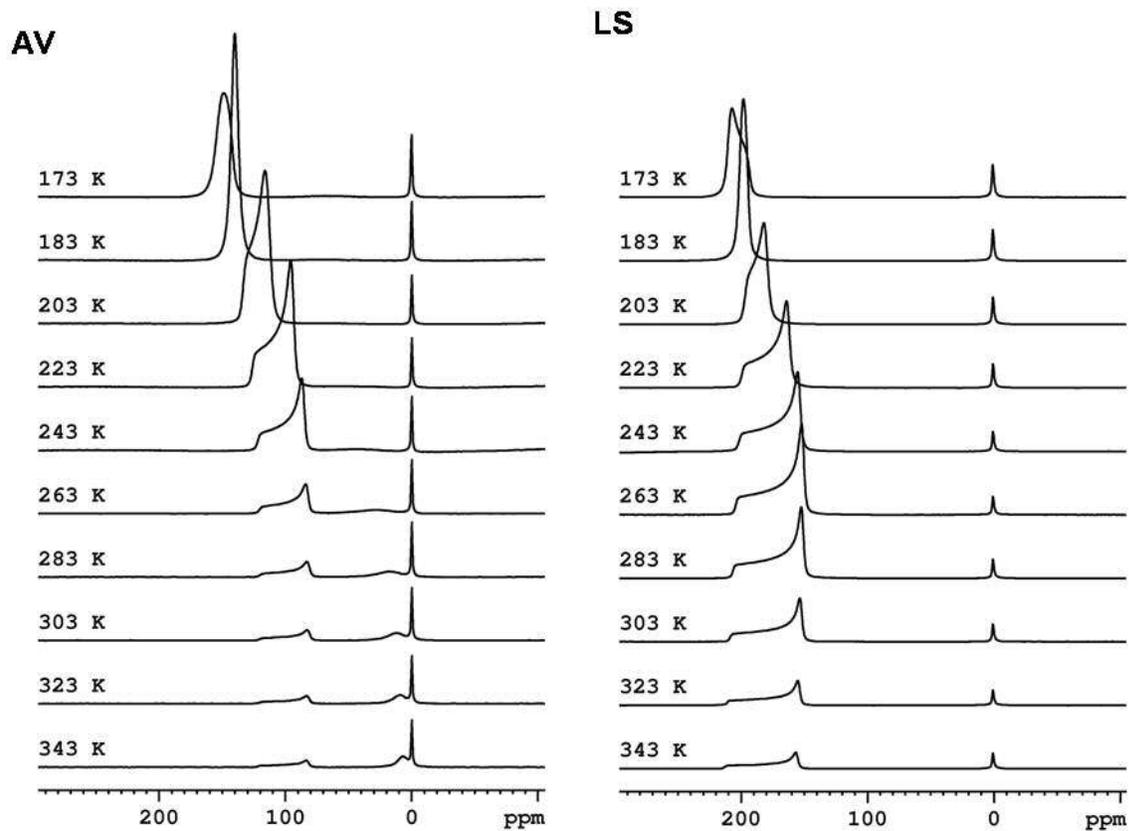
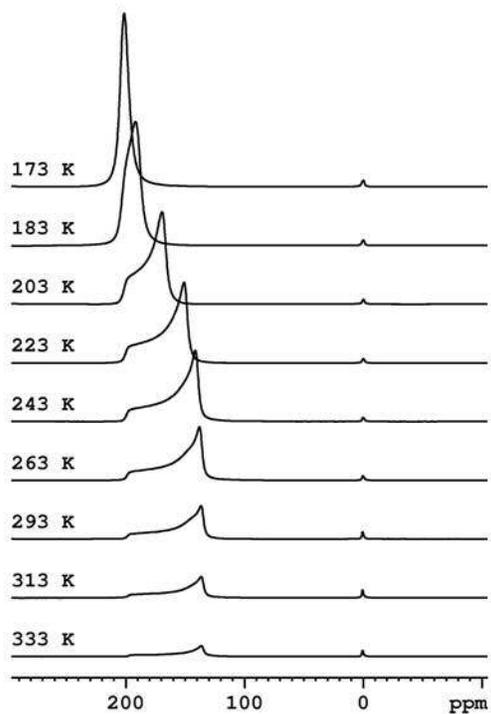
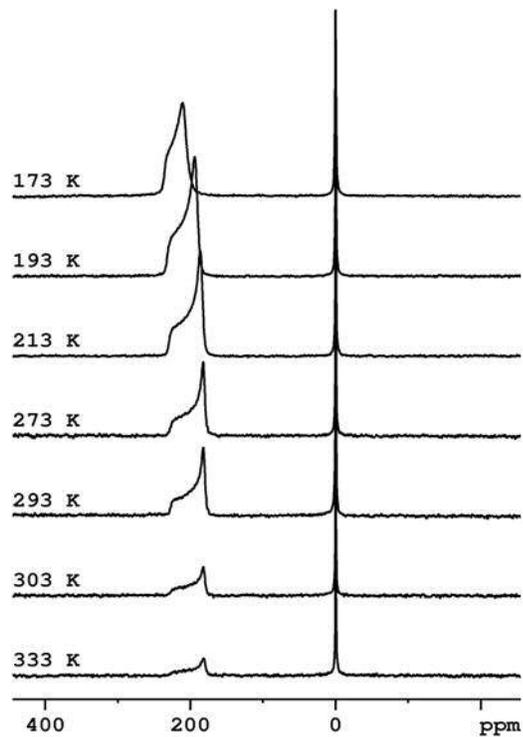
