Supporting Information

Probing the role of Anions in Influencing the Structure, Stability and Properties in Neutral N-donor Linker based Metal-Organic Frameworks

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Figures:

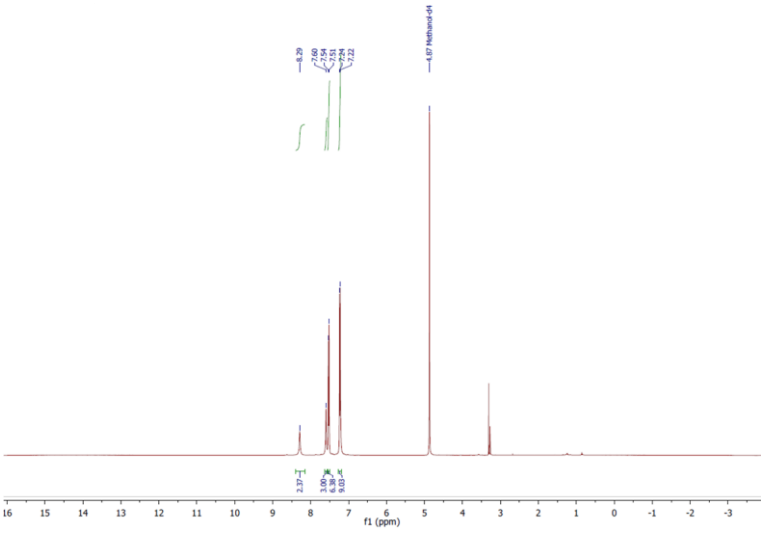

Figure S1: ^{1}H-NMR for ligand (L) recorded in CD_3OD.

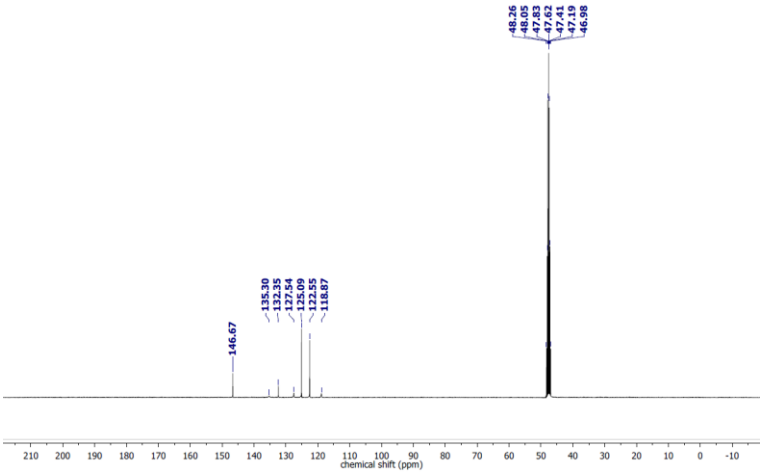

Figure S2: ^{13}C-NMR for ligand (L) recorded in CD_3OD.

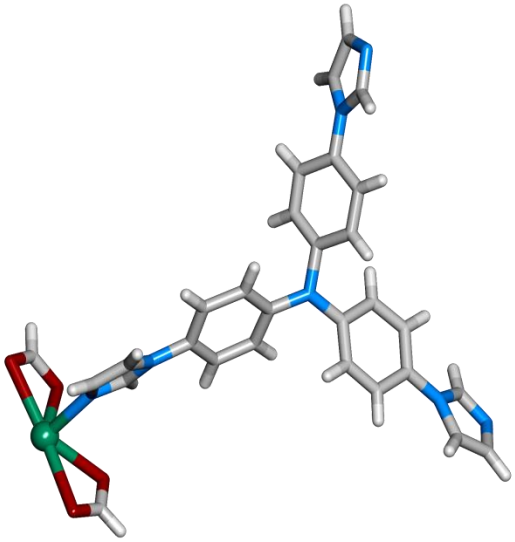

Figure S3: Asymmetric unit of **IPM-311**. (Colour code: C, grey; N, blue; Cd, green; O, dark red; H, white)

