Electronic Supplementary Material (ESI) for RSC Advances.

The Hierarchies of Hydrogen Bond in Cocrystals/ Salts of Isoniazid and its Schiff Base-Case Study

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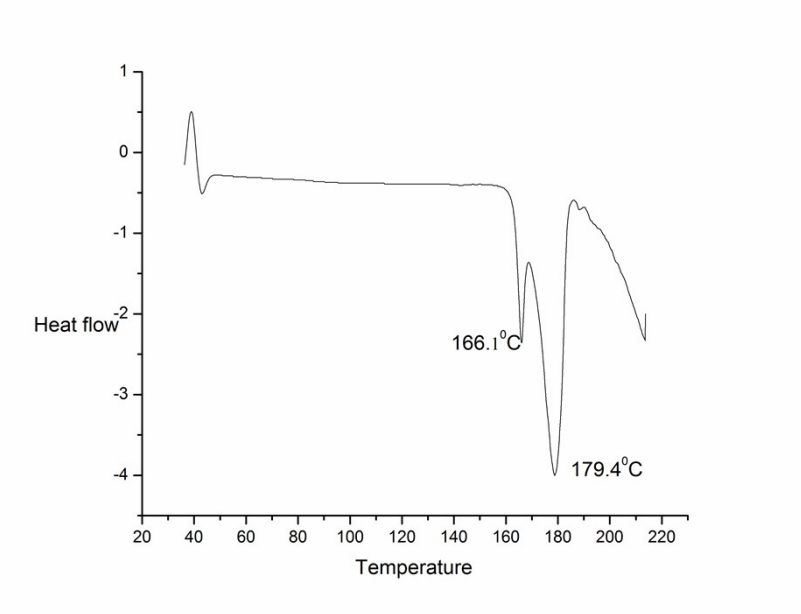

