

S1 Table. Comparison of expected and measured ¹H-NMR spectrum for TM-2-51.

| Proton(s) | Expected δ (ppm) ^a Acetone-D ₆ , 400 MHz | Measured δ (ppm) Acetone-D ₆ , 300 MHz |
|-----------|--|---|
| N | - ^b | - ^b |
| N' | 10.3 (bs, 1H) | - ^b |
| C3, C7 | 8.06 - 8.04 (m, 2H) | 8.11 - 8.08 (m, 2H) |
| C2', C6' | 7.78 - 7.76 (m, 2H) | 7.84 - 7.81 (m, 2H) |
| C5 | 7.69 - 7.64 (m, 1H) | 7.72 - 7.69 (m, 1H) |
| C4, C6 | 7.57 - 7.53 (m, 2H) | 7.63 - 7.60 (m, 2H) |
| C3', C5' | 7.43 - 7.38 (m, 2H) | 7.48 - 7.45 (m, 2H) |
| C4' | 7.28 - 7.24 (m, 1H) | 7.32 - 7.27 (m, 1H) |

^a From reference [17].

^b Not observed.