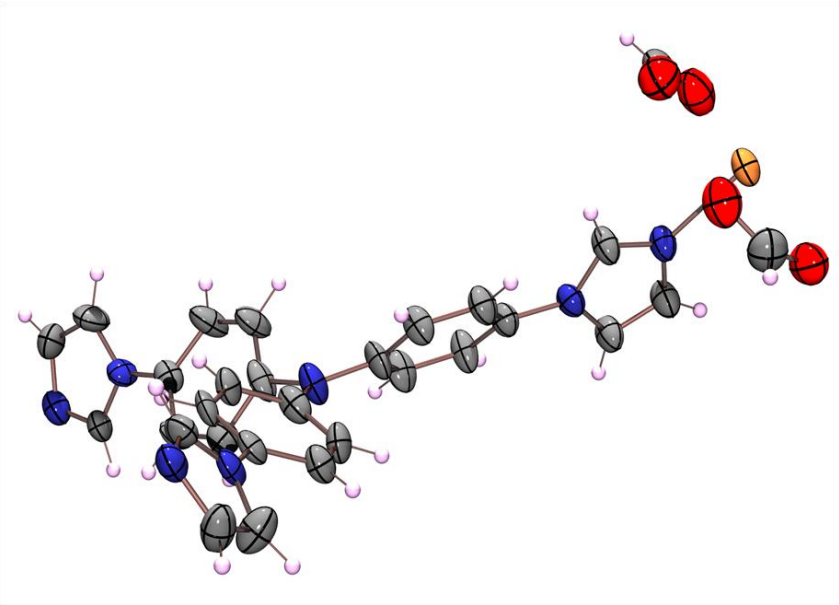

Figure S4: ORTEP diagram of **IPM-311** in thermal ellipsoids 50% probability. (Colour code: C, grey; N, blue; Cd, orange; O, dark red; H, pink)

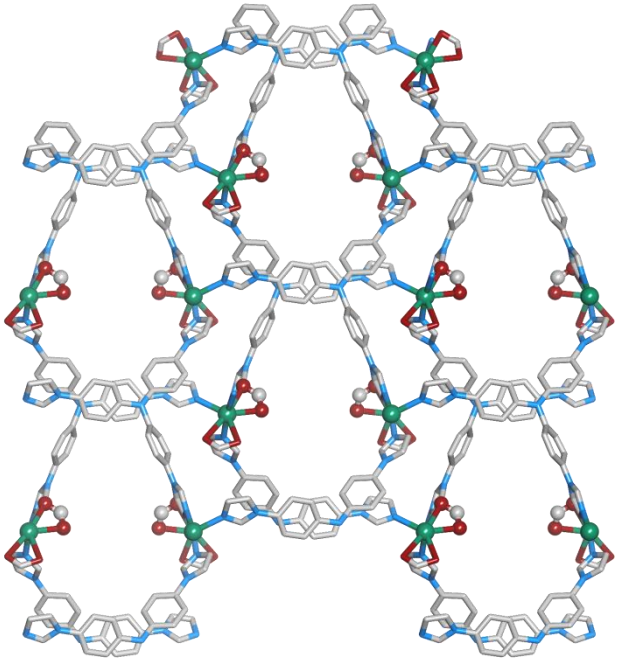

Figure S5: Figure showing packing of **IPM-311** along crystallographic *c*-axis, (Hydrogen atoms have been omitted for clarity. Colour code: C, grey; N, blue; Cd, green; O, dark red)

