Support information

Comprehensive analysis of crystal structure, spectroscopic properties, quantum chemical insights, and molecular docking studies of two pyrazolopyridine compounds: Potential anticancer agents

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Table SI-1. NMR data compound **4a** (DMSO-d_6) and **4b** ($CDCl_3$)

4a		4b	
δ_C (ppm)	δ_H (ppm)	δ_C (ppm)	δ_H (ppm)
12.2 (CH_3)	2.59 (s)	15.6 (CH_3)	2.23 (s)
28.5 (CH_2)	3.23 (t, *J* = 6.3 Hz)	28.3 (CH_2)	3.28-3.32 (m)
36.1 (CH_2)	2.76-2.80 (m)	36.8 (CH_2)	2.77-2.80 (m)
116.9 (C)	-	40.2 (2 x CH_3)	3.06 (s)
120.5 (2xCH)	8.22 (d, *J* = 7.8 Hz)	110.9 (2xCH)	7.53 (t, *J* = 8.0 Hz)
125.0 (C)	-	116.0 (C)	-
126.0 (CH)	7.35 (t, *J* = 7.4 Hz)	119.4 (C)	-
127.2 (2xCH)	7.57 (t, *J* = 7.9 Hz)	121.5 (2 x CH)	6.81 (d, *J* = 8.0 Hz)
129.2 (CH)	8.54 (s)	121.8 (C)	-
138.6 (C)	-	126.1 (CH)	7.31-7.33 (m)
145.8 (C)	-	129.0 (2 x CH)	7.31-7.33 (m)
152.9 (C)	-	130.7 (2xCH)	8.25 (d, *J* = 8.0 Hz)
174.6 (C)	-	139.0 (C)	-
203.4. (C=O)	-	145.9 (C)	-
		147.7 (C)	-
		150.9(C)	-
		153.3 (C)	-
		175.1 (C)	-
		202.8 (C=O)	-