Figure S1: DSC thermogram of 2a

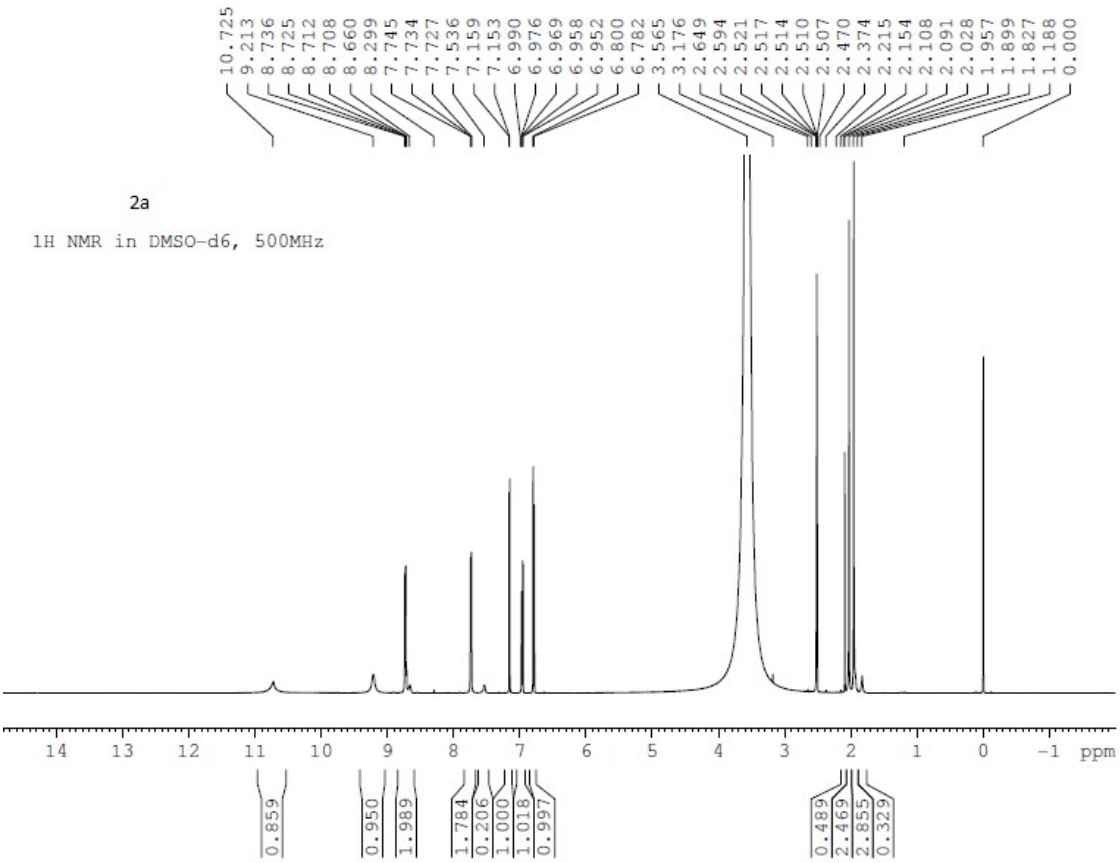

Figure S2a: NMR spectrum of 2a

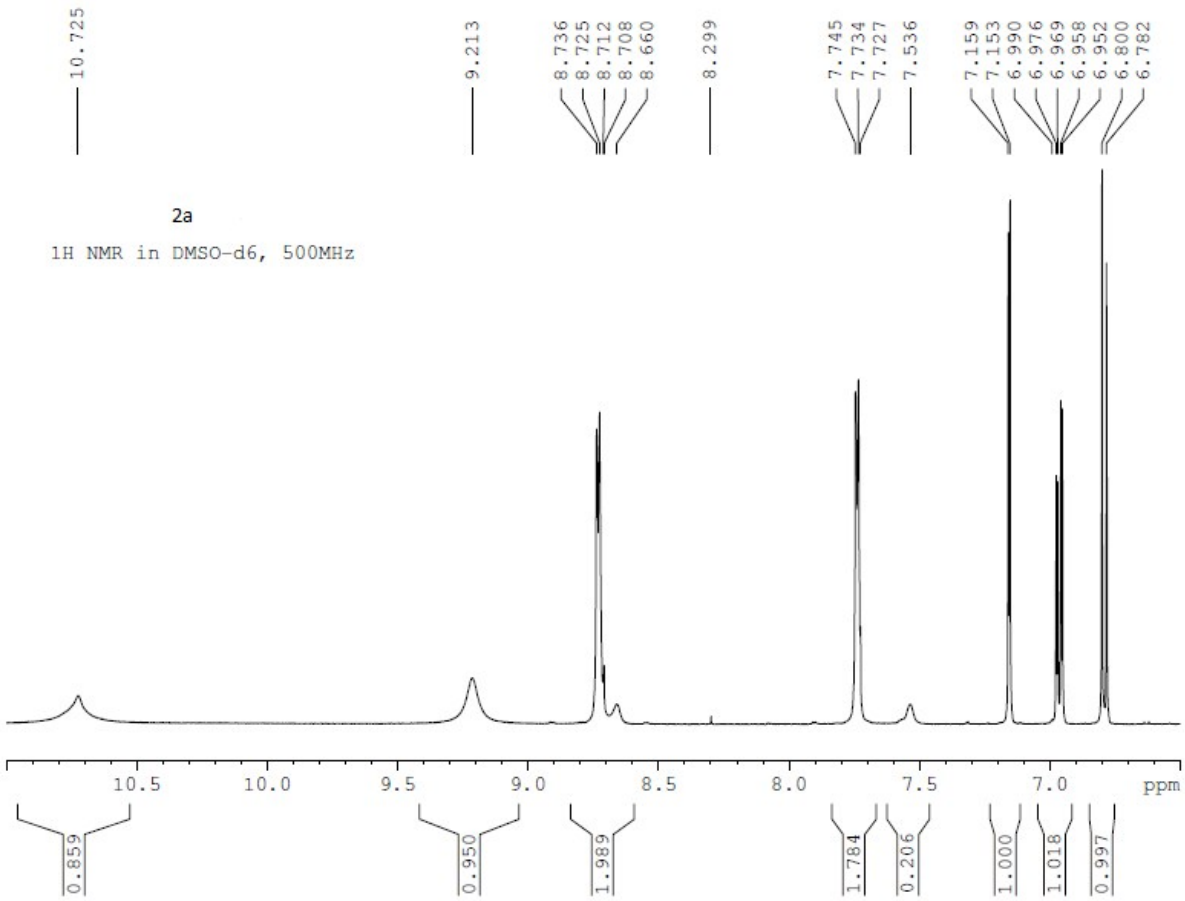

Figure S2b: NMR spectrum of 2a

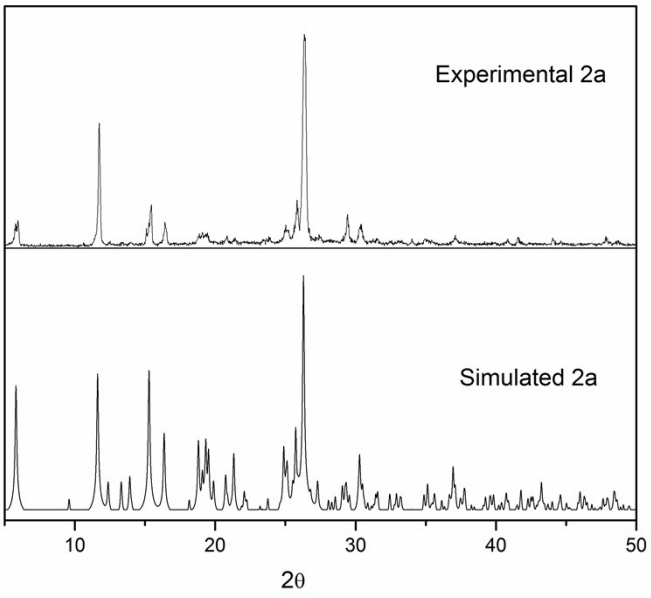

Figure S3: XRPD of 2a

