

Table S3: Percentage of secondary structures for simulations A – J.

		Turn	β -sheet	Bridge	α -helix	3_{10} -helix	π -helix	Coil
A β 16	(A)	73.52	0.00	0.07	0.00	4.69	0.00	21.72
	(B)	67.77	0.00	2.57	0.00	0.73	0.03	28.90
	(C)	77.21	0.00	0.00	0.00	0.00	0.00	22.79
	(D)	66.20	0.00	0.00	0.00	0.00	0.00	33.80
	(E)	58.09	0.00	0.00	0.00	0.00	0.00	41.91
Pt(A β 16)	(F)	41.62	0.00	0.00	0.00	16.35	0.00	42.03
	(G)	82.66	0.00	0.00	0.00	0.00	0.00	17.34
	(H)	55.90	0.00	0.00	0.00	0.00	0.00	44.10
	(I)	82.68	0.00	0.00	0.00	0.00	0.00	17.32
	(J)	53.27	0.00	0.00	0.00	0.00	0.00	46.73