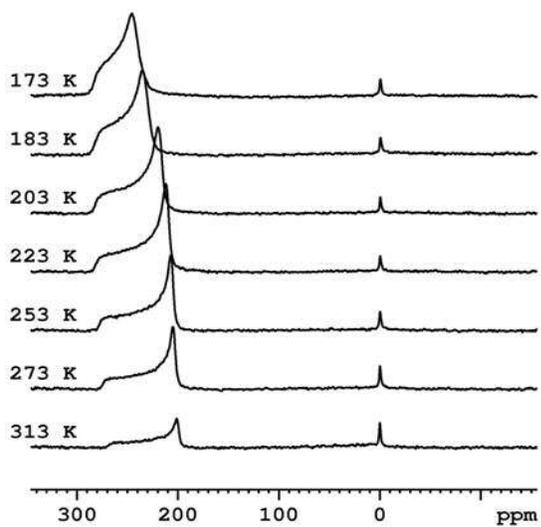
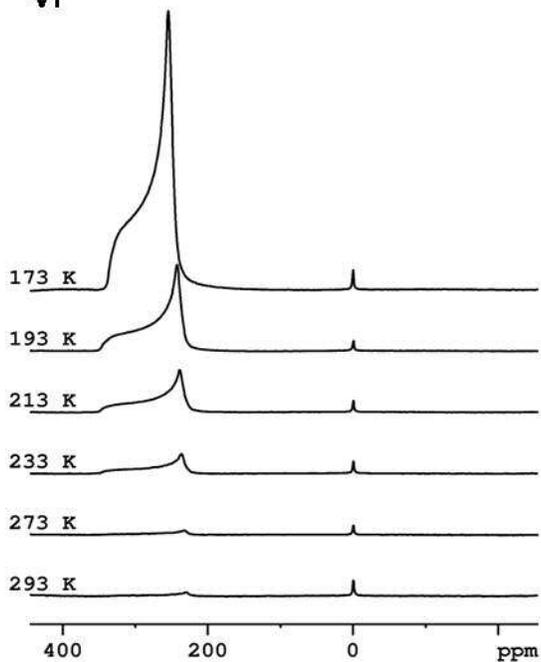


