Supplementary Information to "Monitoring the site-specific solid-state NMR data of oligopeptides" by Czernek & Brus (*Int. J. Mol. Sci*. **2020**)

Table S1: The values (in ppm) of principal elements of the $^{15}N_{amid}$ chemical shielding (σ) / shift (δ) tensors as actually used.

site	the least shielded component		the mid shielded component		the most shielded component	
	σ	δ	σ	δ	σ	δ
G G* G	1.3897	209.2667	152.2426	67.4667	187.4243	32.8667
V G* G	-16.4992	219.5333	148.5507	78.2333	176.0899	43.3333
P G* G	-3.7239	209.2000	163.5715	59.1000	169.0626	51.8000
A G* G	-1.1447	210.1000	165.1714	55.8000	169.8787	48.5000
F G* G	-18.9621	223.4000	152.3791	71.1000	166.8488	53.2000
G G* V	-8.5323	219.8000	160.2319	62.8000	169.2221	55.8000
N-Ac-Aib-OH	-39.6744	244.0	116.5271	144.0	144.9013	68.0
N-Ac-Leu-OH	-28.5929	233.5	132.7600	94.5	157.4859	55.0
A P* G	-14.9525	231.0	82.2485	127.0	187.5769	38.0

Table S2: The values (in ppm) of principal elements of the $^{13}C_{\alpha}$ chemical shielding (σ) / shift (δ) tensors as actually used.

site	the least shielded component		the mid shielded component		the most shielded component	
	σ	δ	σ	δ	σ	δ
G G* G	109.7816	58.1000	123.7610	48.9000	151.4309	22.9000
V G* G	109.2250	57.8000	126.7013	48.1000	151.3295	23.1000
P G* G	98.0611	69.4667	131.2338	40.7667	155.4482	18.7667
A G* G	97.6568	69.9333	130.6169	41.8333	159.2736	16.9333
F G* G	97.9261	69.6333	129.2557	43.3333	153.9203	20.5333
G G* V	97.3389	70.6333	129.8342	42.0333	152.7927	21.7333

Figure S1: The linear relationship between theoretical and experimental eigenvalues of the $^{15}N_{amid}$ chemical shielding/shift tensors of the central glycines in GGG, VGG, PGG, AGG, FGG and GGV tripeptides described in the main text; $\sigma = -1.0876*\delta + 226.50$ ppm (18 data points); standard deviation 3.2 ppm, adjusted $R^2 = 0.99846$.

