Electronic Supplementary Information

Protein binding by dinuclear polypyridyl ruthenium(II) complexes and the effect of cucurbit[10]uril encapsulation

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Table S1. ^{1}H NMR chemical shifts of the aromatic protons of free ΔΔ-Rubb$_{12}$ and changes in chemical shift (Δδ) upon encapsulation by Q[10] after complete equilibrium. All chemical shifts are displayed in ppm. Negative numbers indicate an upfield shift.

	Free ΔΔ-Rubb$_{12}$	**Q[10]-bound ΔΔ-Rubb$_{12}$**	**Δδ**
Mebpy			
H3	8.39	9.22	0.83
H5	6.17	7.10	0.93
H6	6.93	7.41	0.48
H3'	8.36	7.93	-0.43
H5'	6.52	5.80	-0.72
H6'	7.33	7.16	-0.17
CH_3	2.37	2.64	0.27
CH_2a*	2.58	2.36/1.19	-0.22/-1.39
CH_2b*	2.44	0.98/0.77	-1.46/-1.67
CH_2c*	1.17	-0.12/-0.36	-1.29/-1.53
CH_2d*	0.98	-0.69	-1.67
CH_2e*	0.77	-0.23	-1.00
CH_2f*	0.72	-0.58	-1.30
Phen A			
H2	8.14	7.98	-0.16
H3	7.75	8.12	0.37
H4	8.64	8.69	0.05
H5	8.21	8.21	0/0.1
H6	8.17	8.21(or 8.31)	0.04 (or 0.14)
H7	8.26	8.69	0.43
H8	7.85	7.91	0.06
H9	8.61	9.33	0.72
Phen B			
H2	7.95	7.85	-0.10
H3	7.55	7.48	-0.07
H4	8.55	8.52	-0.03
H5	8.17	8.22	0.05
H6	8.19	8.21(or 8.31)	0.02 (or 0.12)
H7	8.46	8.69	0.23
H8	7.42	7.67	0.25
H9	7.80	8.10	0.30

* The CH_2 protons adjacent to bipyridine are nominated as CH_2a, and the CH_2 protons in the middle of the methylene chain are nominated as CH_2f.