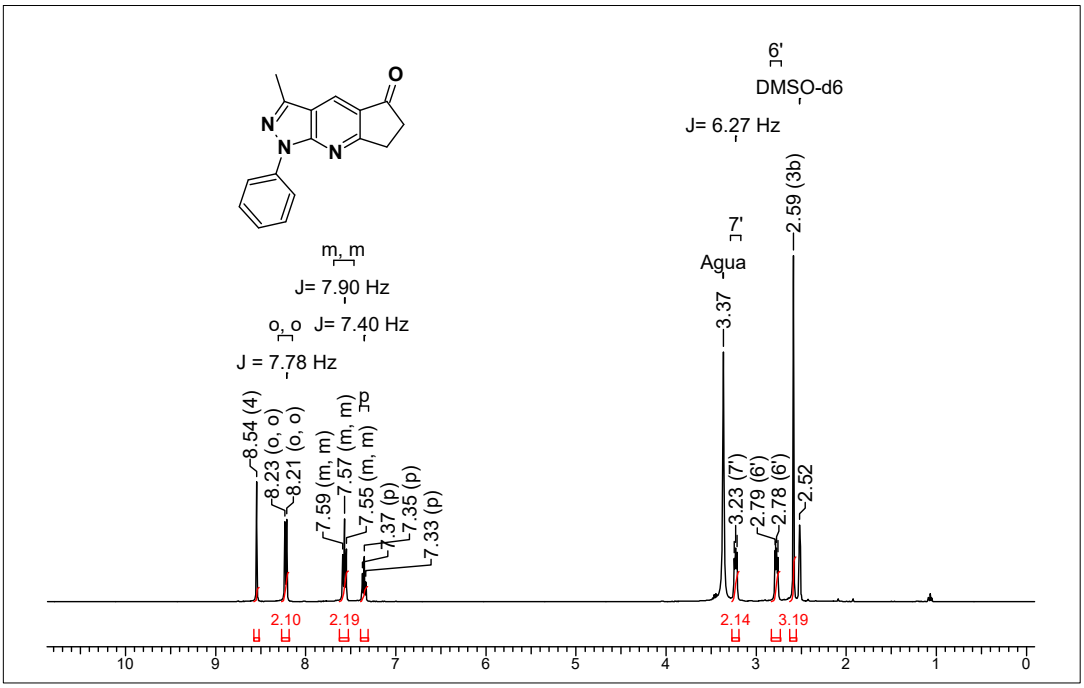

Figure SI-1. ^{1}H-NMR spectrum of compound **4a**

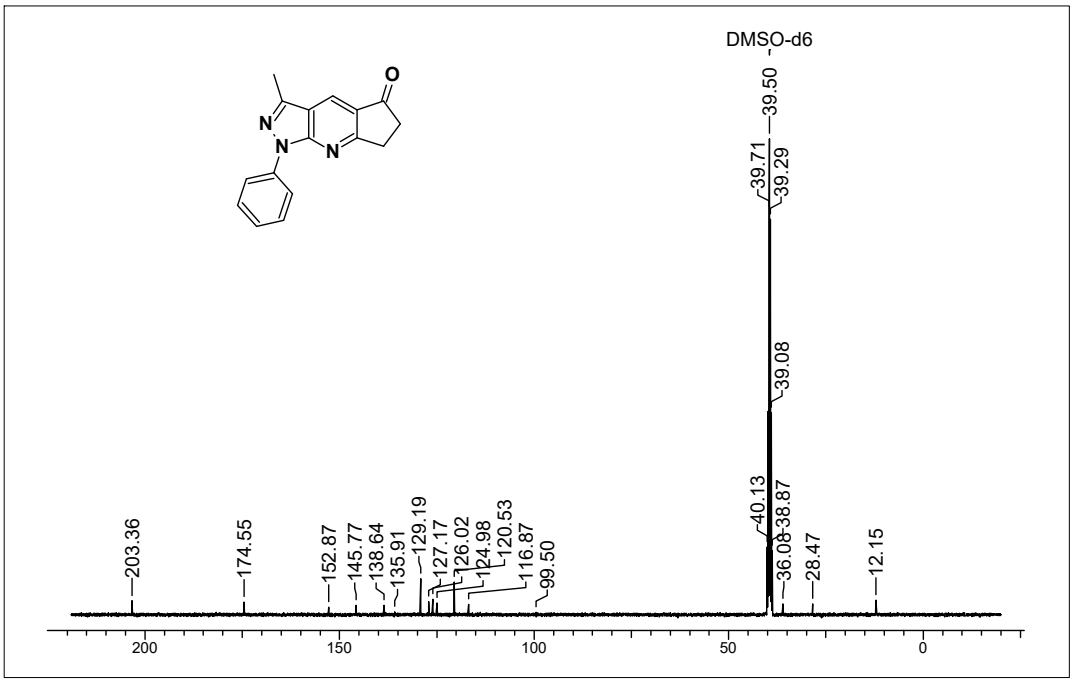

Figure SI-2. ^{13}C-NMR spectrum of compound **4a**

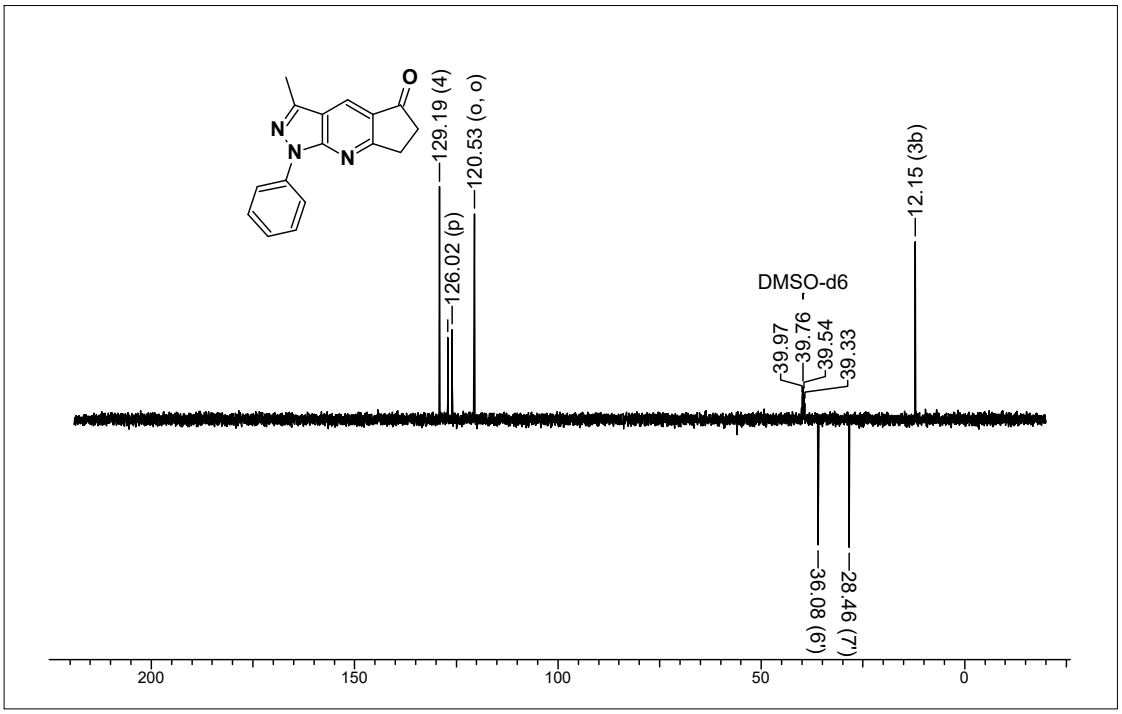