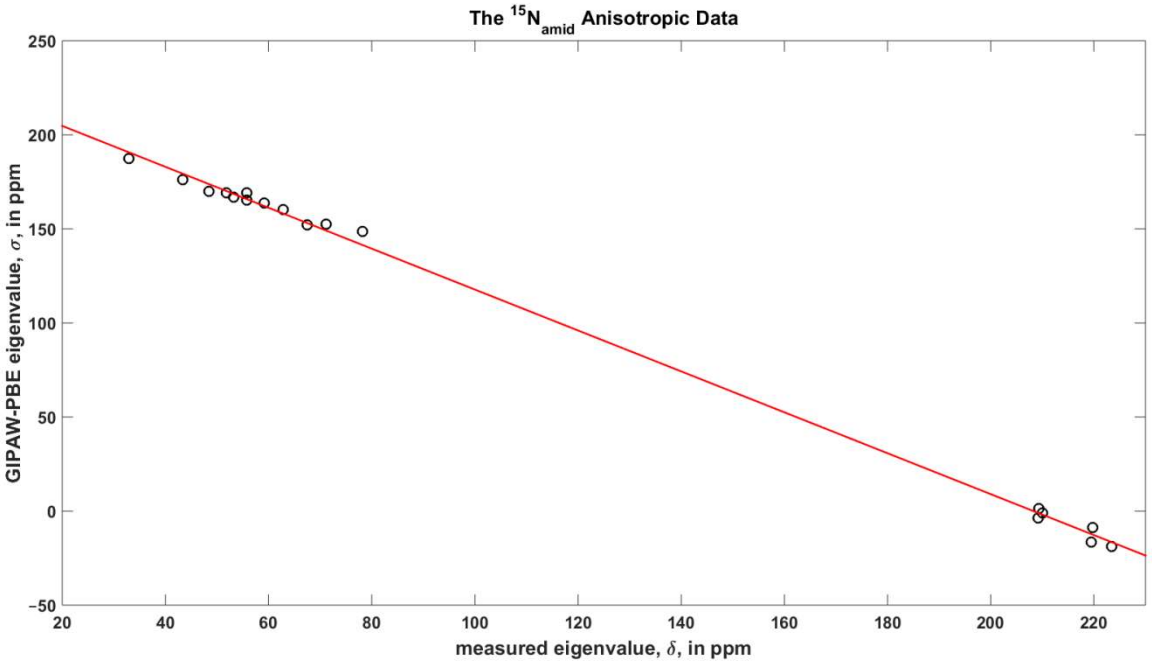

Figure S2: The linear relationship between theoretical and experimental eigenvalues of the $^{13}C_\alpha$ chemical shielding/shift tensors of the central glycines in GGG, VGG, PGG, AGG, FGG and GGV tripeptides described in the main text; $\sigma = -1.1475*\delta + 178.10$ ppm (18 data points); standard deviation 1.4 ppm, adjusted $R^2 = 0.99619$.

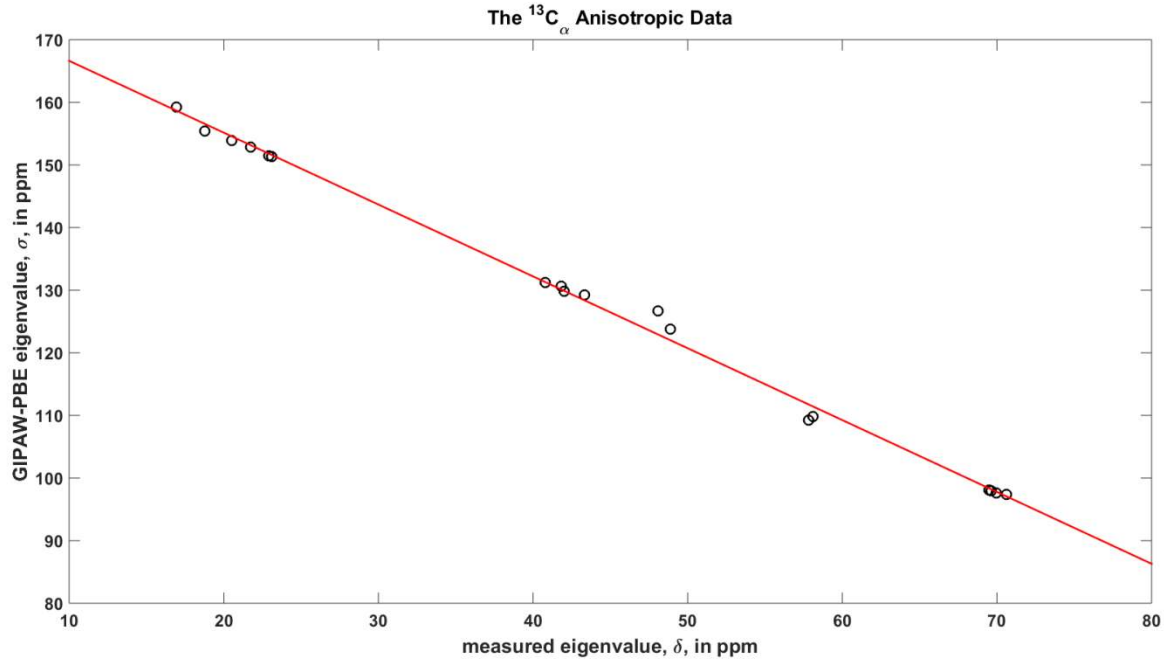

Table S3: Atom numbers in the optimized structure (named ‘Samara1final.pdb’ and available in Supplementary Materials) of samarosporin I used to extract distances and angles which are described in the main text.

site	atom #		
	N_{amid}	H_{amid}	C_{α}
Phe1	7	18	8
Aib2	27	33	28
Aib3	40	46	41
Aib4	53	59	54
Val5	66	73	67
Gly6	82	86	83
Leu7	89	97	90
Aib8	108	114	109
Aib9	121	127	122
Gln11	149	158	150
Iva12	166	173	167
Aib14	197	203	198
Fol15	210	221	211