

**S3 Table.** Comparison of expected and measured <sup>1</sup>H-NMR spectrum for TM-2-104.

Proton(s)	Expected $\delta$ (ppm) <sup>a</sup> CDCl <sub>3</sub> , 400 MHz	Measured $\delta$ (ppm) CDCl <sub>3</sub> , 300 MHz
N	10.90 (d, J = 6.4 Hz, 1H)	11.02 (d, 1H)
N'	8.75 (bs, 1H)	9.02 (bs, 1H)
C3, C7	7.63 - 7.61 (m, 2H)	7.70 - 7.67 (m, 2H)
C5	7.43 - 7.39 (m, 1H)	7.48 - 7.43 (m, 1H)
C5', C7'	7.33 - 7.28 (m, 2H)	7.36 - 7.31 (m, 2H)
C4, C6, C4', C8'	7.21 - 7.15 (m, 4H)	7.25 - 7.23 (m, 4H)
C6'	7.11 - 7.07 (m, 1H)	7.17 - 7.11 (m, 1H)
C2'	5.45 - 5.38 (m, 1H)	5.54 - 5.44 (m, 1H)
C1'	1.46 (d, J = 6.8 Hz, 3H)	1.53 (d, 3H)

<sup>a</sup> From reference [17].