Figure SI-3. DEPT-135 spectrum of compound **4a**

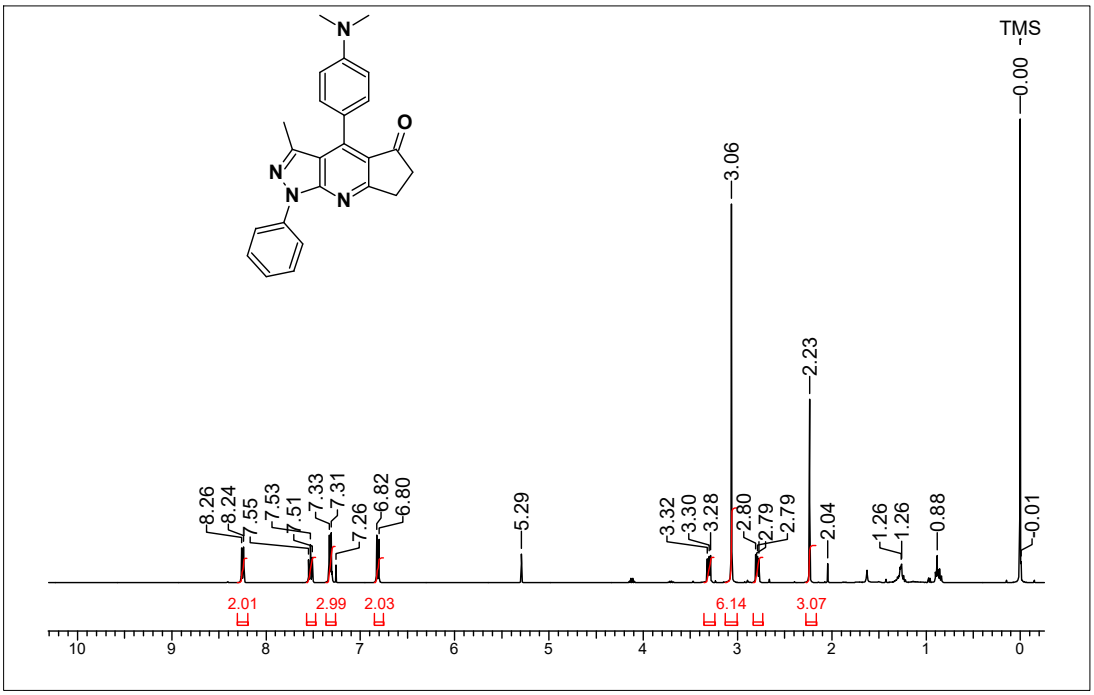

Figure SI-4. ^{1}H-NMR spectrum of compound **4b**

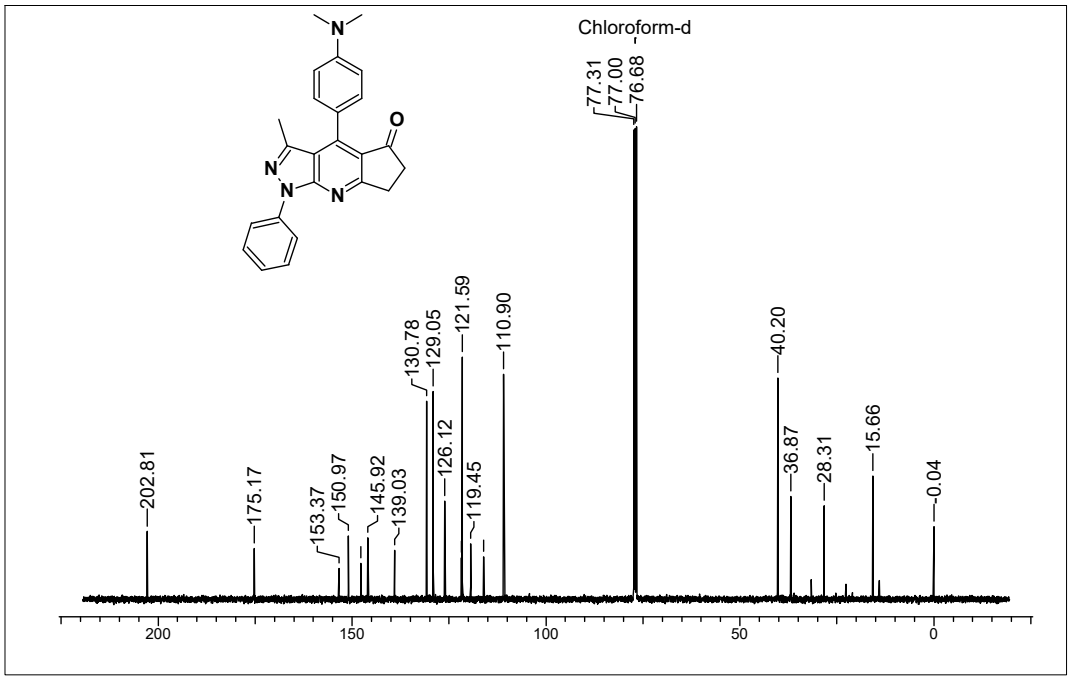

Figure SI-5. ^{13}C-NMR spectrum of compound **4b**

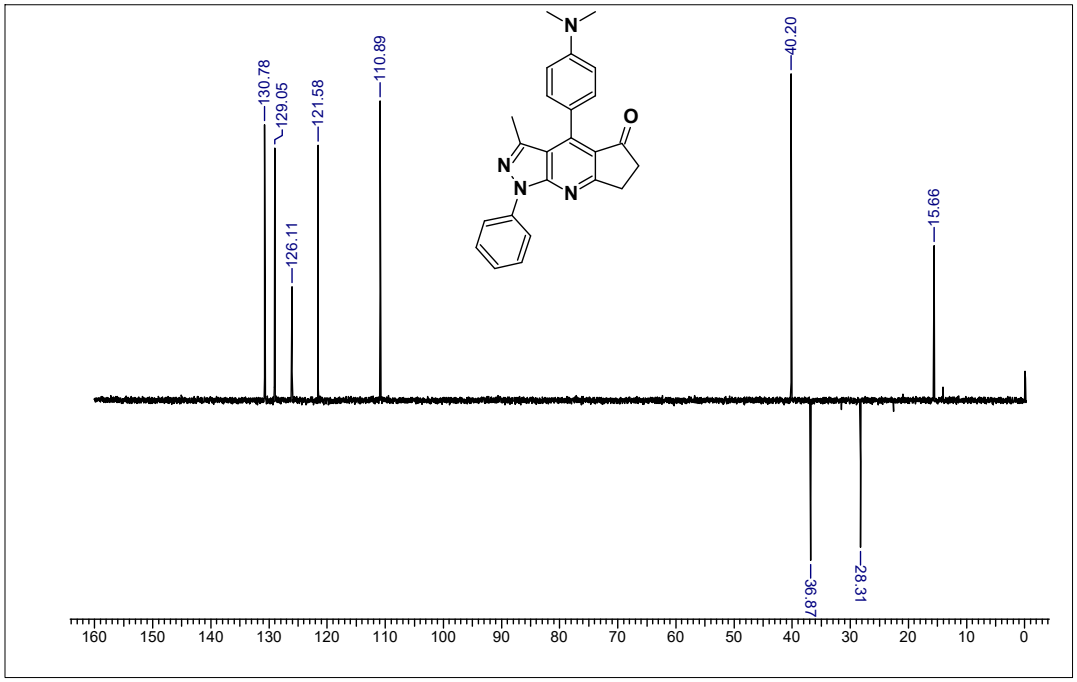

