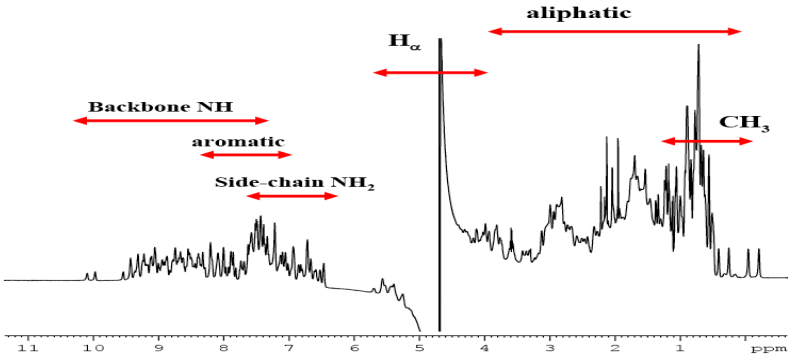
2D ^{15}N HSQC spectrum

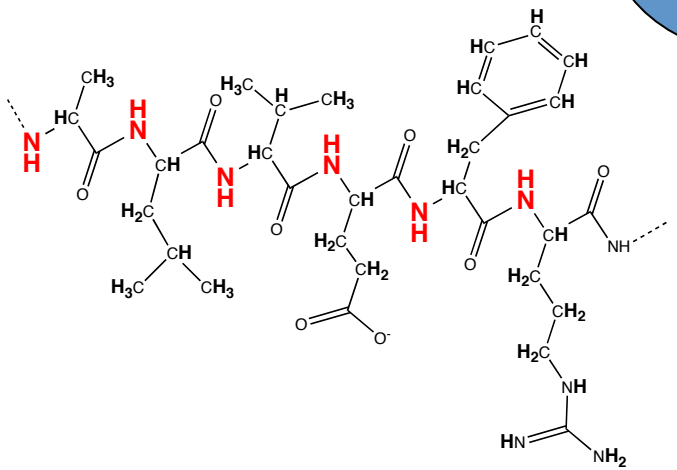


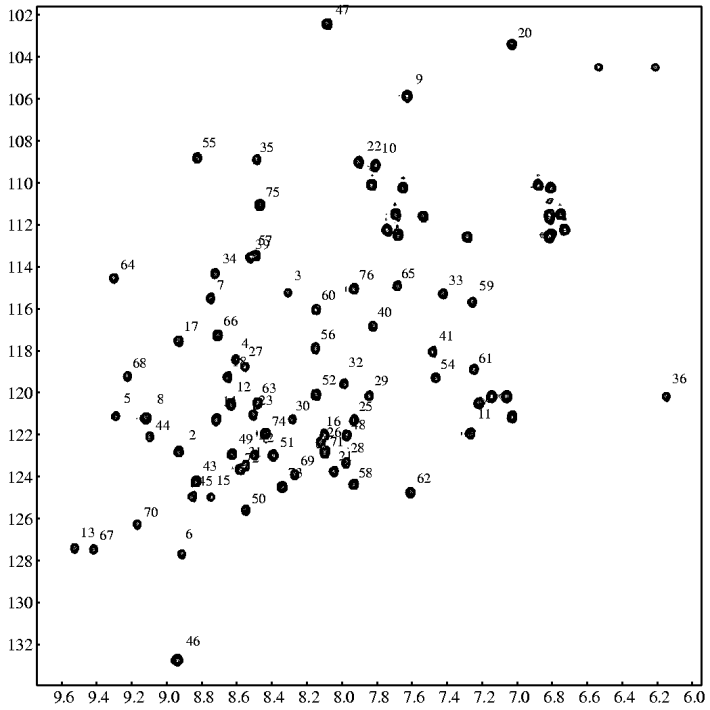
^{1}H

- Selection of ^{1}H bound to ^{15}N

(covalent H-N bond)

