Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information for: Exploring the Geometric, Magnetic and Electronic Properties of Hofmann MOFs for Drug Delivery

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1 Supporting Information

1. Comparison of dispersion corrected binding energies evaluated from GGA-PBE and PBE+U calculations.

2. Spin-resolved electronic band structures as obtained from PBE+U calculation.

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Table S1: Dispersion corrected (D) binding energies evaluated from GGA-PBE and PBE+U (PBEU) calculations. P and B stand for pyrazine and bi-pyridine ligands, respectively.

Drugs	Ni-Fe (kJ/mol)		Ni-Co (kJ/mol)	
	P(PBE-D/PBEU-D)	B(PBE-D/PBEU-D)	P(PBE-D/PBEU-D)	B(PBE-D/PBEU-D)
Fluorouracil	-78.08/-76.86	-68.93/72.81	-63.41/-70.19	-53.44/-62.32
Niacin	-56.33/-61.68	-88.03/-93.74	-38.07/-47.40	-65.93/-74.31

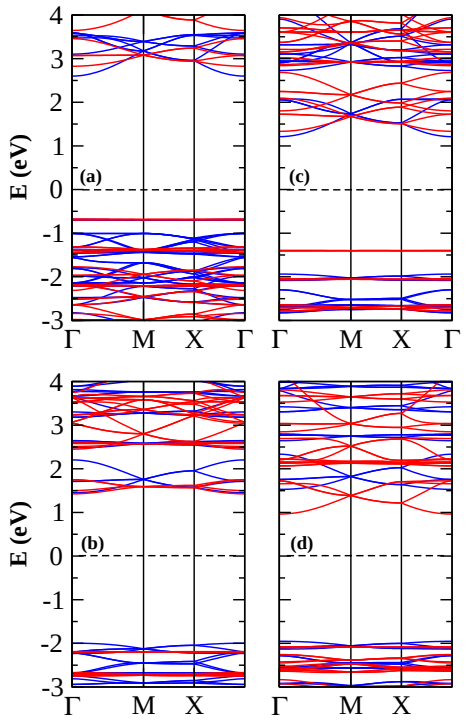

Figure S1: Spin-resolved electronic band structures of (a) Ni-Cr (b) Ni-Mn (c) Ni-Fe and (d) Ni-Co sheets as obtained from PBE+U calculation. The blue (red) line represents the bands for up (down) spin state. The dotted line represents the Fermi level.