

Correlation between average distance matrices

	cell 1	cell 2	cell 3	cell 4	cell 5	cell 6
cell 1	85.2	49.5	57.5	58.2	47.6	49.9
cell 2	46.2	92.1	52.2	51.0	40.9	37.5
cell 3	54.0	46.7	91.5	49.5	51.0	43.0
cell 4	55.1	45.5	45.4	91.1	46.8	45.1
cell 5	44.5	36.0	46.2	42.5	70.6	33.5
cell 6	50.2	33.2	42.5	44.1	36.3	91.3

Table S2: Comparison of distance matrices. Shown are the correlation coefficients between the average distance matrices (in %) for structure ensembles obtained from cell 1 to cell 6. Lower diagonal: ISD ensemble vs ISD ensemble. Upper diagonal: ISD ensemble vs ensemble by Nagano *et al.* Diagonal (shown in bold face): ISD ensemble vs ensemble by Nagano *et al.*