Supporting information

A High Resolution Solid State NMR Approach for Structural Studies of Bicelles

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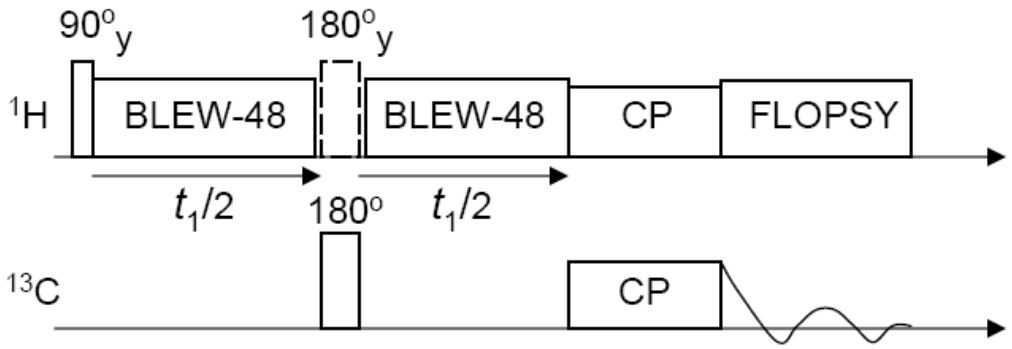
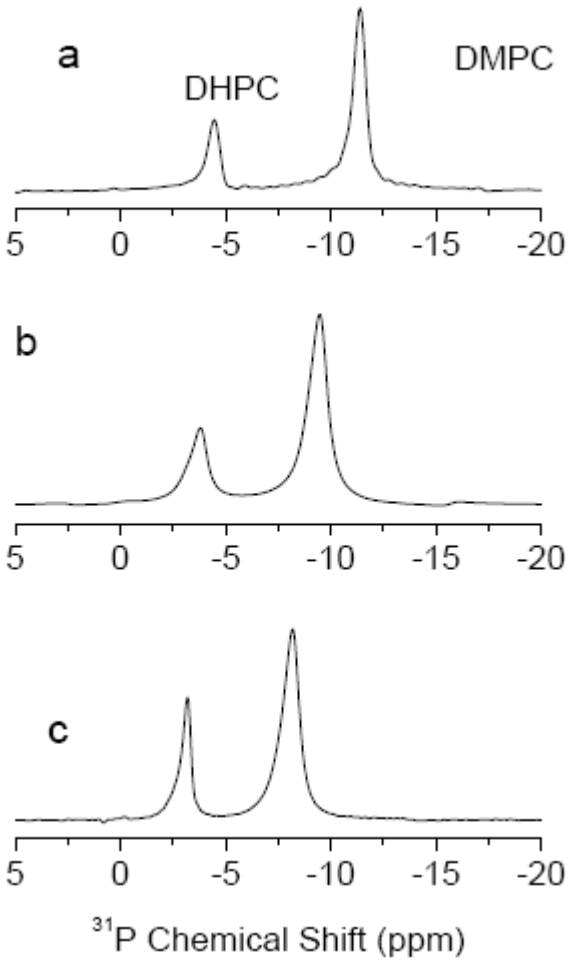
A. Pulse sequence



2D pulse sequence employed in the measurement of $^{13}C–^{1}H$, $^{13}C–^{31}P$ and $^{1}H–^{31}P$ dipolar couplings. In the t_1 period, proton magnetization evolves in the presence of homonuclear proton decoupling sequence BLEW48. After the cross polarization from proton to carbon, the ^{13}C signal is recorded in the presence of proton decoupling by the FLOPSY sequence. In the PDLF experiment with the two simultaneous 180^0 pulses, in the middle of the evolution period (t_1), $^{1}H–^{31}P$, $^{13}C–^{31}P$ couplings and ^{1}H chemical shift are suppressed while the $^{13}C–^{1}H$ dipolar splittings are obtained in the indirect dimension. On the other hand, in the absence of the proton 180^0 pulse, the ^{13}C-^{1}H interactions are refocused while the $^{1}H–^{31}P$ dipolar coupling and ^{1}H chemical shift are present in the indirect dimension. In both cases the dipolar spectra in the indirect dimension are correlated to the ^{13}C chemical shift and ^{13}C-^{31}P dipolar couplings in the direct dimension.

B. ^{31}P chemical shift spectra of bicelles



^{31}P NMR spectra of bicelle samples with different concentrations of MSI-78 peptide: a) 0 mole %, b) 0.5 mole % and c) 2.0 mole % MSI-78. Spectra were obtained by acquiring the FID after a 90^0 rf pulse in the presence of 10 kHz proton decoupling. 64 transients were accumulated with a recycle delay of 3 s. The chemical shift scale was referenced by setting the isotropic peak observed at 10°C to 0 ppm.