## Supporting information

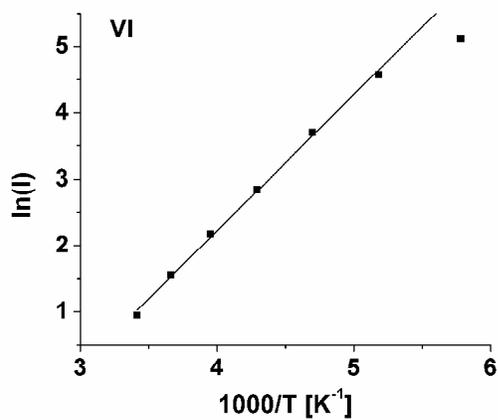
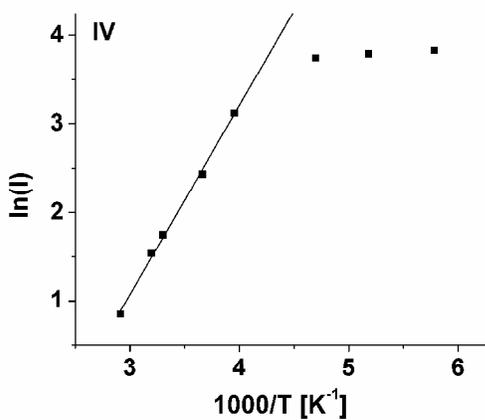
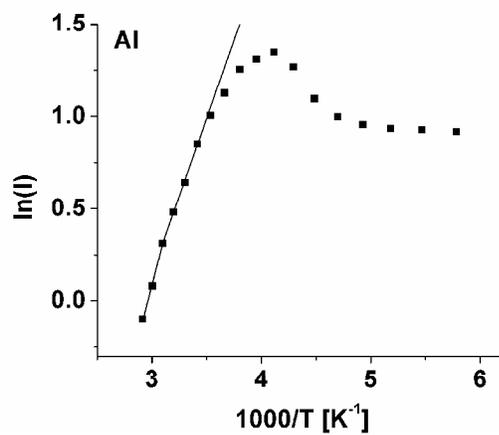
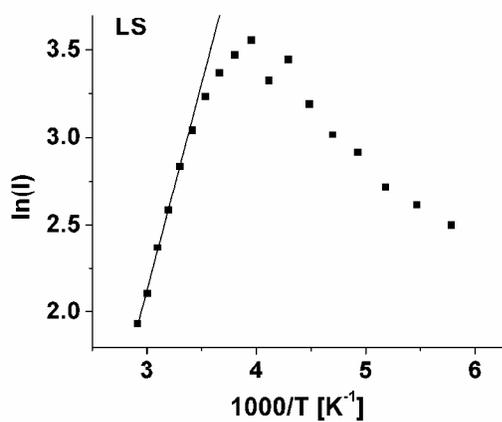
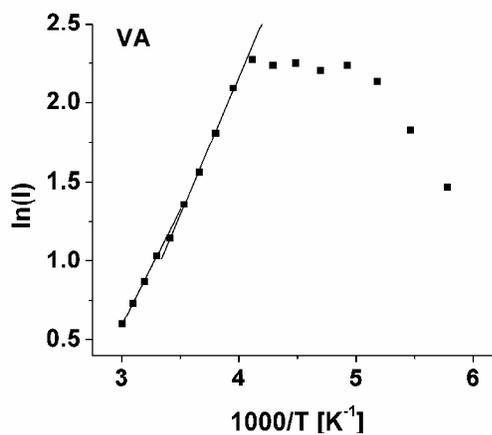
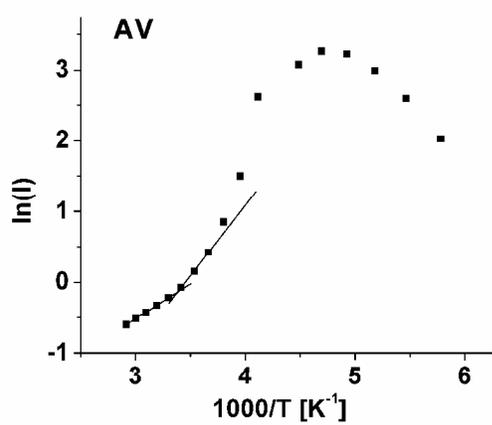
Continuous-flow HP  $^{129}\text{Xe}$  NMR spectra of AV, LS, VV, IA, IV and VI dipeptides in the 173-343 K temperature range