Figure SI-6. DEPT-135 spectrum of compound **4b**

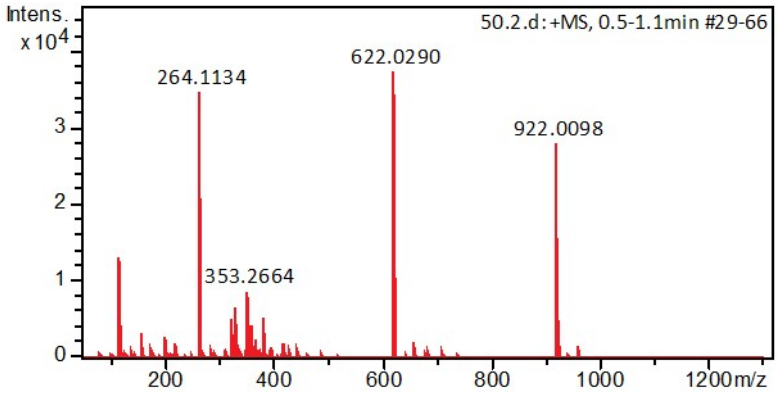

Figure SI-7. MS spectrum of compound **4a**

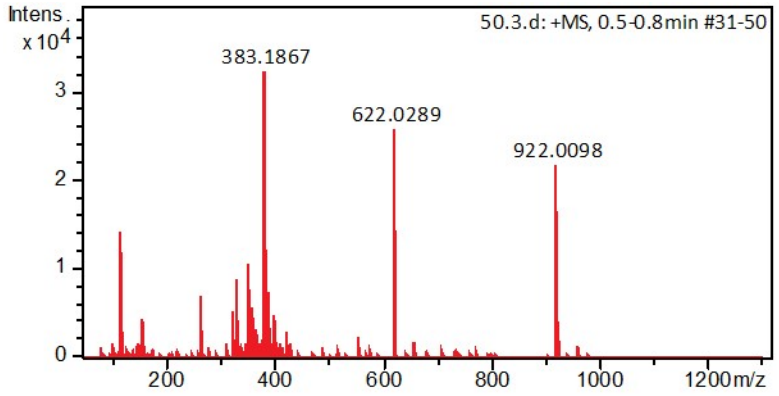

Figure SI-8. MS spectrum of compound **4b**

Figure SI-9. ORTEP plots of compounds **4a** (left) and **4b** (right). Thermal ellipsoids were drawn with 30% of probability. H-atoms were omitted for sake

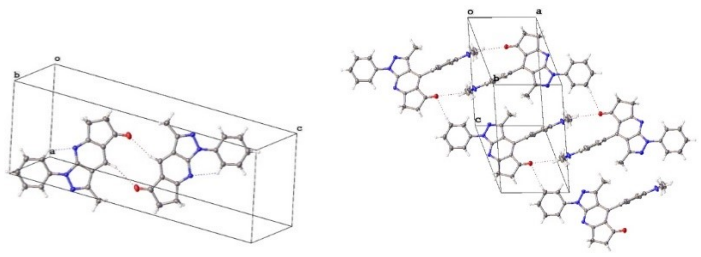

Figure SI-10. Crystal Packing of compounds **4a** (left) and **4b** (right)