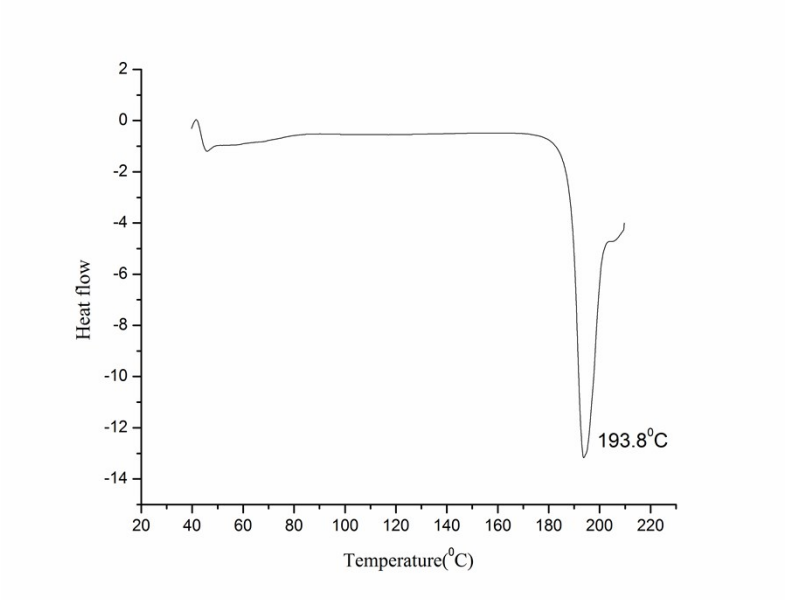

Figure S4: DSC thermogram of 1b

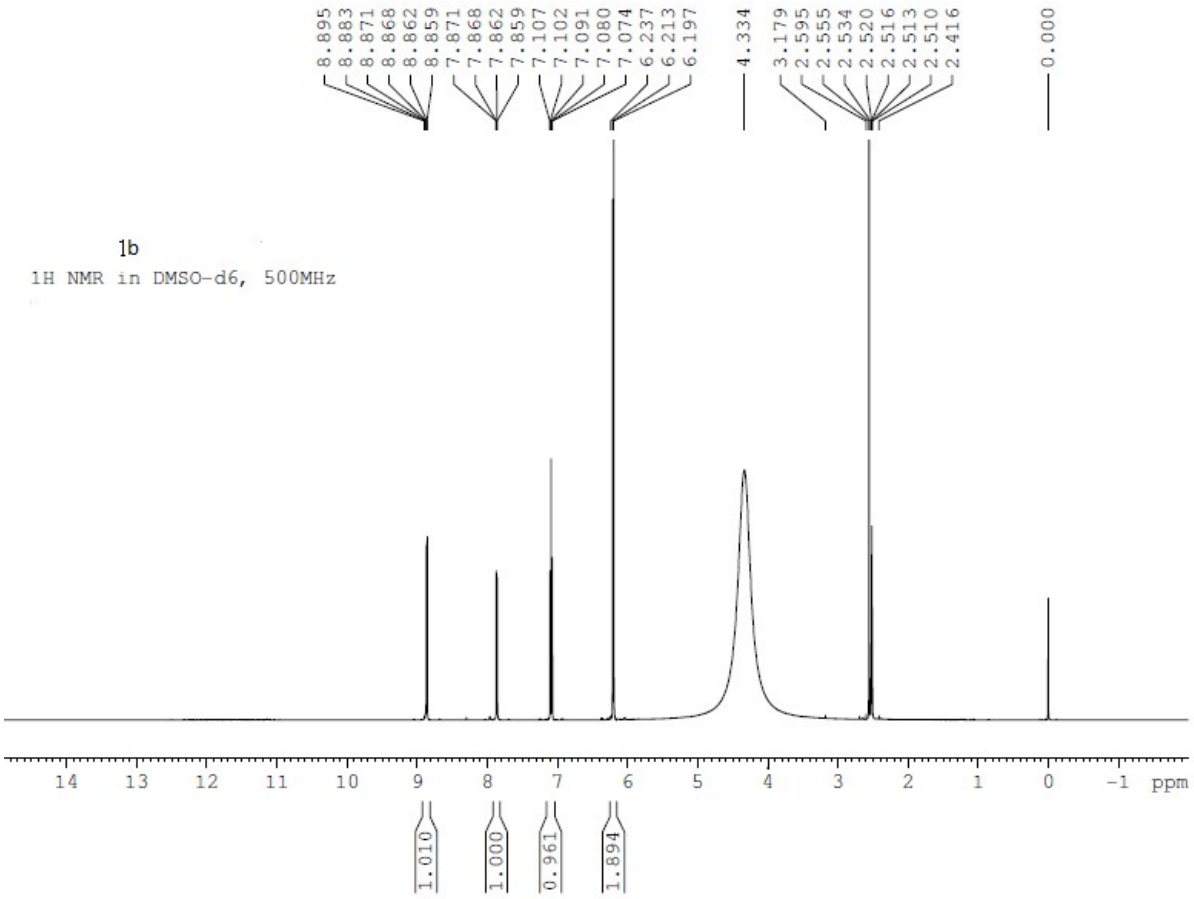

Figure S5a: NMR spectrum of 1b

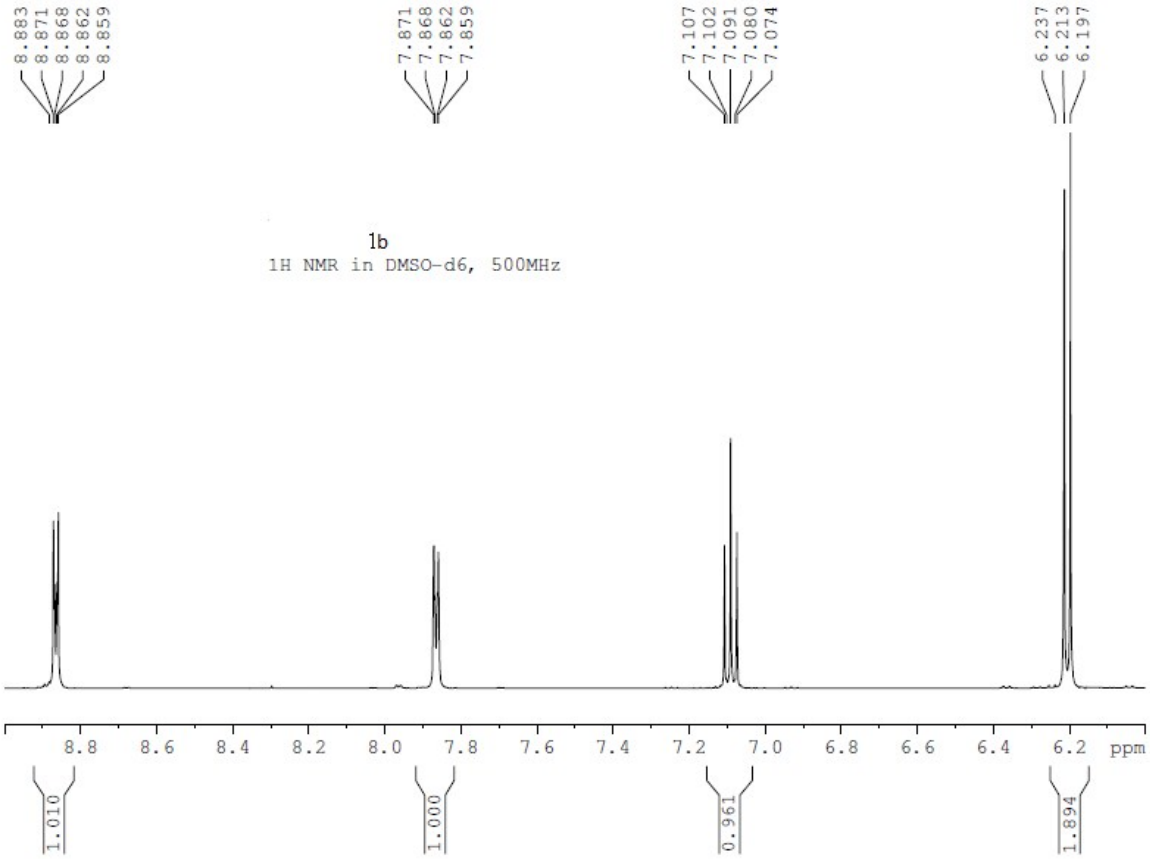

Figure S5b: NMR spectrum of 1b

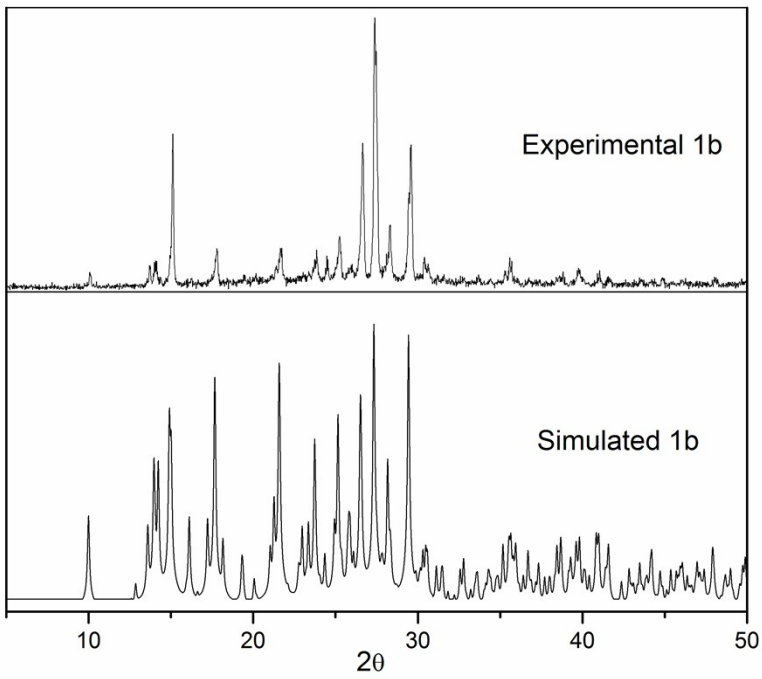