- Chemical shift evolution ^{1}H and ^{15}N

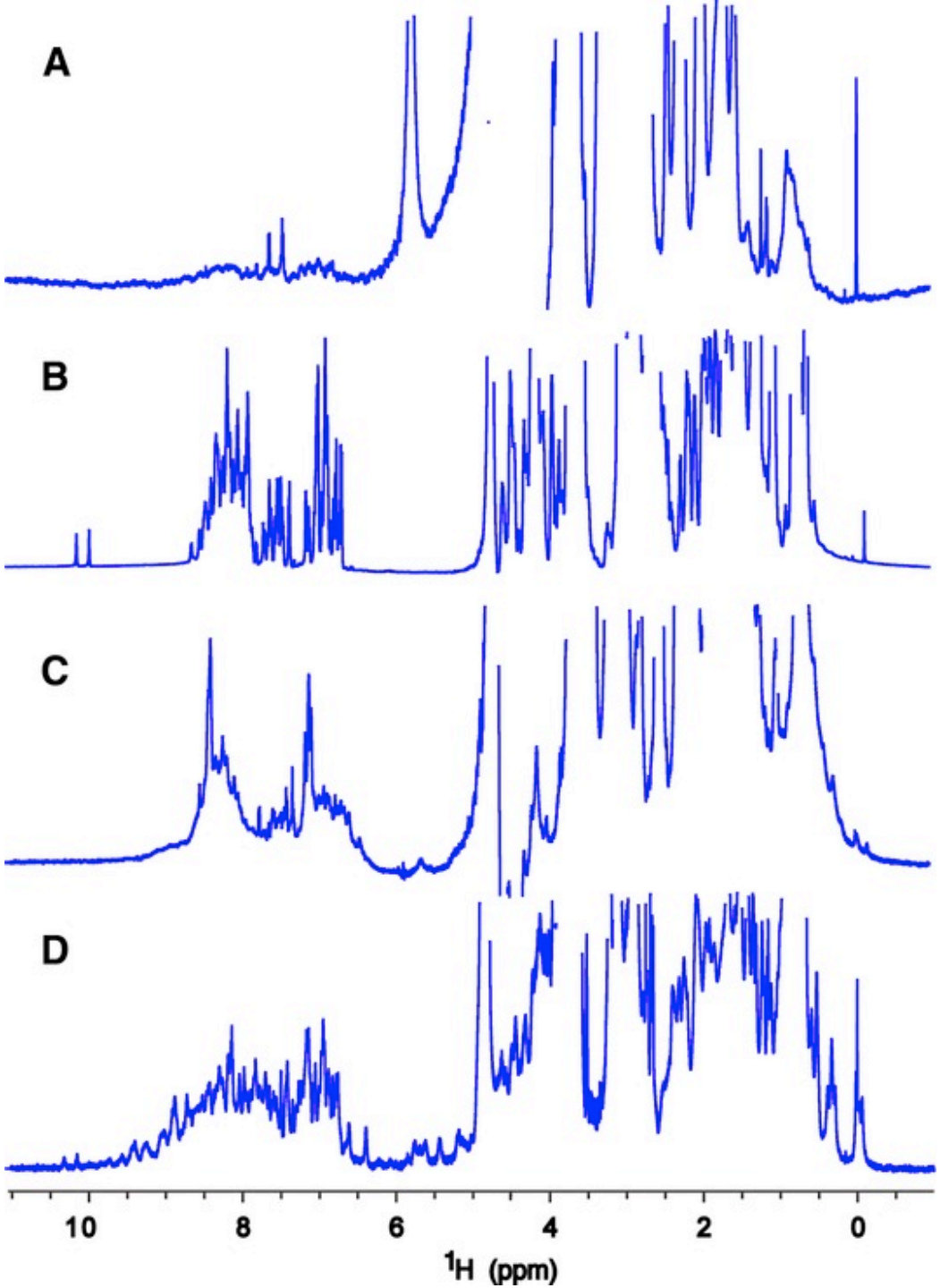




^{15}N (ppm)

^{1}H (ppm)