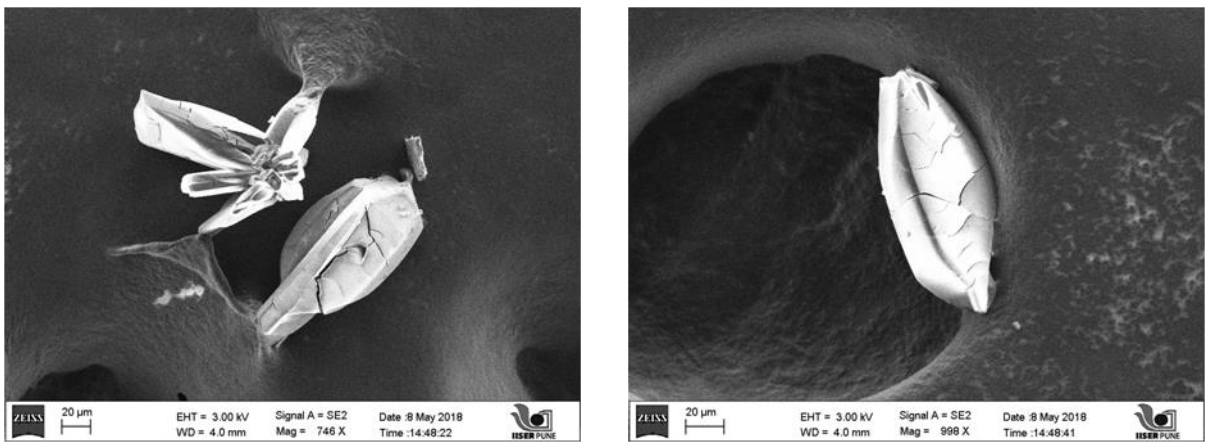

Figure S6: FESEM images for compound **IPM-311.** The images were recorded for the solid sample on carbon tape.

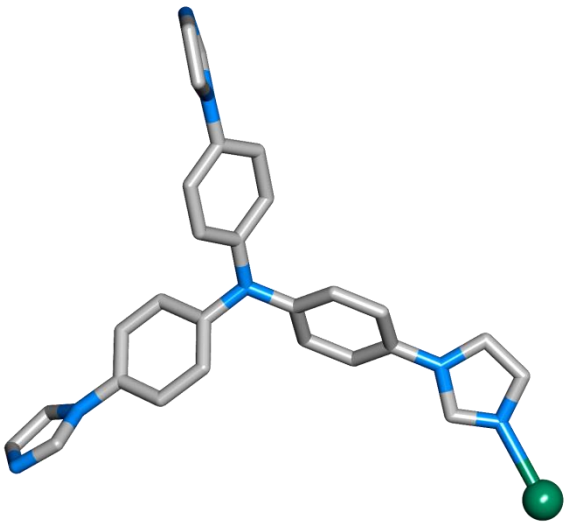

Figure S7: Asymmetric unit of **IPM-206**. (Colour code: C, grey; N, blue; Cd, green. H-atoms are omitted for clarity)

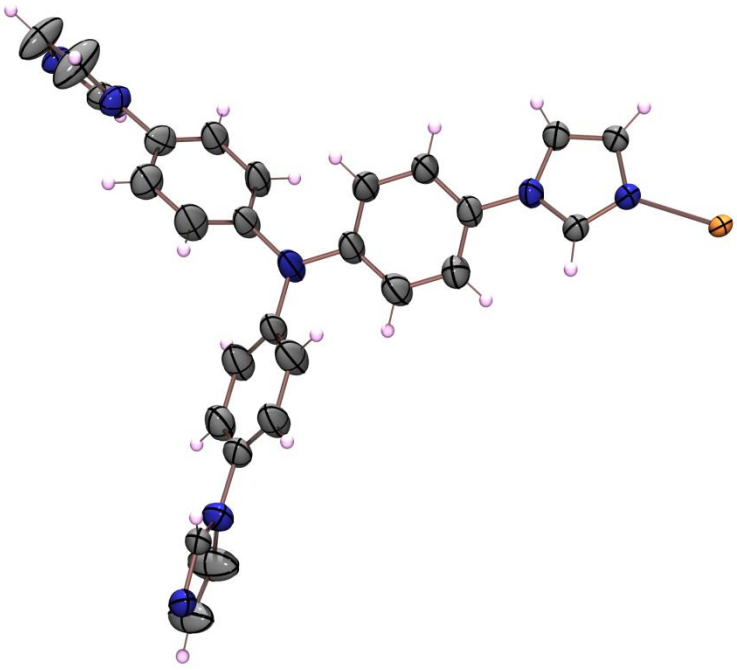

Figure S8: ORTEP diagram of **IPM-206** in thermal ellipsoids 50% probability. (Colour code: C, grey; N, blue; Cd, orange; H, pink)

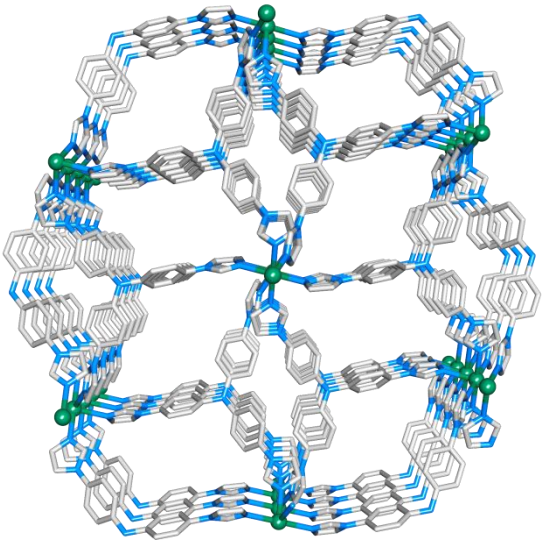

Figure S9: Figure showing packing of **IPM-206** along crystallographic *b*-axis (Hydrogen atoms have been omitted for clarity. Colour code: C, grey; N, blue; Cd, green)

