Supporting Material

A Second Look at Mini-Protein Stability: Analysis of FSD-1 using CD, DSC and Simulations

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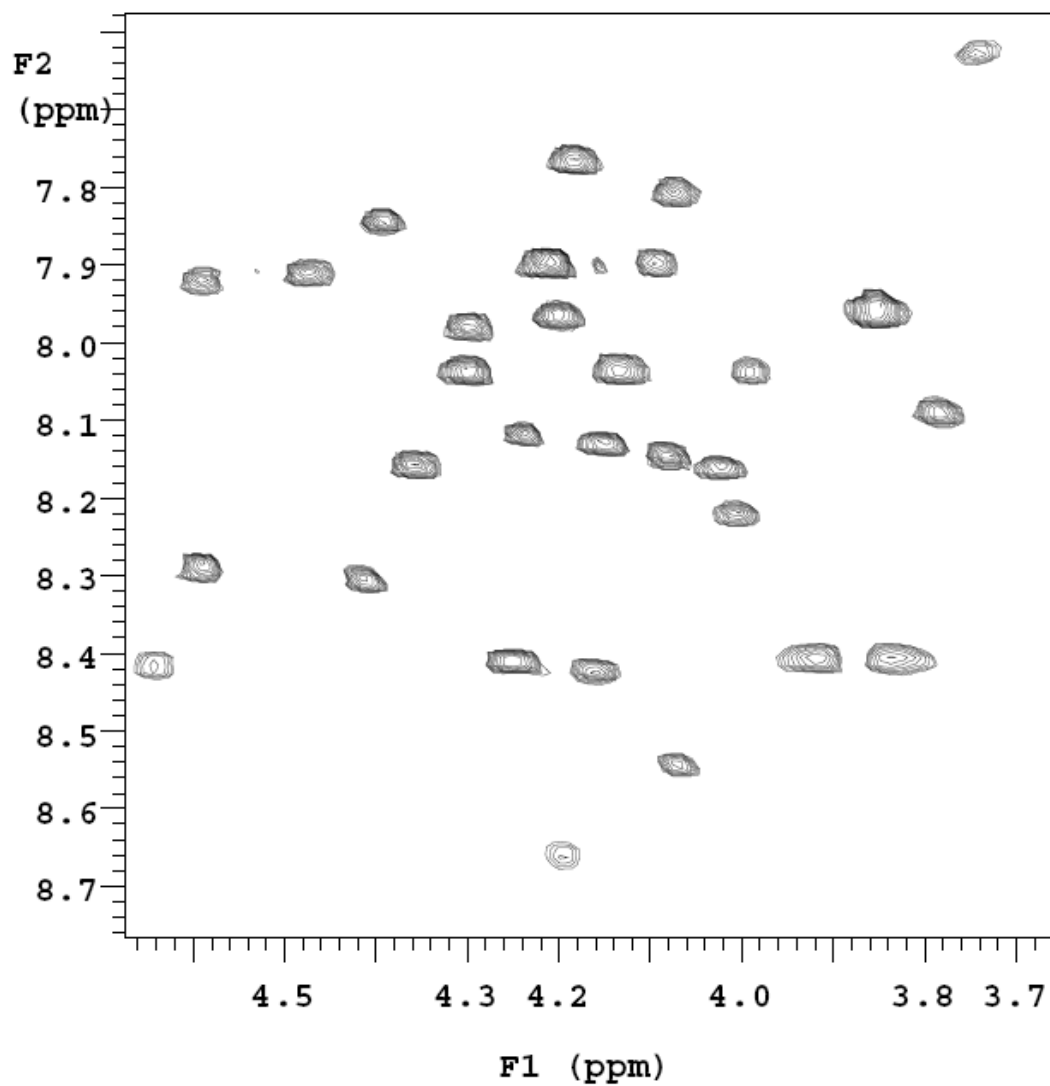E-mail addresses: jafeng@artsci.wustl.edu (JAF), kao@wustl.edu (JK)

Figure S1. TOCSY H$^{\alpha}$-NH fingerprint NMR spectra of FSD-1 at 25 $^{\circ}$C. The cross peaks correspond to 27 unique amino acids.

NMR spectra were recorded with a Varian Inova-600 (Varian Inc., Palo Alto, CA) spectrometer and the data were processed with VNMR software. NMR samples (~2mM) were prepared in H_2O-D_2O (90:10/v:v) with 50 mM sodium phosphate at pH 5.0 (uncorrected glass electrode). The spectra was collected at 25 ^{o}C. The total correlation (TOCSY) spectra were recorded using an MELV-17 mixing sequence of 80 ms flanked by two 2 ms trim pulses. Phase-sensitive 2D spectra were obtained by employing the hypercomplex method. A total of 2 x 256 x 2048 data matrixes with 16 scans per t1 increment were collected. Gaussian and sine-bell apodization functions were used in weighting the t2 and t1 dimensions, respectively. After two-dimensional Fourier transformation, the 2048 x 2048 frequency domain representation was phase and baseline corrected in both dimensions.