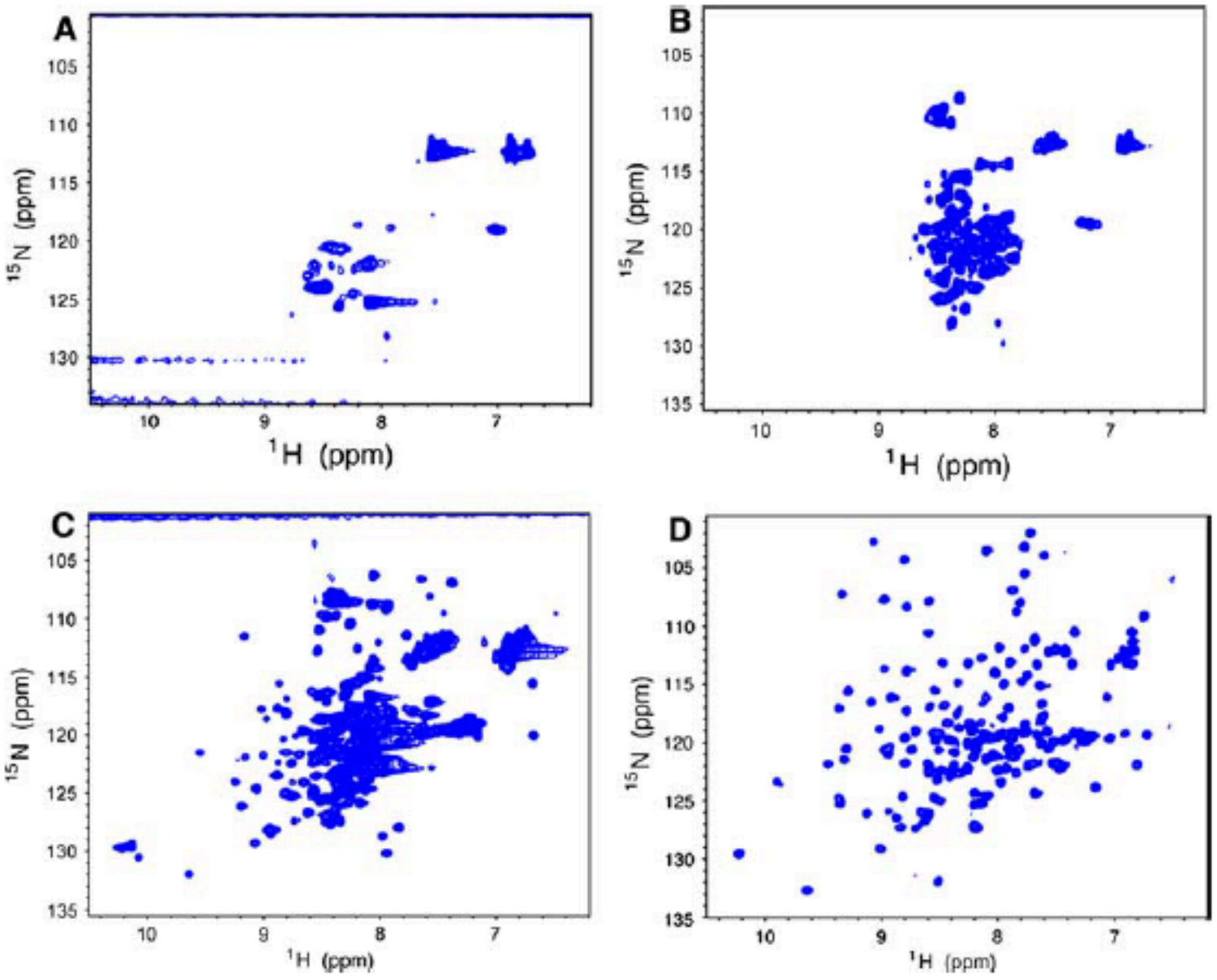
NMR spectrum and protein folding



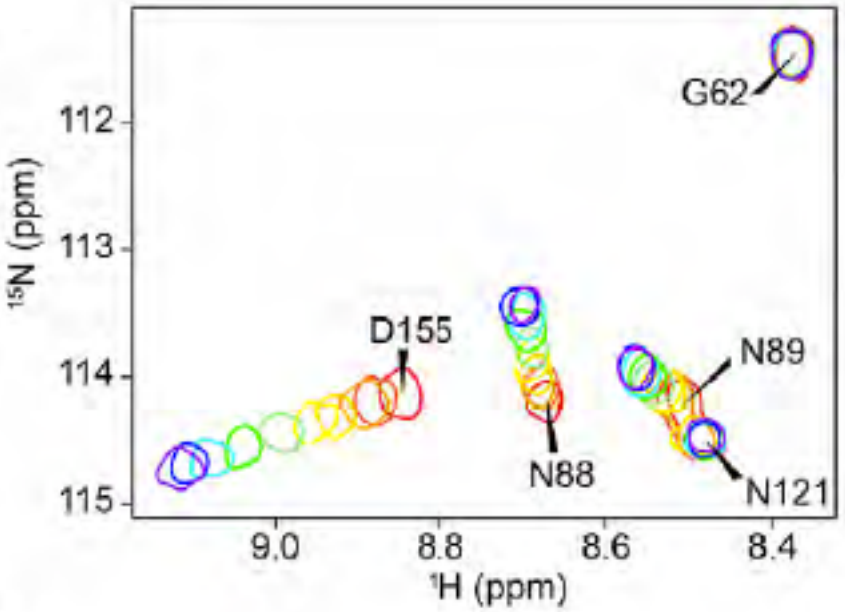
1D ^{1}H NMR spectra with H_2O presaturation of representative NESG targets obtained with a 1.7-mm micro NMR cryoprobe at 20°C with corresponding NESG target IDs. **A** HR3159A spectrum scores as "poor" on account of broad poorly dispersed resonances. **B** LmR69A spectrum scores "unfolded" due to sharp and poorly dispersed peaks in all regions. **C** EwR71A spectrum scores as "promising" with the presence of upfield-shifted methyl peaks but crowding of the amide region (7–9 ppm), and relatively broad peaks. **D** NsR431C spectrum scores "good" with sharp uniform intensity and upfield-shifted methyls

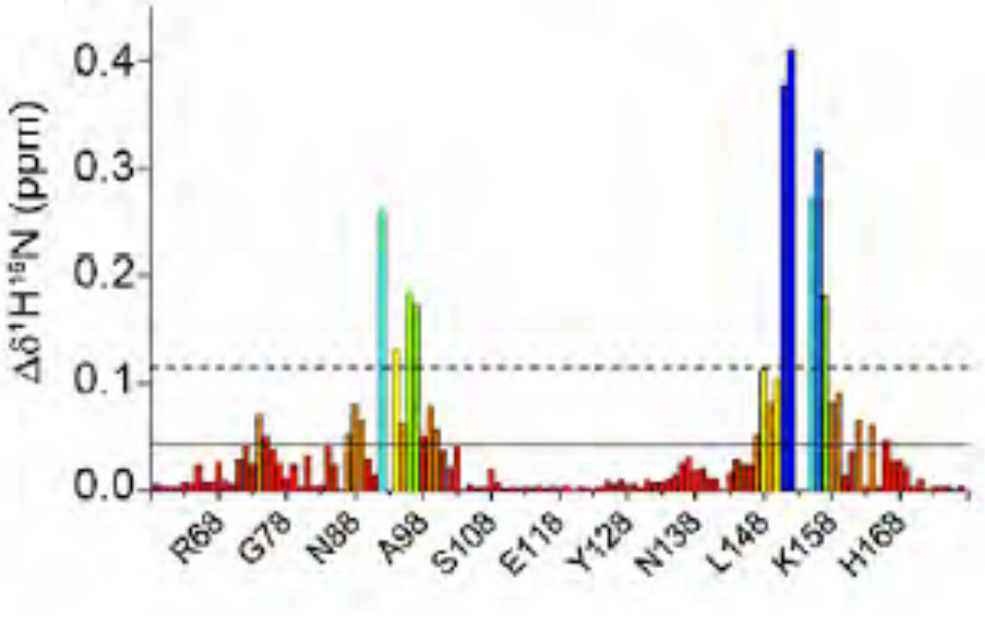
Rossi P. *et al.*
J. Biomol. NMR, **2009**,
46, 11-22