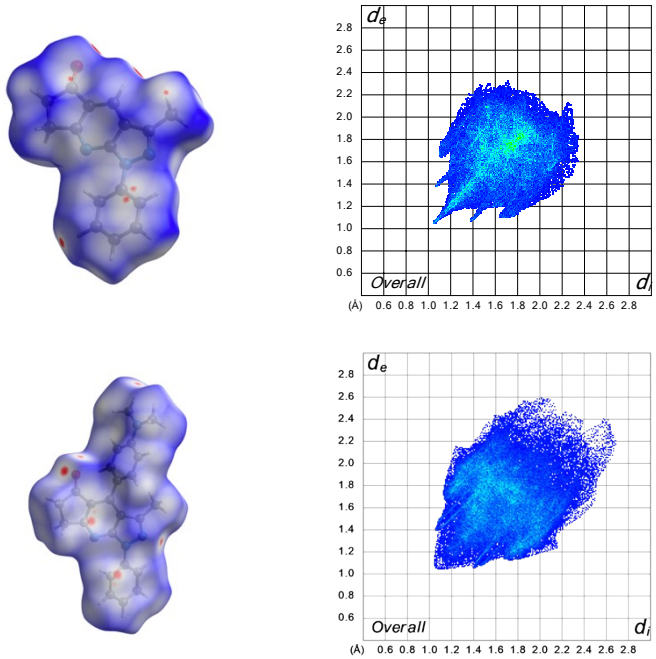

Figure SI-11. Overall Hirshfeld surface (left) for title compound and its fingerprint plot (right) for compounds **4a** (top) and **4b** (bottom)

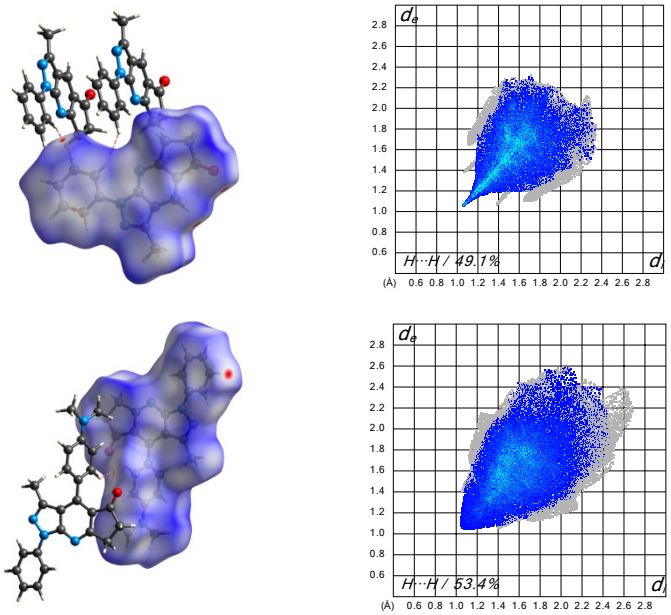

Figure SI-12. Dihydrogen bond-like interactions in compound **4a** (top) and **4b** (bottom)

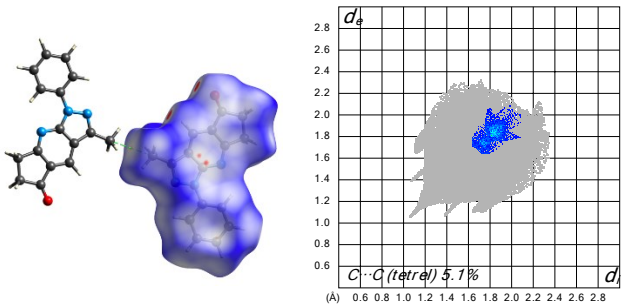

Figure SI-13. Ditetrel bond interaction in compound **4b**

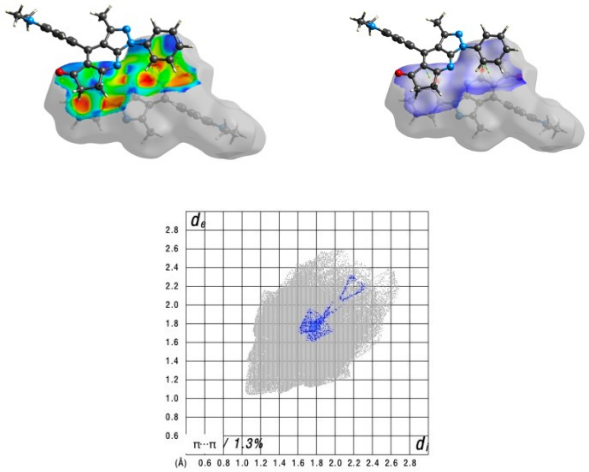

Figure SI-14. Shape index surface (left), and dnorm surface (middle) for compound **4b** and its fingerprint plot (right), showing π···π stacking interactions

