Supplementary material for Mareque Rivas *et al*. (2001) *Proc. Natl. Acad. Sci. USA* **98** (17), 9478–9483. (10.1073/pnas.161257798)

Table 2. Summary of ^{1}H NMR [500 MHz, $CD_3CN/CDCl_3$ (6:1)] data between -20°C and + 55°C for **1**

No metal	-20°C δ, ppm	25°C δ, ppm	55°C δ, ppm
^{t}But	1.11	1.11	1.12
ArH	6.99	6.91	6.99
Heq	3.14	3.16	3.17
Hax	4.54	4.62	4.63
OCH_2CO	4.73	4.74	4.75
OCH_2CO	4.57	4.61	4.67
Val-NH	7.83	7.63	7.49
Val-Hα	4.39	4.42	4.39
Val-Hβ	2.10	2.11	2.12
Val-Hγ	0.84, 0.85	0.84, 0.85	0.84, 0.88
OCH_2Ph	5.03, 5.09	5.06, 5.10	5.07, 5.11
Ph	7.29-7.32	7.29-7.32	7.29-7.32

Na^+	-20 ° C δ (ppm)	25 ° C δ (ppm)	55 ° C δ (ppm)
^{t}But	1.17	1.20	1.24
ArH	7.25-7.29	7.28-7.33	7.28-7.33
Heq	3.32	3.32	3.32
Hax	4.14	4.20	4.23
OCH_2CO	4.54	4.32	4.29
OCH_2CO	4.10	4.34	4.44
Val-NH	6.86	6.75	6.67
Val-Hα	4.68	4.62	4.61
Val-Hβ	2.17	2.17	2.17
Val-Hγ	0.76, 0.90	0.83, 0.92	0.87, 0.94
OCH_2Ph	4.94, 5.13	5.04, 5.16	5.08, 5.18
Ph	7.29-7.32	7.28-7.33	7.28-7.33

K^+	-20 ° C δ (ppm)	25 ° C δ (ppm)	55 ° C δ (ppm)
^{t}But	1.18	1.22	1.23
ArH	7.29-7.34	7.29-7.36	7.29-7.37
Heq	3.30	3.31	4.32
Hax	4.26	4.30	4.33
OCH_2CO	4.52	4.61	4.64
OCH_2CO	4.12	4.08	4.08
Val-NH	6.87	6.75	6.68
Val-Hα	4.60	4.59	4.58
Val-Hβ	2.15	2.17	2.19
Val-Hγ	0.81, 0.93	0.88, 0.96	0.91, 0.98
OCH_2Ph	5.04, 5.12	5.10, 5.17	5.12, 5.18
Ph	7.29-7.34	7.29-7.36	7.29-7.37