2D ^{15}N HSQC spectra

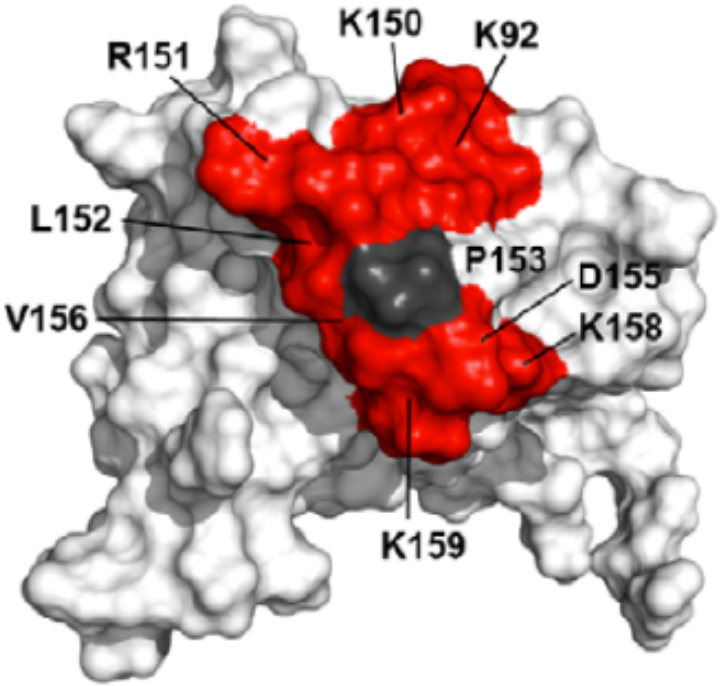


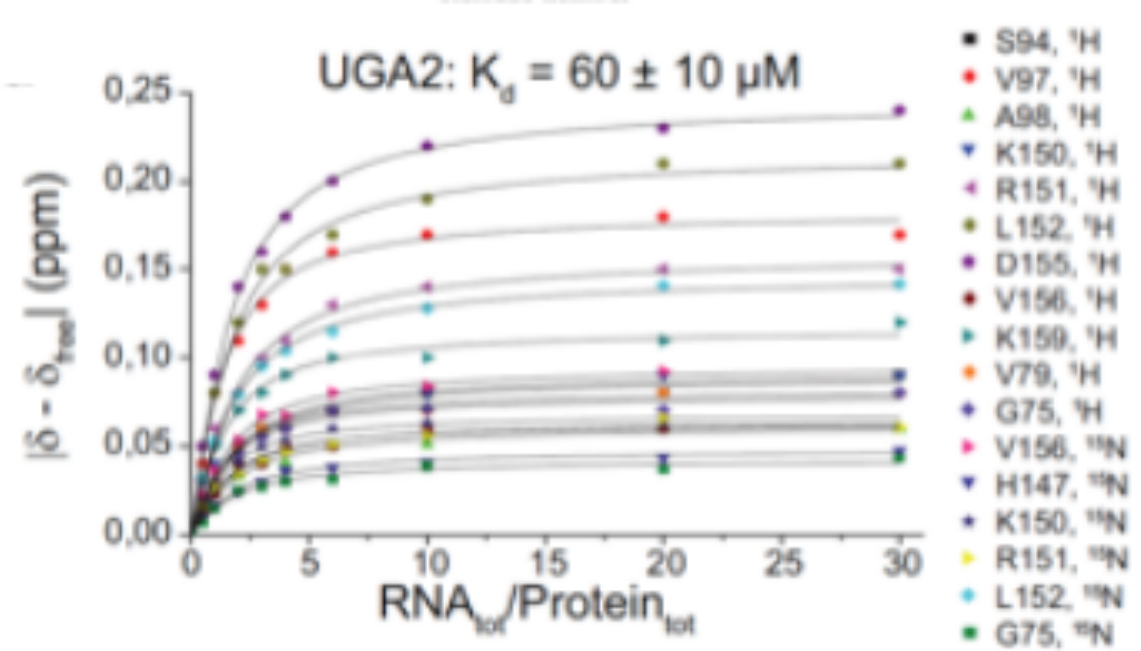
Following a binding event to extract Kd



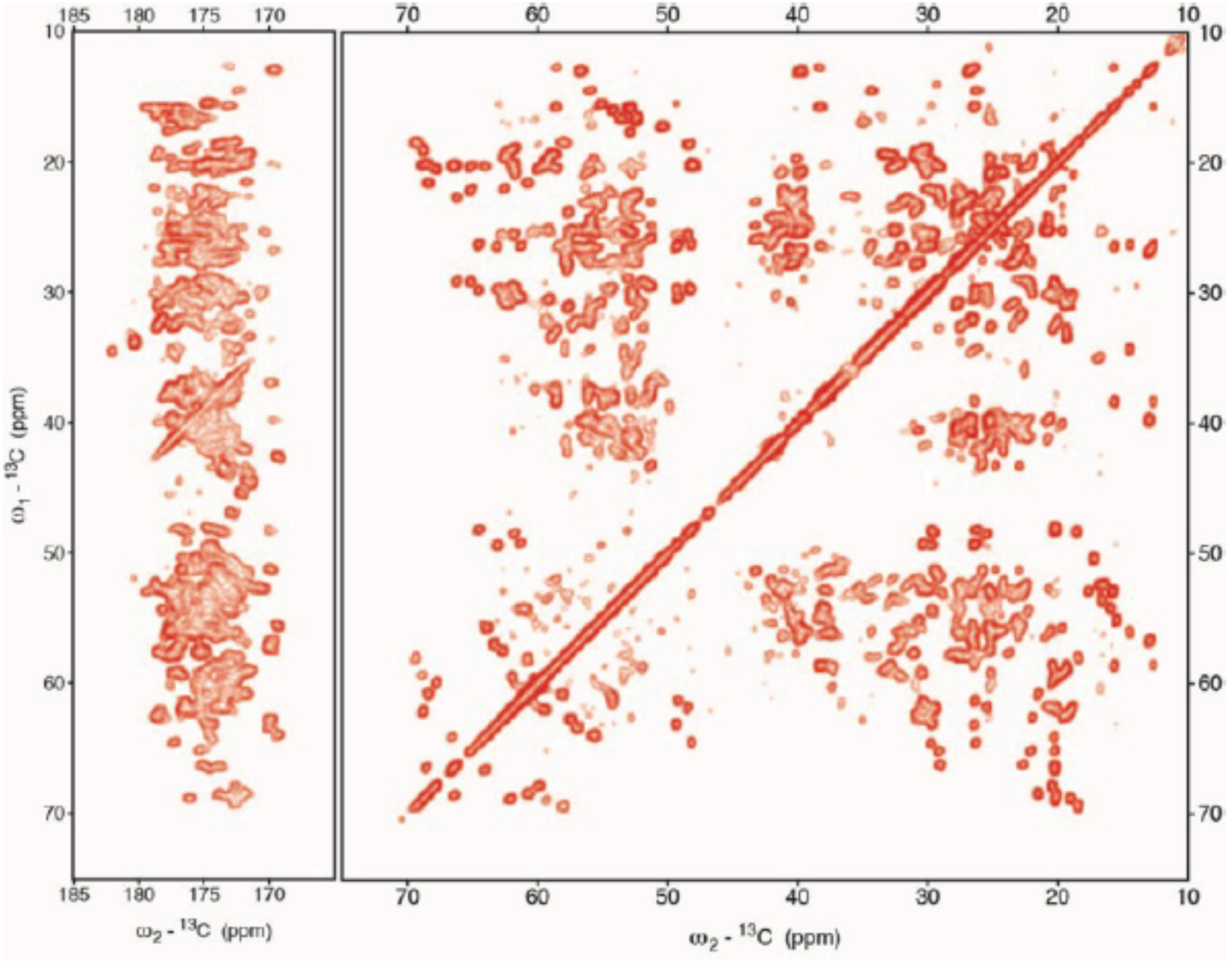