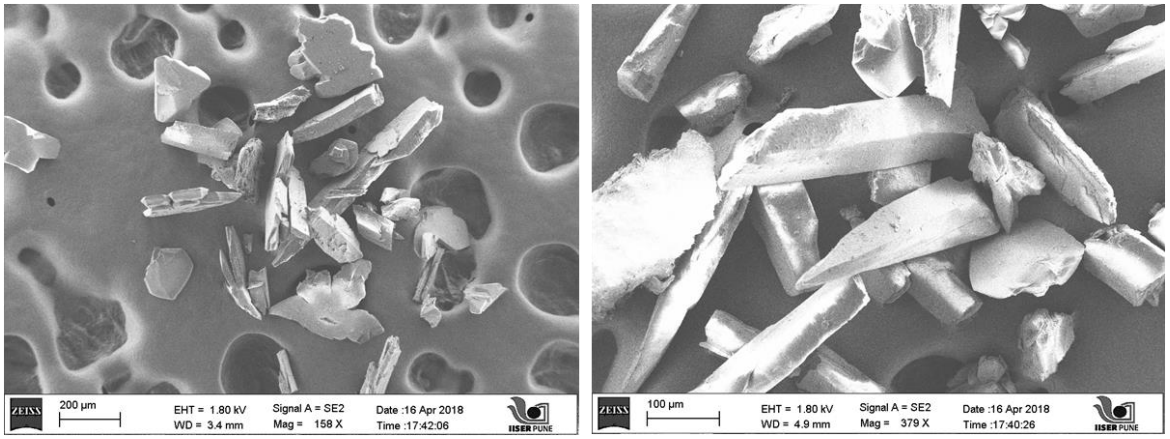

Figure S10: FESEM images for compound **IPM-206.** The images were recorded for the solid sample on carbon tape.

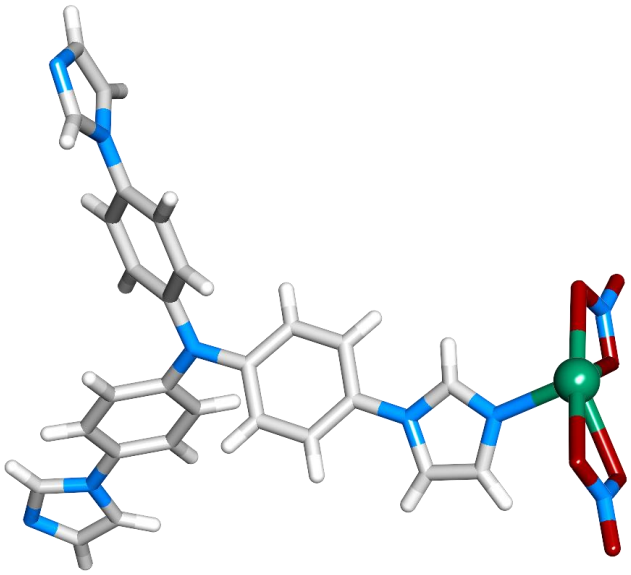

Figure S11: Asymmetric unit of **IPM-310**. (Colour code: C, grey; N, blue; Cd, green; O, dark red; H, white)

