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

**Table 9**. Temperature and metal dependence of the valine and glycine amide proton chemical shifts in **3**

| T, K | Val N-H δ, ppm No metal | Gly N-H δ, ppm No metal | Tyr N-H δ, ppm No metal | Val N-H δ, ppm, $Na^+$ | Gly N-H δ, ppm, $Na^+$ | Tyr N-H δ, ppm, $Na^+$ | Val N-H δ, ppm, $K^+$ | Gly N-H δ, ppm, $K^+$ | Tyr N-H δ (ppm), $K^+$ |
|---|---|---|---|---|---|---|---|---|---|
| 253 | 8.4 | 7.97 | 7.46 | 7.59 | 8.37 | 7.88 | 7.3 | 8.02 | 7.45 |
| 258 | 8.37 | 7.96 | 7.44 | 7.48 | 8.34 | 7.8 | 7.21 | 8 | 7.42 |
| 268 | 8.32 | 7.92 | 7.4 | 7.42 | 8.3 | 7.78 | 7.17 | 7.96 | 7.35 |
| 278 | 8.28 | 7.88 | 7.37 | 7.35 | 8.24 | 7.73 | 7.15 | 7.92 | 7.32 |
| 288 | 8.25 | 7.84 | 7.32 | 7.18 | 8.19 | 7.66 | 7.14 | 7.88 | 7.27 |
| 298 | 8.19 | 7.79 | 7.16 | 7.14 | 8.15 | 7.62 | 7.13 | 7.83 | 7.21 |
| 308 | 8.13 | 7.75 | 7.02 | 7.05 | 8.07 | 7.54 | 7.11 | 7.78 | 7.17 |
| 318 | 8.09 | 7.71 | 6.99 | 6.98 | 8.00 | 7.47 | 7.09 | 7.73 | 7.12 |
| 328 | 7.98 | 7.64 | 6.9 | 6.92 | 7.94 | 7.41 | 7.08 | 7.67 | 7.08 |