Following a binding event to extract Kd

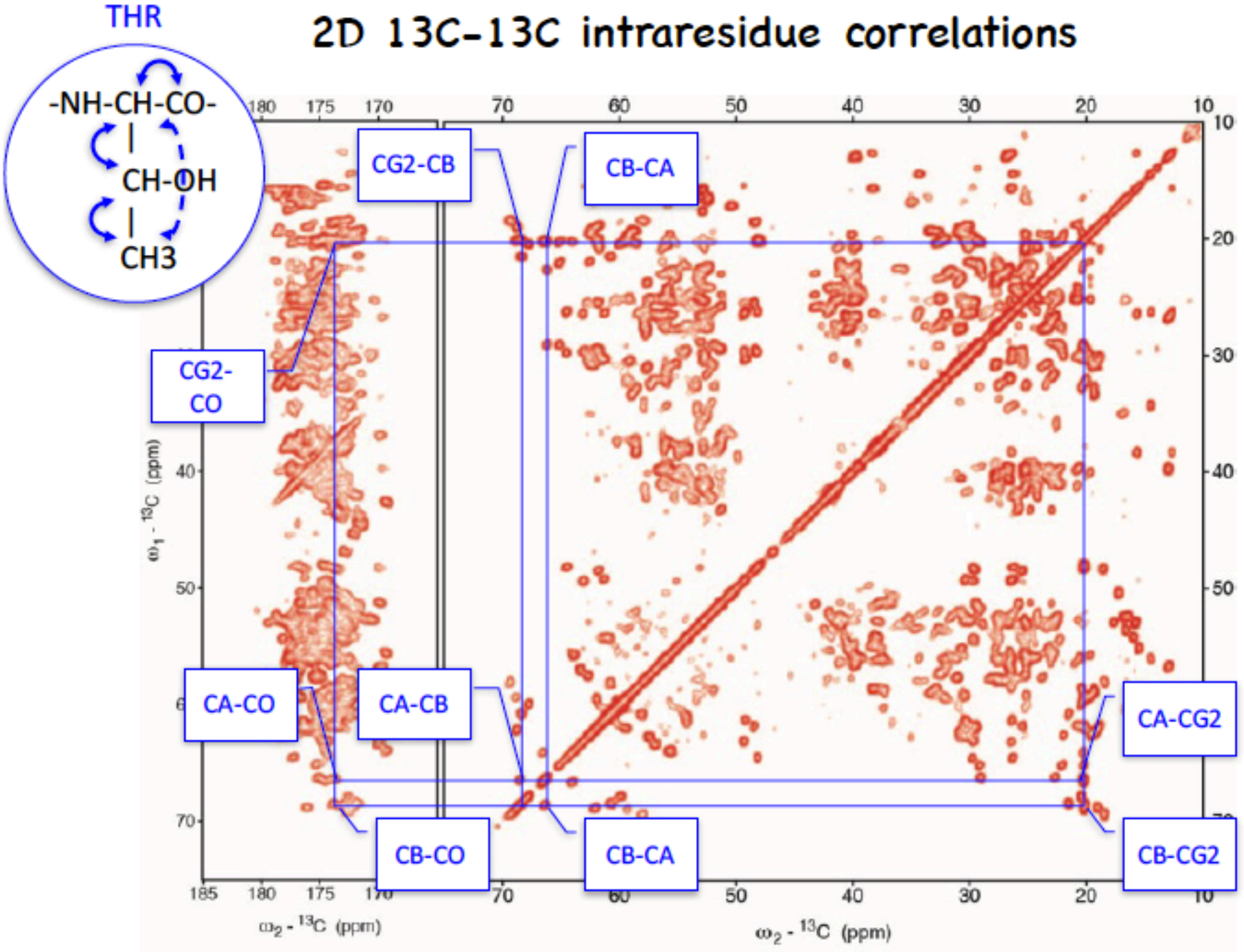




2D ^{13}C-^{13}C or ^{13}C-^{15}N correlation spectrum



2D 13C-13C intraresidue correlations