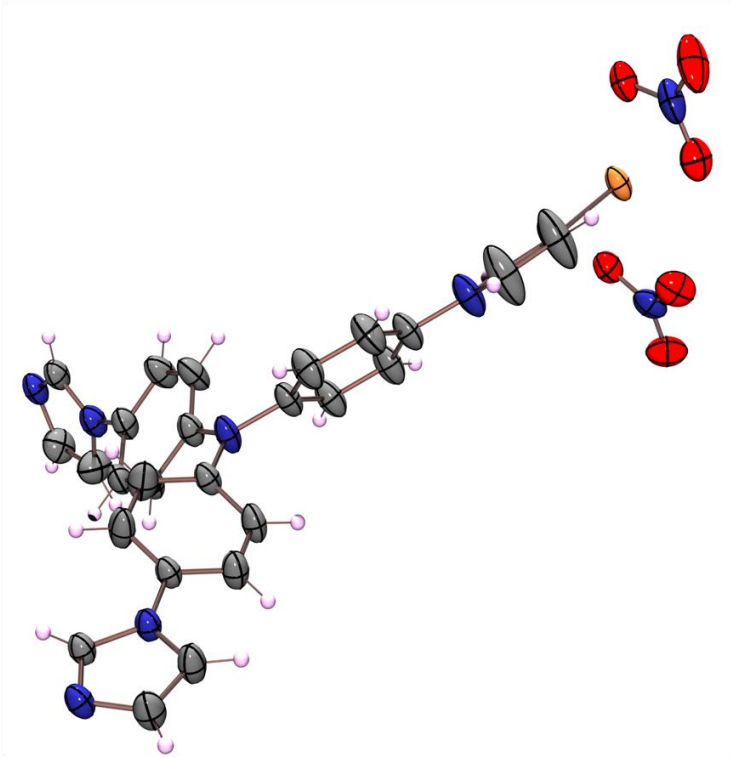

Figure S12: ORTEP diagram of **IPM-310** in thermal ellipsoids 50% probability. (Colour code: C, grey; N, blue; Cd, orange; O, red; H, pink)

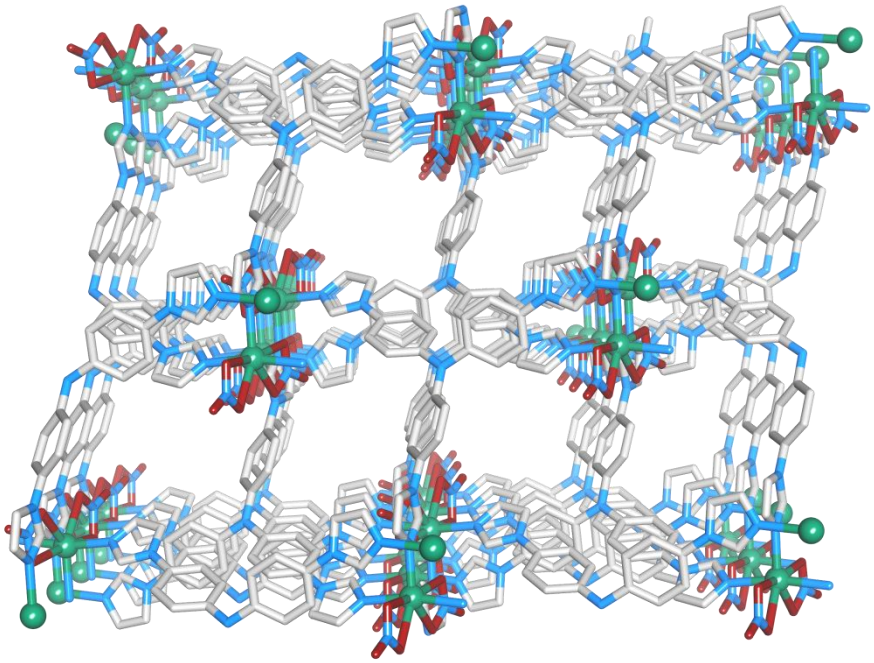

Figure S13: Figure showing packing of **IPM-310** along crystallographic *b*-axis. (Hydrogen atoms have been omitted for clarity. Colour code: C, grey; N, blue; Cd, green)