Figure S6: XRPD of 1b

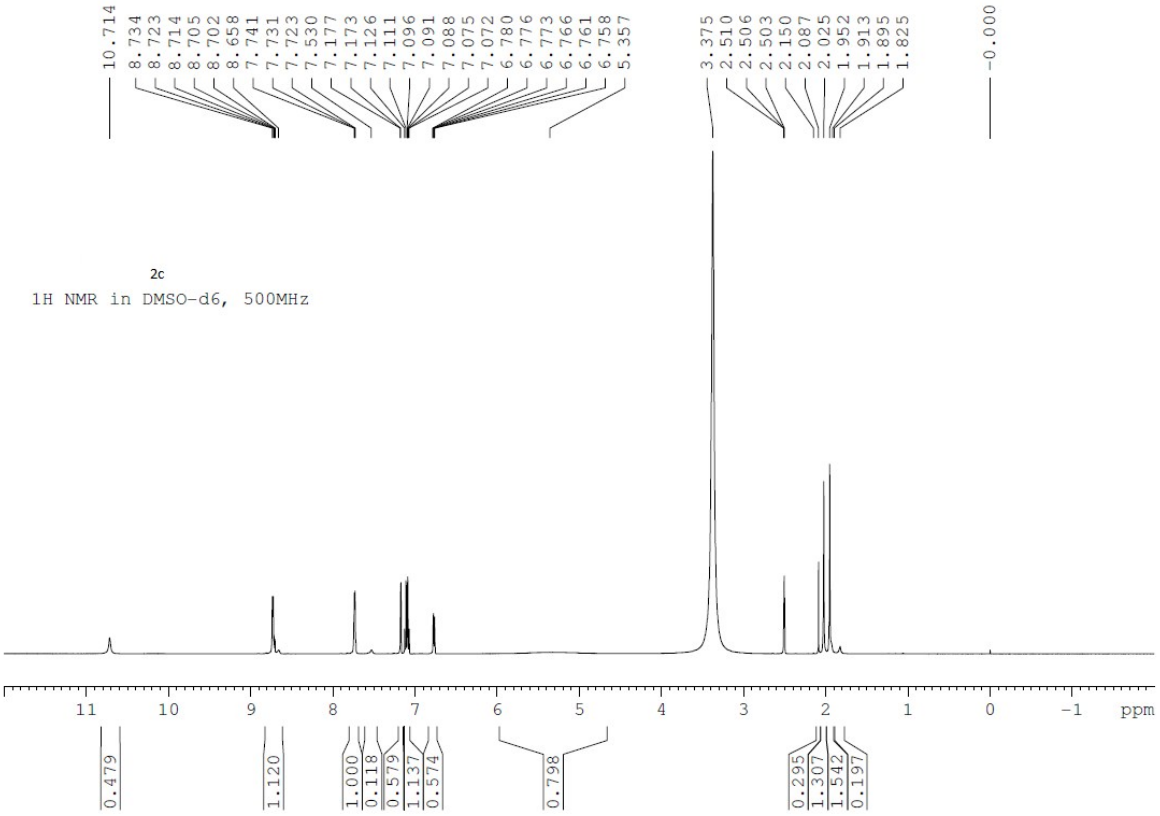

Figure S7a: NMR spectrum of 2c

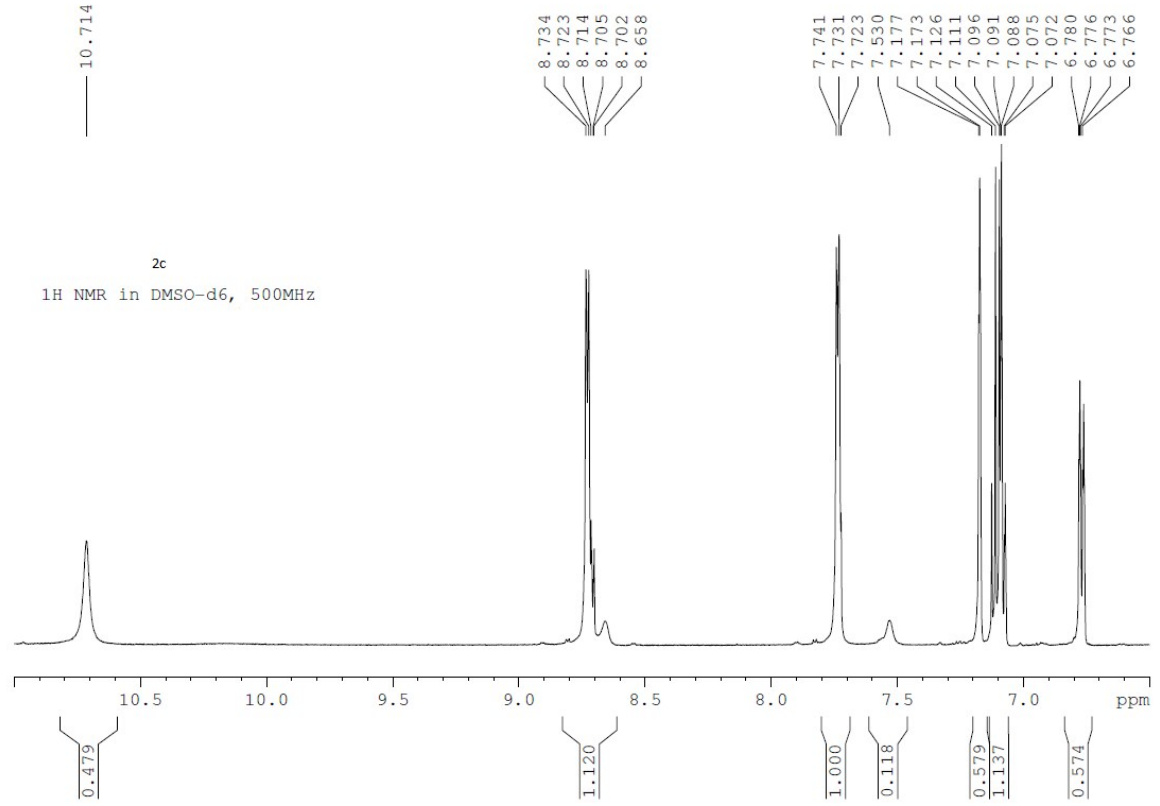

Figure S7b: NMR spectrum of 2c

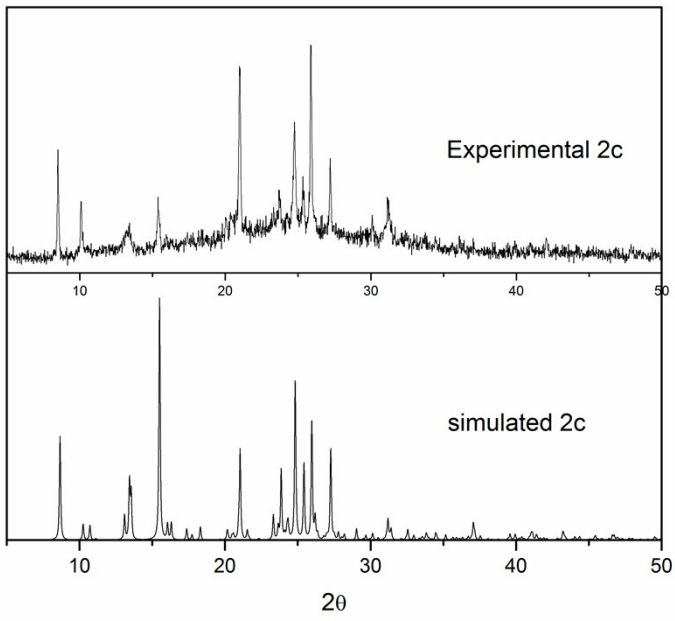

Figure S8: XRPD of 2c