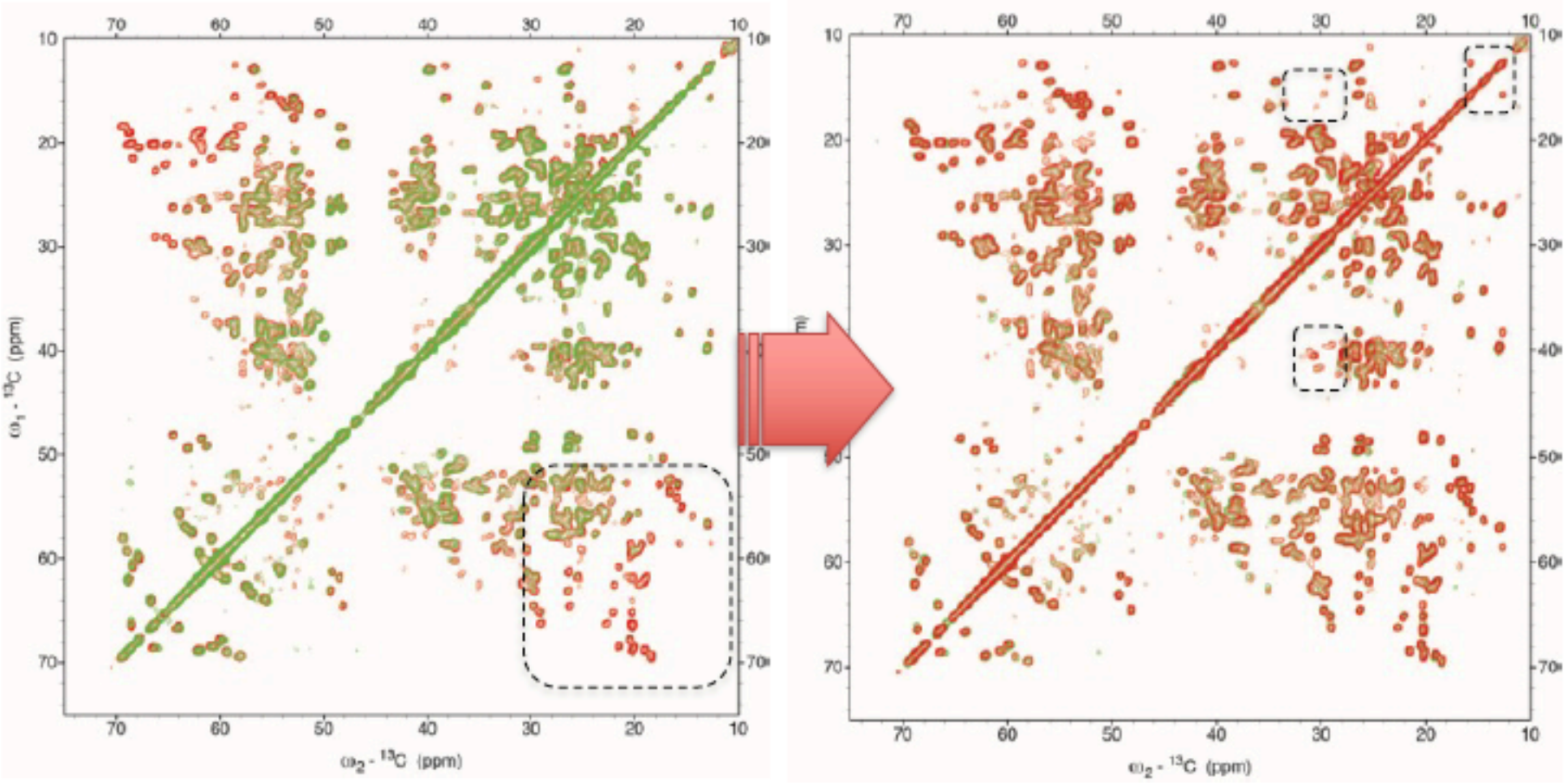
Is higher MAS frequency really beneficial ?

MAS 12 kHz
MAS 18 kHz

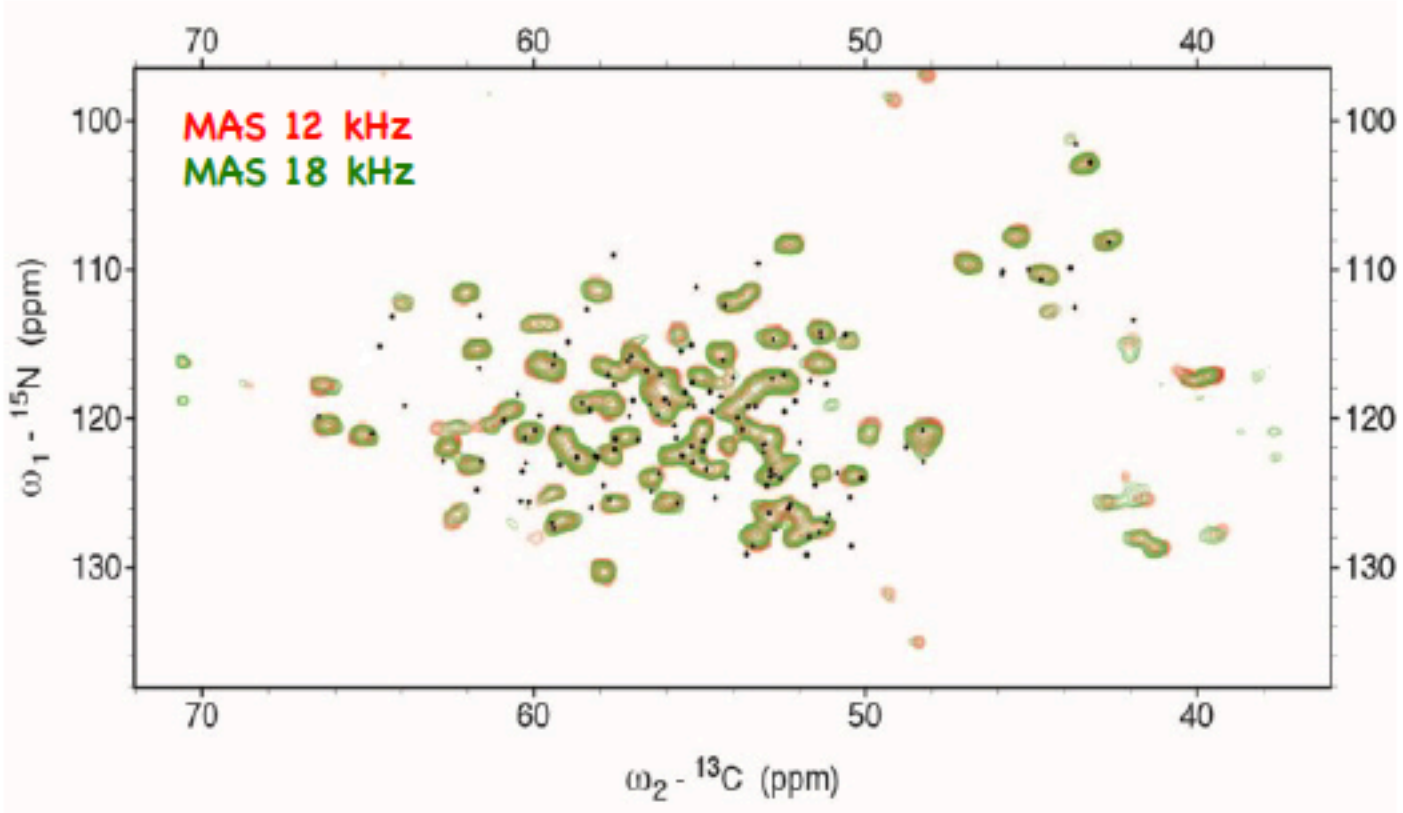
13C-13C dipolar-based transfer efficiency

