Sequence-specific resonance assignment of soluble non-globular proteins by 7D APSY-NMR spectroscopy

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Supplementary Material

Selection of projection angles. The selection of projection angles for the three APSY-NMR experiments recorded in this work with urea-denatured OmpX was guided by three principal considerations. (i) For the complete set of projections used in a given experiment, the sampled angles should be distributed evenly in the space of all possible projection angles, subject to practical limitations imposed by (ii) and (iii). (ii) Since the sensitivity for the recording of the 2D projection spectra is proportional to $2^{-q/2}$, where q is the number of projection angles that differ from 0° or 90°, projections with large q-values are disfavoured. (iii) The C^{β} position has a large chemical shift dispersion in denatured proteins, when compared to the backbone nuclei. In the 5D APSY-HNCOCACB and 7D APSY-seq-HNCO(CA)CBCANH experiments, "dispersion-optimized projection angles" were therefore used to accommodate this situation. These angles project the sweep widths of different correlated indirect dimensions to the same size. The complete sets of projection angles used are listed in the tables ST1 to ST3.

Table ST1. Projection angles used to record a set of 60 2D projections for the 5D APSY-HNCOCACB experiment with urea-denatured OmpX.

α	β	γ
± 35°	0°	0°
0°	0°	± 75°
0°	± 82°	0°
90°	± 84°	0°
0°	90°	± 35°
90°	0°	± 82°
0°	0°	90°
0°	90°	0°
90°	0°	0°
0°	0°	0°
0°	± 82°	± 60°
± 35°	0°	± 60°
± 35°	± 66°	0°
90°	± 84°	± 66°
± 35°	± 66°	± 50°
0°	0°	± 32°
0°	± 41°	0°
± 70°	0°	0°
90°	0°	± 41°

$$\begin{vmatrix} 90° & \pm 42° & 0° \\ 0° & 90° & \pm 17° \\ 0° & \pm 41° & \pm 60° \\ 0° & \pm 82° & \pm 30° \end{vmatrix}$$

Table ST2. Projection angles used to record a set of 40 2D projections for the 6D APSY-seq-HNCOCANH experiment with urea-denatured OmpX.

α	β	γ	δ
90°	± 45°	0°	0°
0°	0°	90°	± 45°
± 45°	0°	0°	0°
0°	0°	0°	90°
0°	0°	± 45°	0°
90°	0°	0°	0°
0°	90°	0°	0°
0°	± 45°	0°	± 45°
0°	0°	0°	0°
0°	± 45°	± 45°	0°
90°	± 45°	± 45°	0°
± 50°	0°	± 40°	± 25°
90°	± 50°	± 40°	± 25°

Table ST3. Projection angles used to record a set of 100 2D projections for the 7D APSY-seq-HNCO(CA)CBCANH experiment with urea-denatured OmpX.

α	β	γ	δ	ε
0°	0°	0°	0°	90°
0°	0°	0°	90°	0°
0°	0°	90°	0°	0°
0°	90°	0°	0°	0°
90°	0°	0°	0°	0°
0°	0°	0°	0°	0°
0°	0°	90°	± 31°	0°
0°	90°	0°	± 80°	0°
90°	0°	0°	0°	± 84°
90°	0°	0°	± 77°	0°
0°	0°	± 59.3°	0°	0°
0°	± 9.5°	0°	0°	0°
± 13°	0°	0°	0°	0°
0°	90°	0°	± 80.5°	± 66.3°
0°	90°	± 84.3°	± 30.6°	0°
90°	0°	± 82.2°	± 30.5°	0°
90°	± 36°	0°	± 74°	0°
90°	± 36°	± 80.4°	0°	0°
0°	0°	0°	± 45°	± 58.6°

0°	0°	± 59.3°	± 27.1°	0°
0°	± 9.5°	0°	± 44.6°	0°
0°	± 9.5°	± 58.9°	0°	0°
± 13°	0°	0°	± 44.3°	0°
± 13°	± 9.3°	0°	0°	0°
0°	0°	90°	0°	± 27°
90°	0°	0°	0°	± 42°
0°	0°	0°	0°	± 33°
0°	0°	± 30°	0°	0°
90°	0°	0°	± 38°	± 33°
90°	0°	± 41°	0°	± 27°
90°	± 63°	0°	0°	± 41°
0°	0°	0°	± 23°	± 29°
0°	0°	± 30°	0°	± 25°
± 52°	0°	0°	0°	± 33°
0°	0°	90°	± 15°	0°