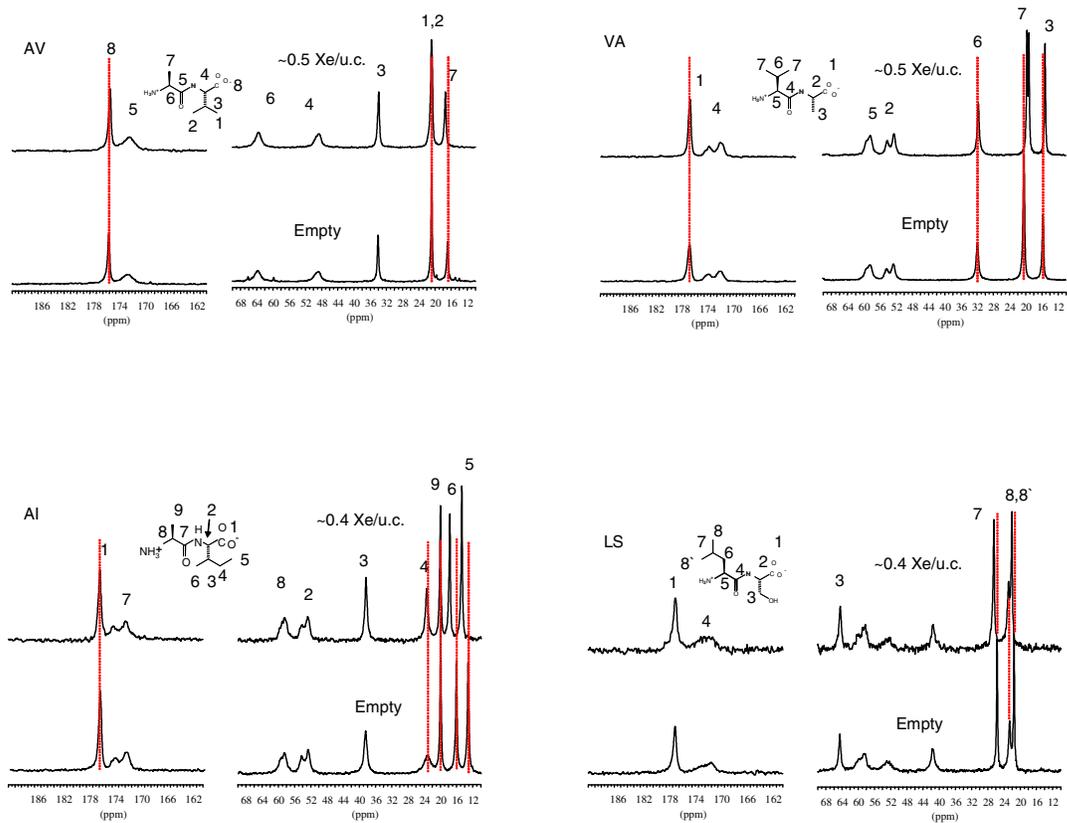
**Figure 1S A:** Continuous-flow HP  $^{129}\text{Xe}$  NMR spectra of AV and LS dipeptides in the 173-343 K temperature range.

