

J-9308-m1

## Supplementary material

The figure S1 shows a 2D HNNCA spectrum obtained with a scheme derived from the *ct*-HNNCA pulse sequence of Grzsiak & Bax,<sup>20</sup> using the same sample and the same experimental conditions as described in Fig.1. A Bruker AMX 600 spectrometer equipped with four channels was used. 140 ( $t_1$ ) \* 512 ( $t_2$ ) complex points were accumulated, with  $t_{1max}({}^{15}\text{N}, {}^{13}\text{C}^\alpha) = 11.4$  ms and  $t_{2max}({}^1\text{H}^{\text{N}}) = 65$  ms. 192 scans per increment were acquired, resulting in a total measuring time of 17 hours. Phase-sensitive detection was achieved using States-TPPI<sup>16</sup> in  $t_1$ , so that peaks are observed at  $\Omega({}^{15}\text{N}) \pm \Omega({}^{13}\text{C}^\alpha)$  along the frequency axis  $\omega_1$ . Since in this experiment the chemical shift of  ${}^{13}\text{C}^\alpha$  is not recorded in a phase-sensitive manner, the carrier of the pulses applied to  ${}^{13}\text{C}^\alpha$  was set to the edge of the spectral range covered by the  ${}^{13}\text{C}^\alpha$ -resonances in order to allow unambiguous assignments. The water signal was reduced by a purge pulse (see Fig. 2) and with the convolution method of Marion *et al.*<sup>21</sup>. The digital resolution after zero-filling was 24 Hz along  $\omega_1$  and 7.6 Hz along  $\omega_2$ . Prior to Fourier transformation the data were multiplied with a cosine window in  $t_1$  and a sine window shifted by  $45^\circ$  in  $t_2$ .<sup>22</sup> The spectrum was processed using the program PROSA.<sup>23</sup> (A) Contour plot. The peaks at the  $\omega_2$  amide proton frequency of Ile 38 are connected with a vertical line. (B) Cross section along  $\omega_1$  at  $\omega_2({}^1\text{H}^{\text{N}})$  of Ile 38. Four peaks are observed in this cross section: one pair of peaks (solid arrow) represents the intraresidual connectivity between  ${}^{15}\text{N}$  and  ${}^{13}\text{C}^\alpha$  of residue Ile 38, the other one (dotted arrow) the sequential  ${}^{15}\text{N}_i$ - ${}^{13}\text{C}^\alpha_{i-1}$  connectivity between Asp 37 and Ile 38. The  ${}^{13}\text{C}^\alpha$  chemical shifts of Asp 37 (11.8 ppm) and Ile 38 (25.2 ppm) are relative to the  ${}^{13}\text{C}$  carrier position (40.1 ppm). The  ${}^{15}\text{N}$  chemical shift of Ile 38 (120.4 ppm), around which the pairs of peaks are centered, is indicated by a vertical arrow.

"Reduced Dimensionality in Triple-Resonance NMR experiments"

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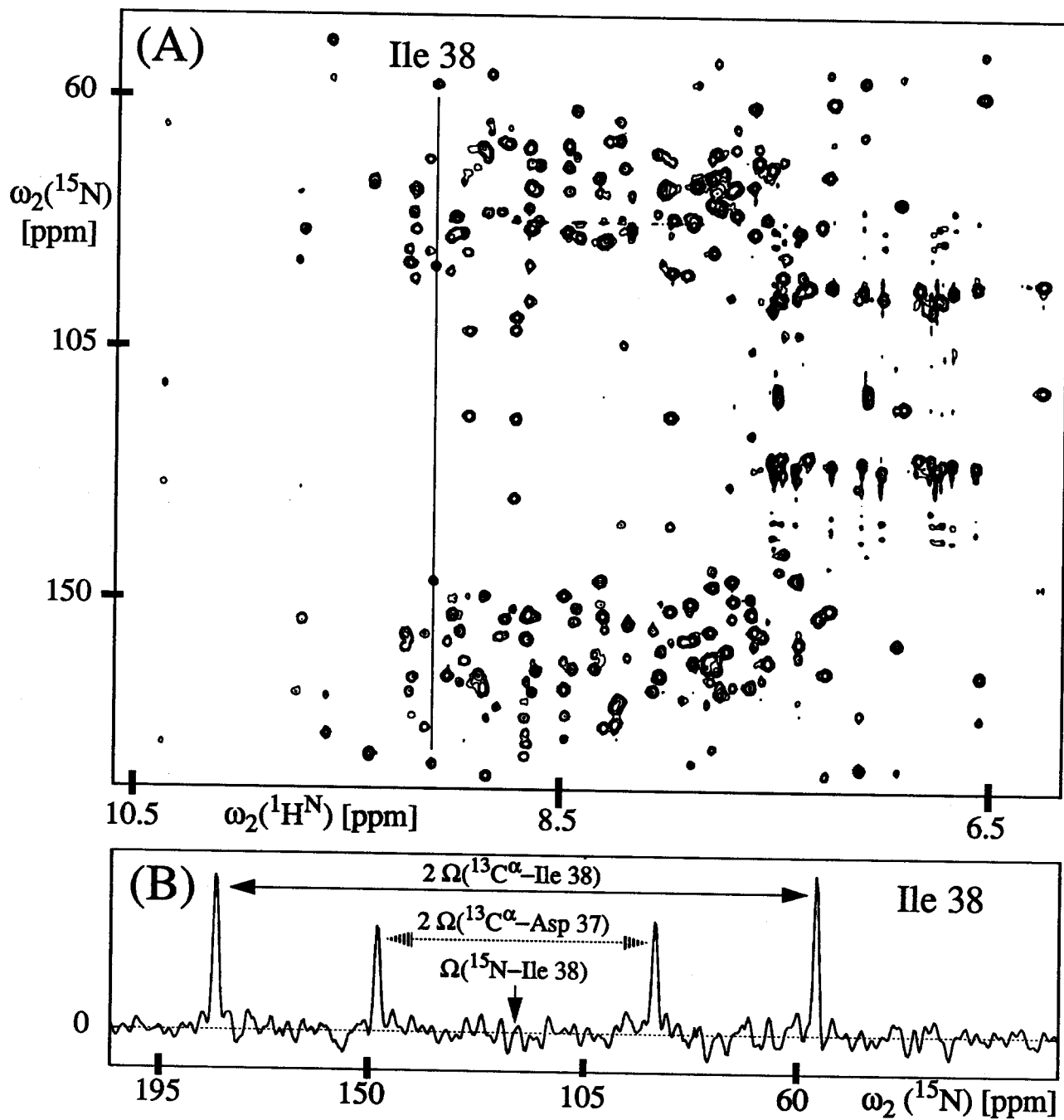


Fig. S1