## Supplementary Figure S1.



**Supplementary Fig. S1.** Histogram showing weighted average chemical shift changes  $(\Delta\delta(N,H)_{av} = [(\Delta\delta_{NH})^2 + (\Delta\delta_N/5)^2]^{1/2})$  for kurtoxin amide resonances between in presence and absence of CD<sub>3</sub>CN. The solid and dotted lines indicate the average value (0.06) and average plus one standard deviation value (0.11) of all residues of kurtoxin, respectively.

## **Supplementary Figure S2.**



**Supplementary Fig. S2.** Summary of the sequential and medium range NOE connectivities,  ${}^{3}J_{\text{NH-C}\alpha\text{H}}$  coupling constants, and slowly exchanging backbone NH protons observed in kurtoxin. These structural parameters were used for sequence-specific assignments and for identification of secondary structural elements. The sequential and medium range NOEs  $d_{\text{NN}}$ ,  $d_{\alpha\text{N}}$ ,  $d_{\beta\text{N}}$ ,  $d_{\text{NN}}(i, i+2)$ ,  $d_{\alpha\text{N}}(i, i+2)$ ,  $d_{\alpha\text{N}}(i, i+3)$  and  $d_{\alpha\beta}$  (*i*, *i*+3) are indicated by bars between two residues. The classification of NOEs as strong, medium or weak is indicated by the height of the filled bars. Values of the  ${}^{3}J_{\text{NH-C}\alpha\text{H}}$  coupling constants are indicated by  $\uparrow (\geq 8 \text{ Hz})$  and  $\downarrow (\leq 5.5 \text{ Hz})$ . Filled circles indicate backbone amide protons that were still observed in the TOCSY spectra after 25 h in D<sub>2</sub>O. The chemical shift index is indicated by a ternary index with a value of -1, 0 or +1. Values of -1 and +1 indicate a shift deviation from the random-coil value of greater than 0.1 p.p.m. upfield and downfield, respectively; those within the range of the random-coil values are given a value of 0.

## **Supplementary Figure S3.**



Supplementary Fig. S3. Schematic diagram of anti-parallel  $\beta$ -sheet structure of kurtoxin. Red dotted lines and blue dotted arrows indicate interstrand hydrogen bond and interstrand NOEs, respectively. The residues number is labeled on the C $\alpha$  atoms.