**VV****IA****IV****VI**

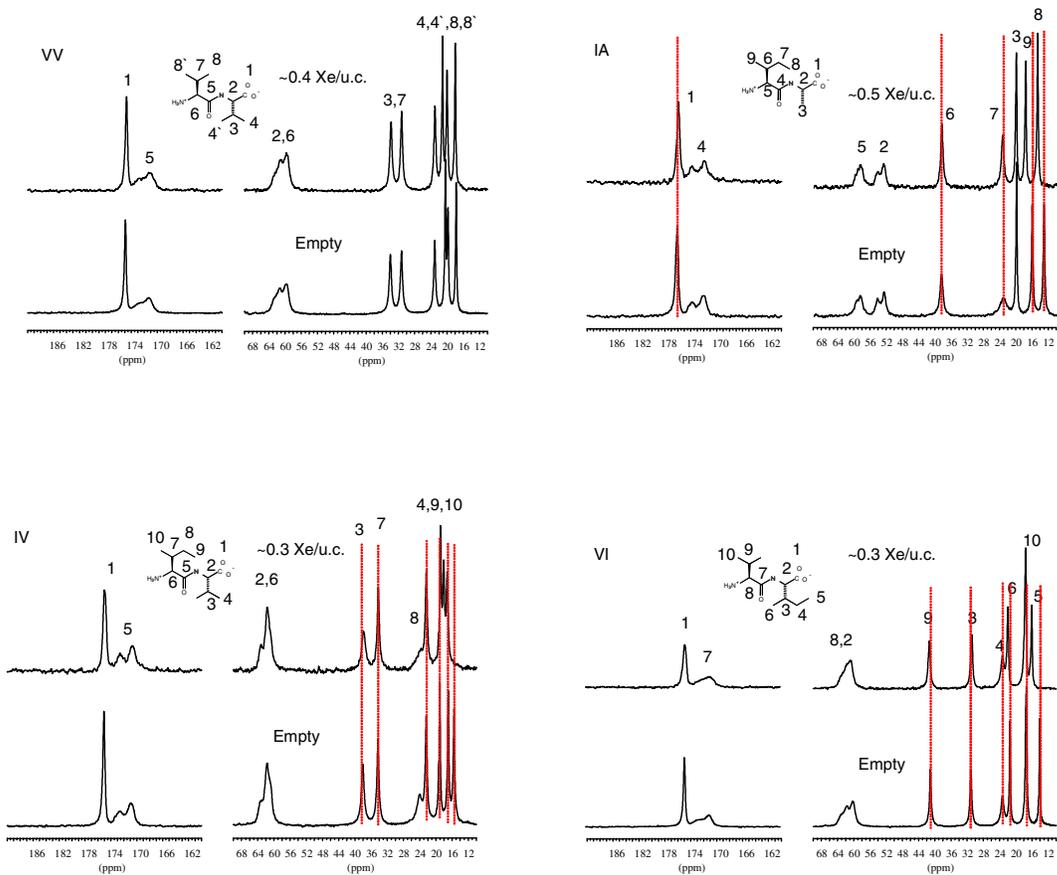
**Figure 1S B :** Continuous-flow HP  $^{129}\text{Xe}$  NMR spectra of VV, IA, IV and VI dipeptides in the 173-343 K temperature range



**Figure 2S:** Experimentally observed  $\ln(I) - 1000/T$  dependences for AV, VA, LS, AI, IV and VI dipeptides and linear fits of the data in the high-temperature regions.



**Figure 3S A :**  $^{13}\text{C}$  CP MAS spectra of empty and Xe-loaded porous dipeptides.



**Figure 3S B :**  $^{13}\text{C}$  CP MAS spectra of empty and Xe-loaded porous dipeptides.

Table 1 S. Change in the  $^{13}\text{C}$  chemical shift of  $\text{CH}_3$  groups in porous dipeptides upon adsorption of Xe (Hz, SF=50.1 MHz)

	AV	VA	AI	LS	VV	IA	IV	VI
$\text{CH}_3'$	9	-39	-45	-39	-35	-3	10	-25
$\text{CH}_3''$	-3	-62	-48	-12	-10	-81	-56	-9
$\text{CH}_3'''$	-26	-27	-51	-27	-11	-78	-85	-98