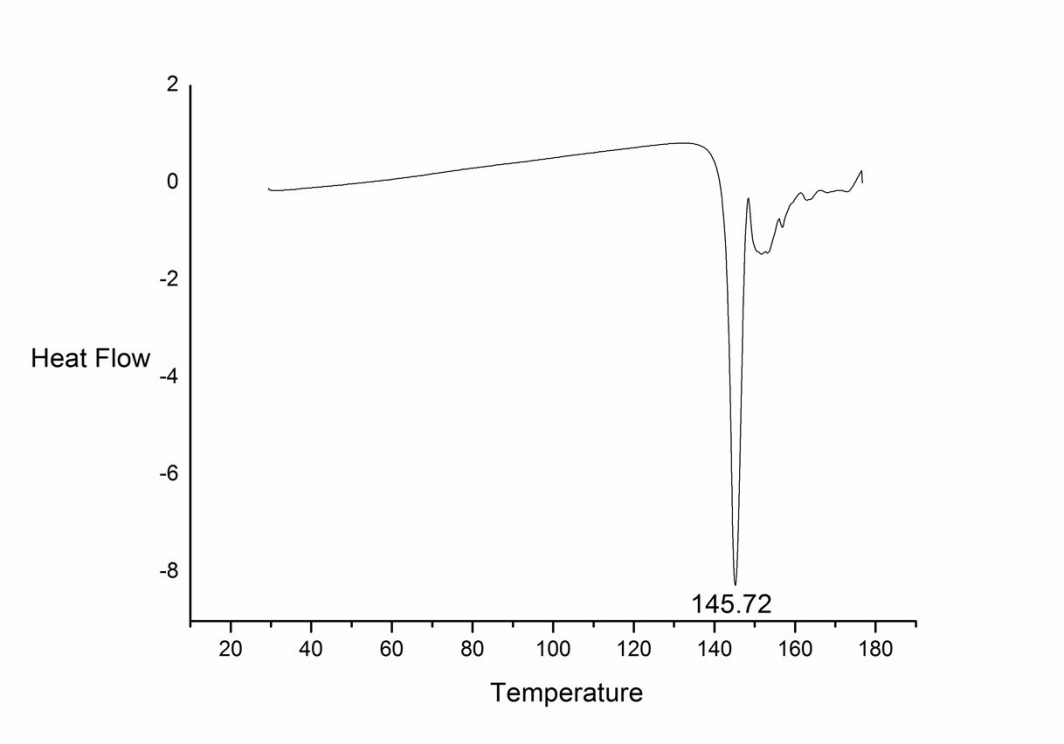

Figure S9: DSC thermogram of 1d

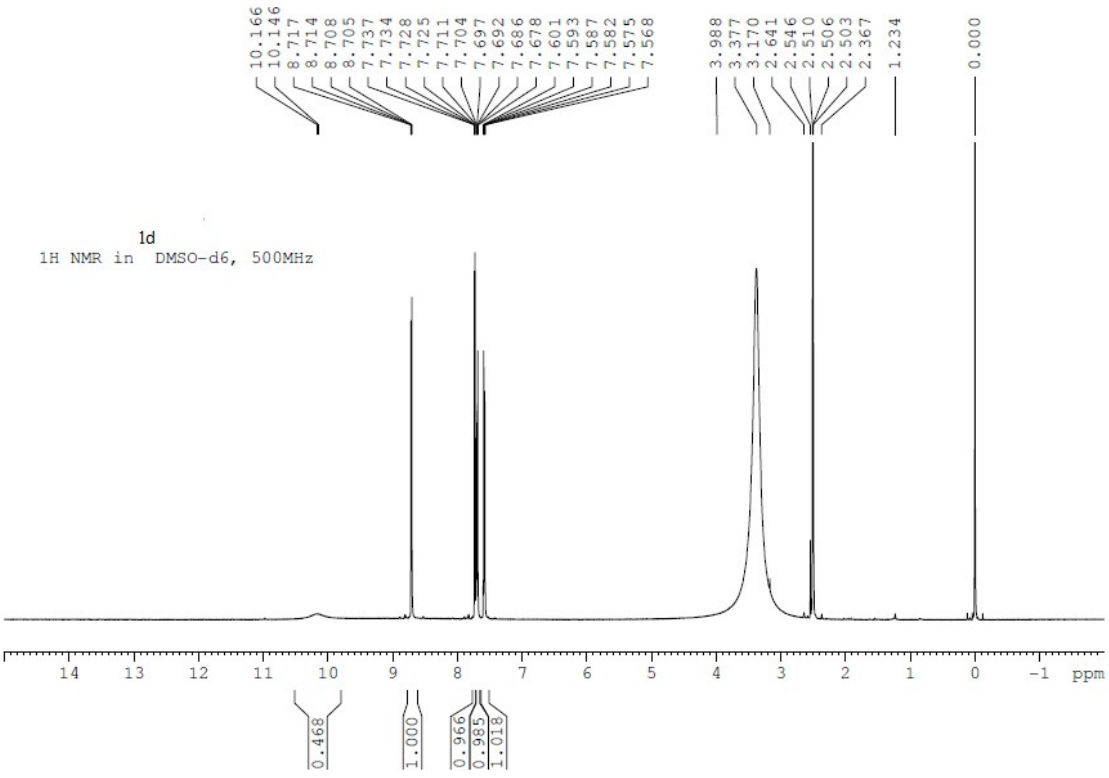

Figure S10a: NMR spectrum of 1d

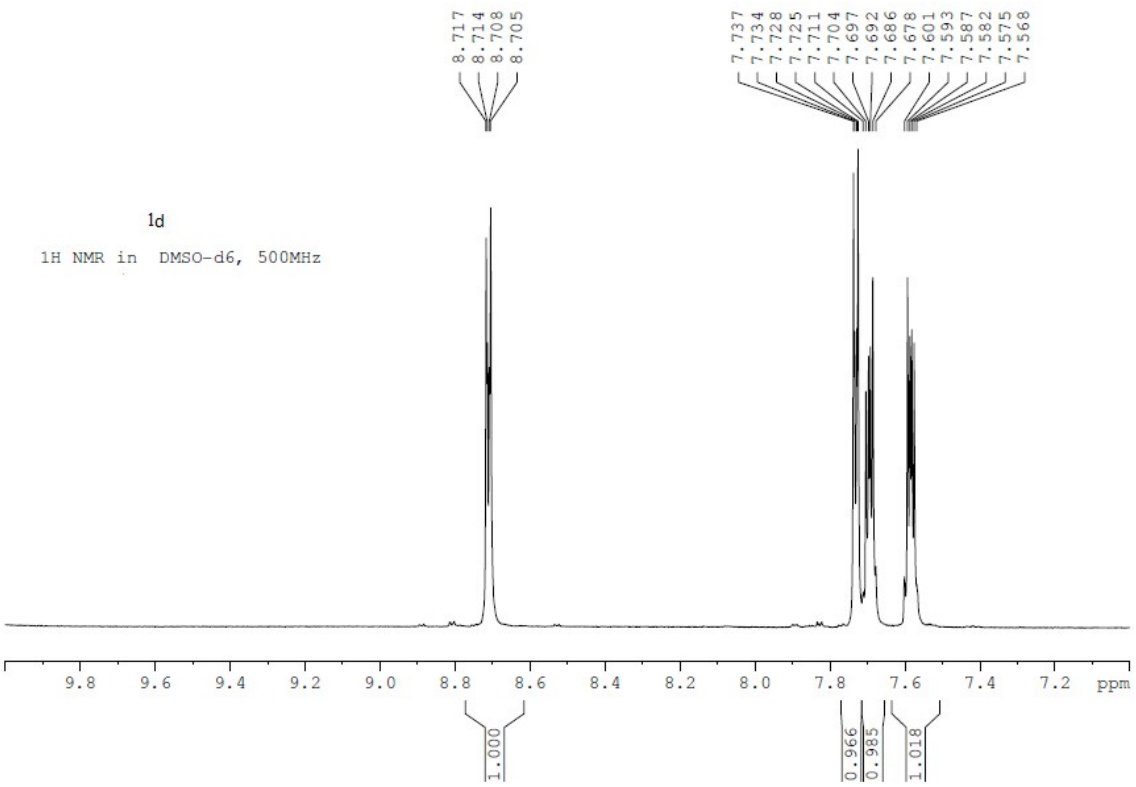

Figure S10b: NMR spectrum of 1d

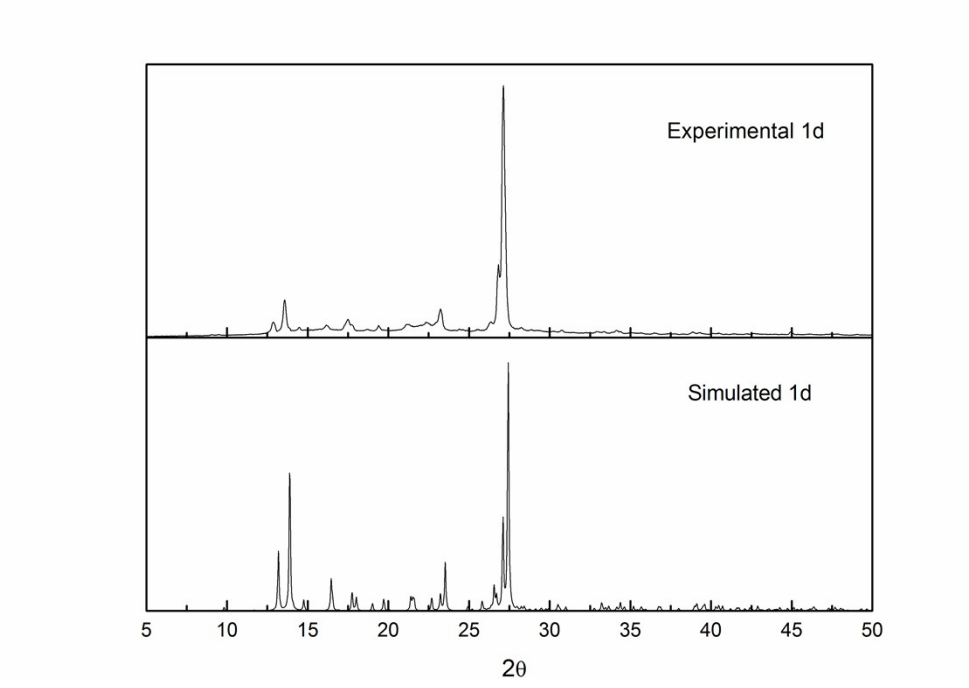