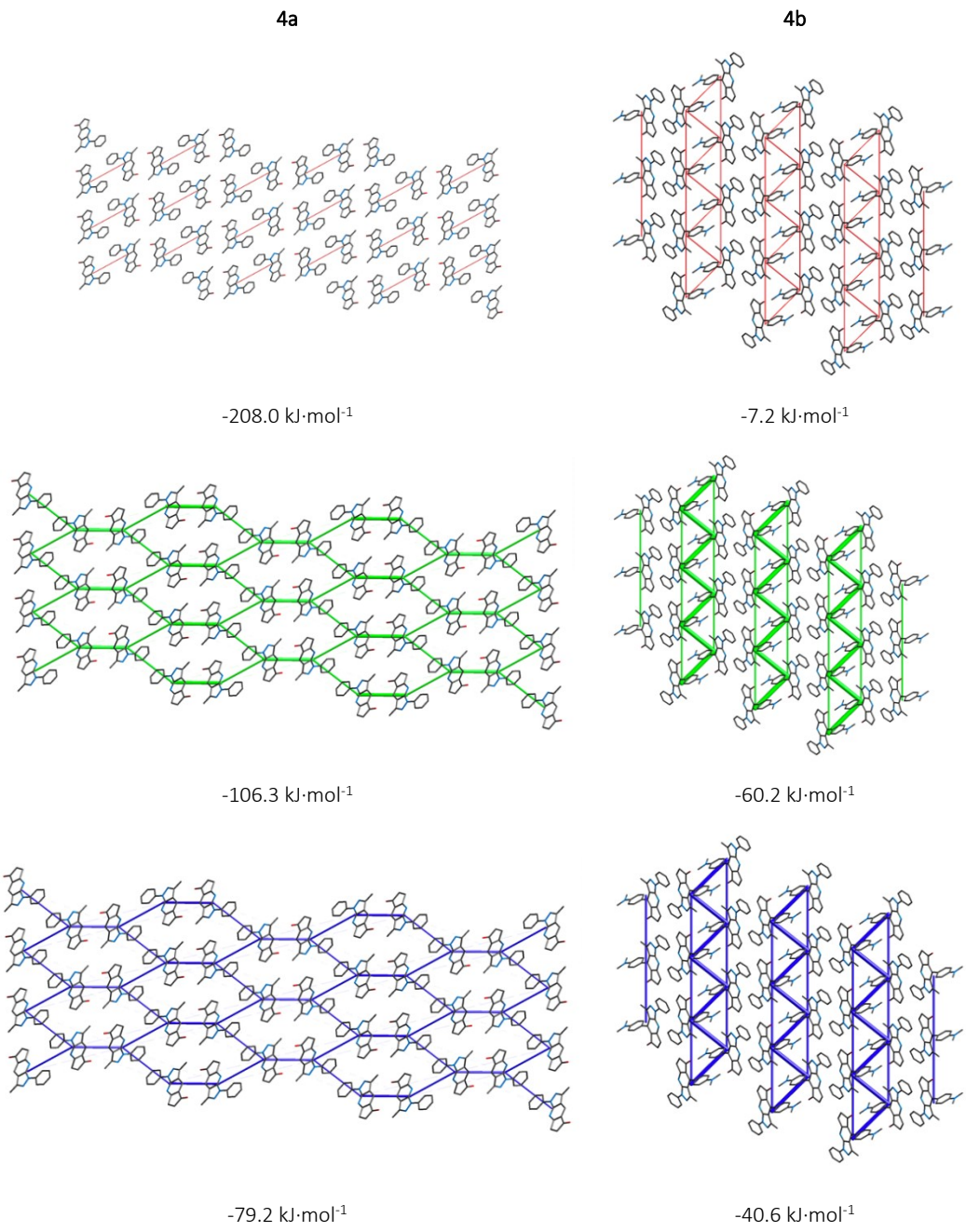

Figure SI-15. Energy framework of the compounds **4a** (left), and **4b** viewed along [100] direction