectrometer, except that different water suppression schemes were used. The common parameters were: $t_{1\text{max}} = 51$ ms and $t_{2\text{max}} = 102$ ms, 16 scans per FID, sweep widths of 10000 Hz in both dimensions, recycle delay 1.1 s (excluding the acquisition time but including the water suppression period by selective water irradiation or SWET, respectively), and selective water irradiation during the evolution time with an amplitude of 15 Hz. The water signal was reduced by subtraction of a 5th order polynomial from each FID and the dispersive tails of the diagonal peaks were minimized by multiplication of the data with an unshifted sine-bell window function in both dimensions prior to Fourier transformation. No baseline correction was applied after Fourier transformation. In both spectra the contours were plotted at the same heights, using an exponential scale with a factor of 1.4 between subsequent contour levels. (a) Overview of the COSY spectrum recorded with water suppression by preirradiation during 1 s immediately prior to the first 90° pulse with an amplitude of 40 Hz. (b) Overview of the COSY spectrum recorded with water suppression by SWET during the 96 ms immediately prior to the first 90° pulse with an average irradiation amplitude of 15 Hz. The pulse sequence of Fig. 2 was used. (c) and (d) Expansions of the spectra shown in (a) and (b), respectively. The position of the water resonance in the indirect dimension is indicated by an arrow. Water suppression by SWET resulted in less attenuation of the $\text{H}^\alpha$-$\text{H}^\text{N}$ cross-peaks at chemical shifts near the water resonance and less saturation transfer to some of the $\text{H}^\alpha$ resonances at other chemical shifts.
Fig. S2
Fig. S2(c)

Fig. S2(d)