Figure S11: XRPD of 1d

Characterization by ^{1}H NMR:

NMR(500 MHz, DMSO-d_6): 1a: 8.7 (dd, J=12Hz, 2H), 7.7 (d, J=9Hz, 2H), 7.1(d, J=3Hz, 1H), 6.9(dd, J=9Hz, 1H), 6.8(d, J=9Hz, 1H),

NMR(500 MHz, DMSO-d_6): 1b: 8.8(dd, J=4.5Hz, 2H), 7.8(dd, J=4.5Hz, 2H), 7.8(dd, J=4.5Hz, 2H), 6.2(d, J=8Hz, 2H), 7.0(t, J=4.2Hz, 1H).

NMR(500 MHz, DMSO-d_6): 1c: 8.7(dd, J=9Hz, 2H), 7.7(dd, J=9Hz, 2H), 7.1(d, J=2Hz, 1H), 6.7(dd, J=3.5Hz, 1H), 7.0(d, J=7.5Hz, 1H), 7.1(d, J=8Hz, 1H).

NMR(500 MHz, DMSO-d_6): 1d: 8.7(d, J=4.5Hz, 2H), 7.7(d, J=4.5Hz, 2H), 7.6(m, J=9Hz, 2H), 7.5(m, J=10Hz, 2H)

Characterization by FT-IR:

1a: 1601(m), 1656(s) 3211.4(s).
1b: 1580(m), 1636(s), 1580(m), 3054(s)
1c: 1601.6(m), 1669.6(s), 3071(s).
1d: 1632.3(m), 1659.6(s), 3306.1(s).