2D PDSD (mix=50 ms)

2D DARR (mix=50 ms)

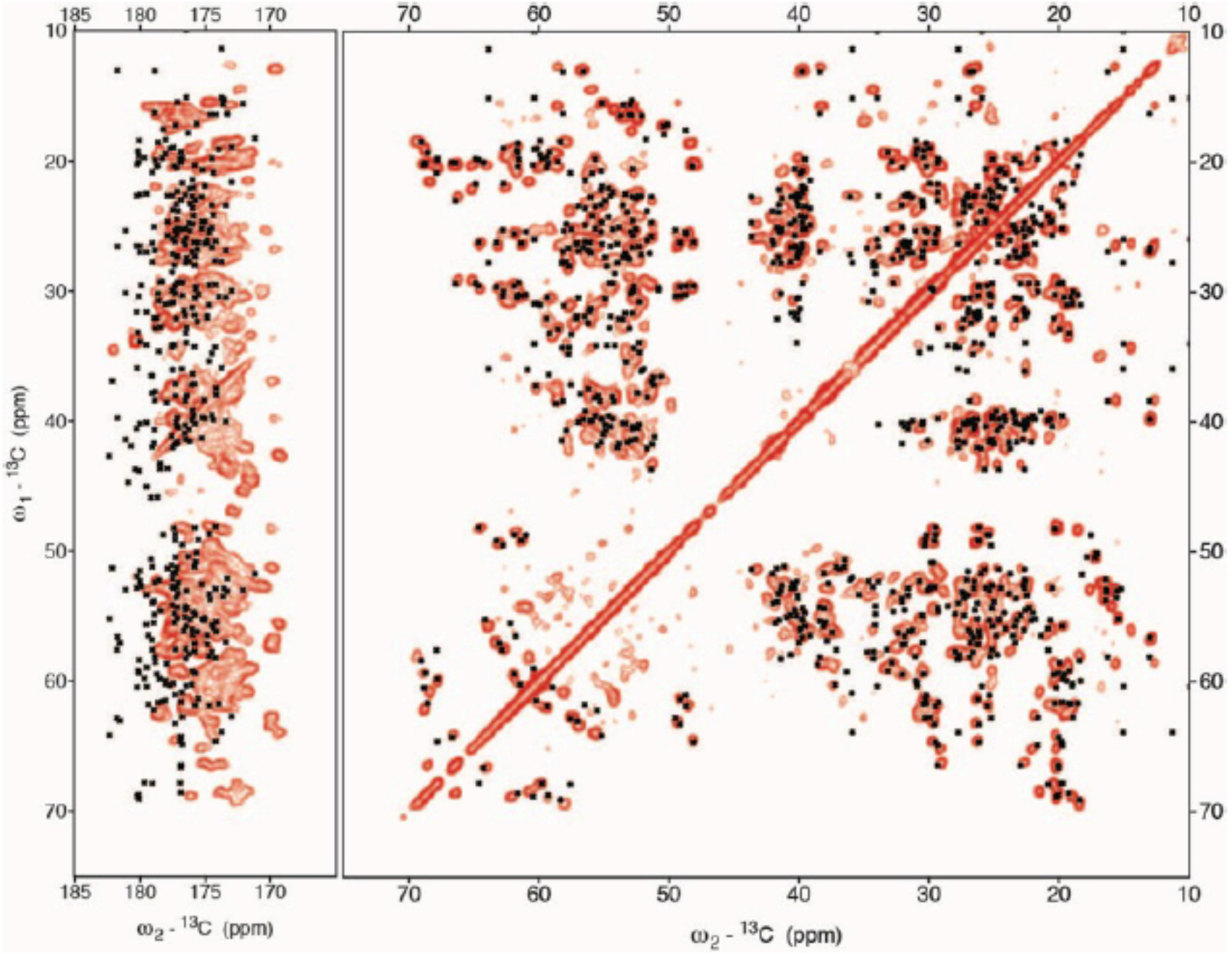


Is higher MAS frequency really beneficial ?

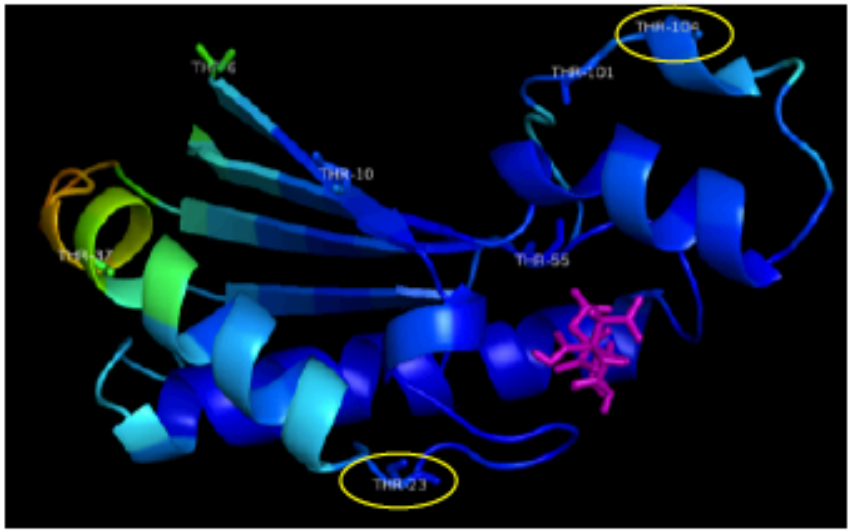


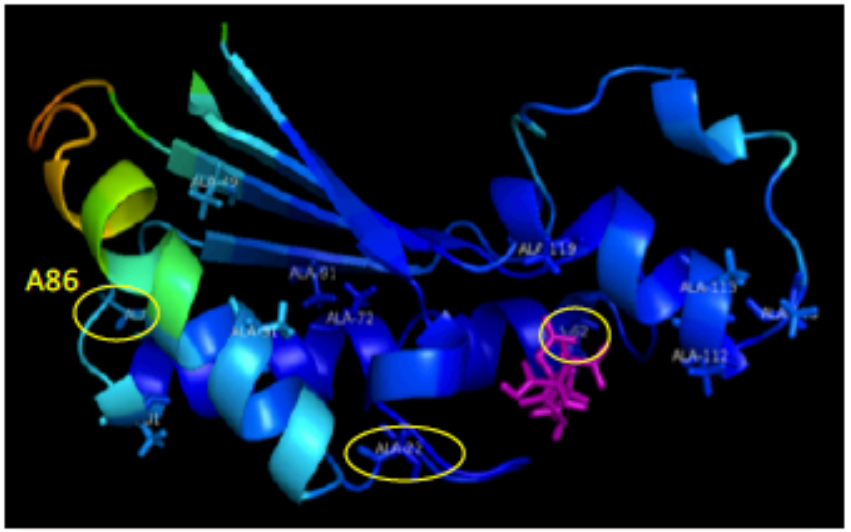
	13C linewidth	15N linewidth
MAS 12 kHz	100 Hz (≈ 0.6 ppm)	80 Hz (≈ 1.1 ppm)
MAS 18 kHz	100 Hz (≈ 0.6 ppm)	70 Hz (≈ 1.0 ppm)

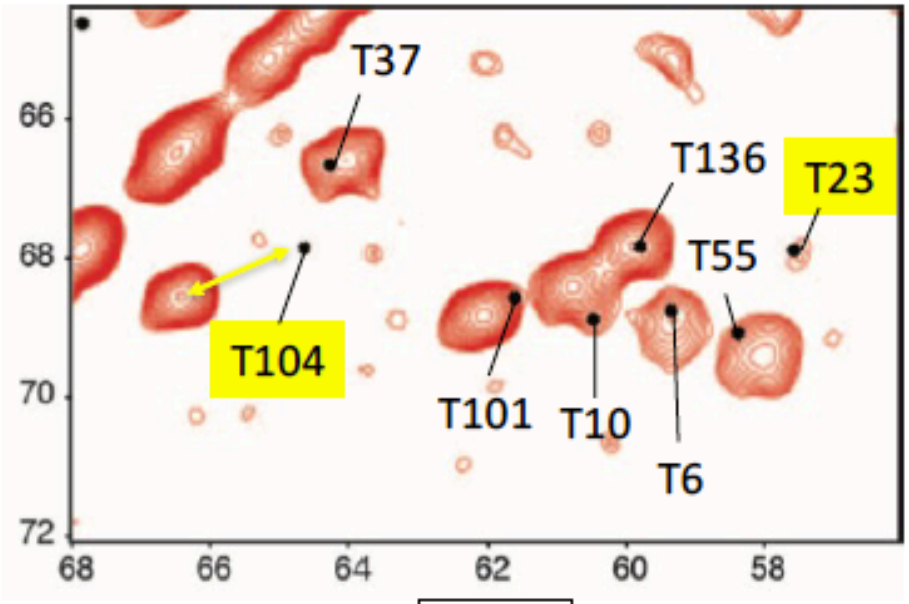
Comparison with solution NMR data



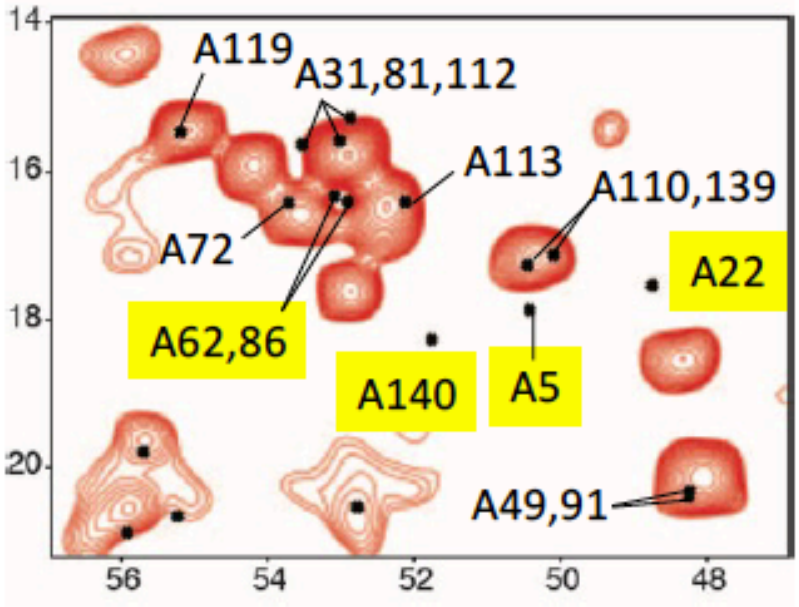
Comparison with solution NMR data







8 THR



15 ALA