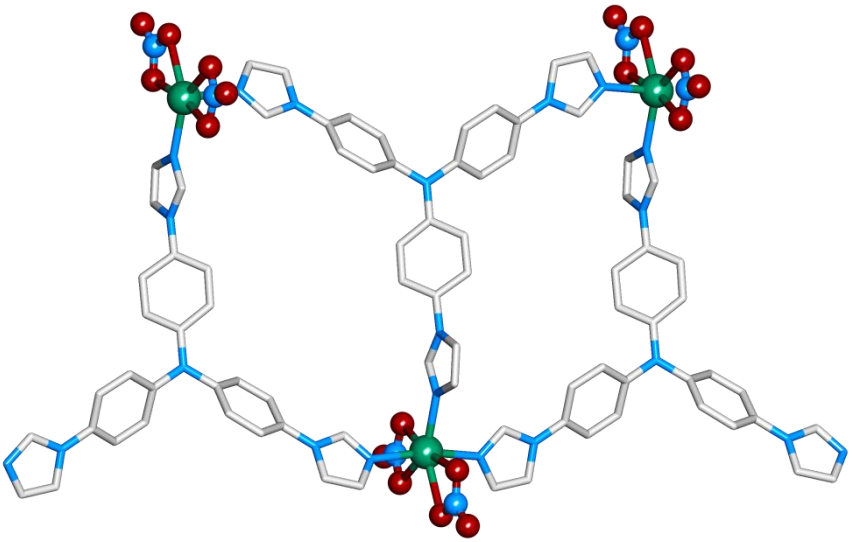

Figure S14: Figure showing one-dimensional packing of **IPM-310** showing coordinated nitrate anions. (Hydrogen atoms have been omitted for clarity. Colour code: C, grey; N, blue; Cd, green; O, red)

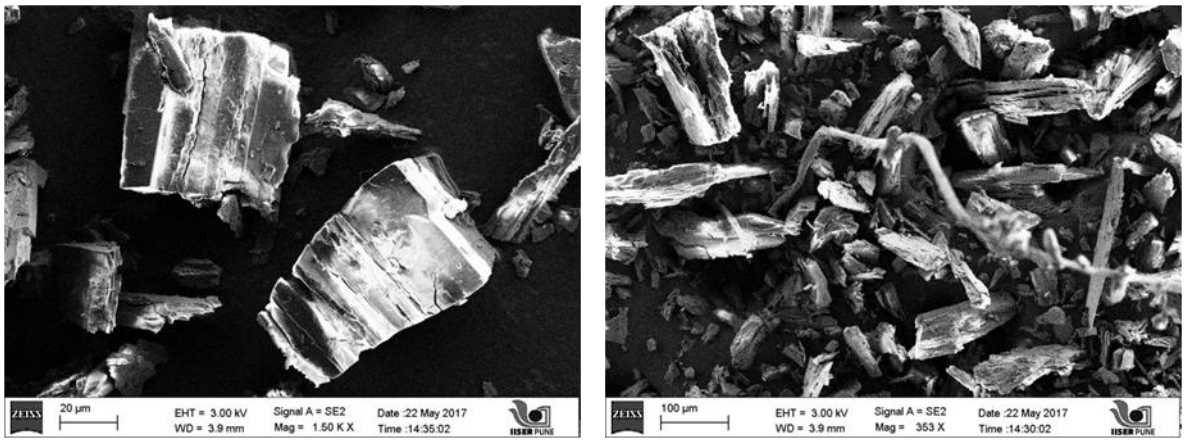

Figure S15: FESEM images for compound **IPM-310**. The images were recorded for the solid sample on carbon tape.

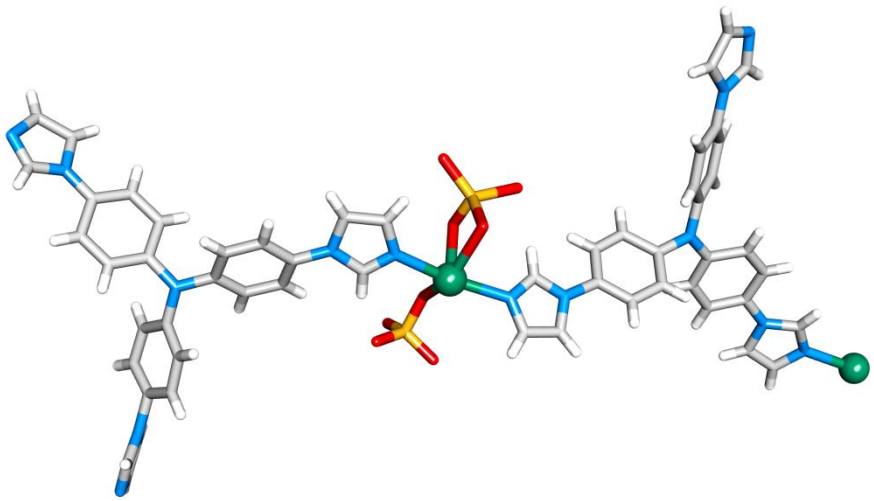

Figure S16: Asymmetric unit of **IPM-312**. (Colour code: C, grey; N, blue; Cd, green; O, dark red; H, white; S, yellow)

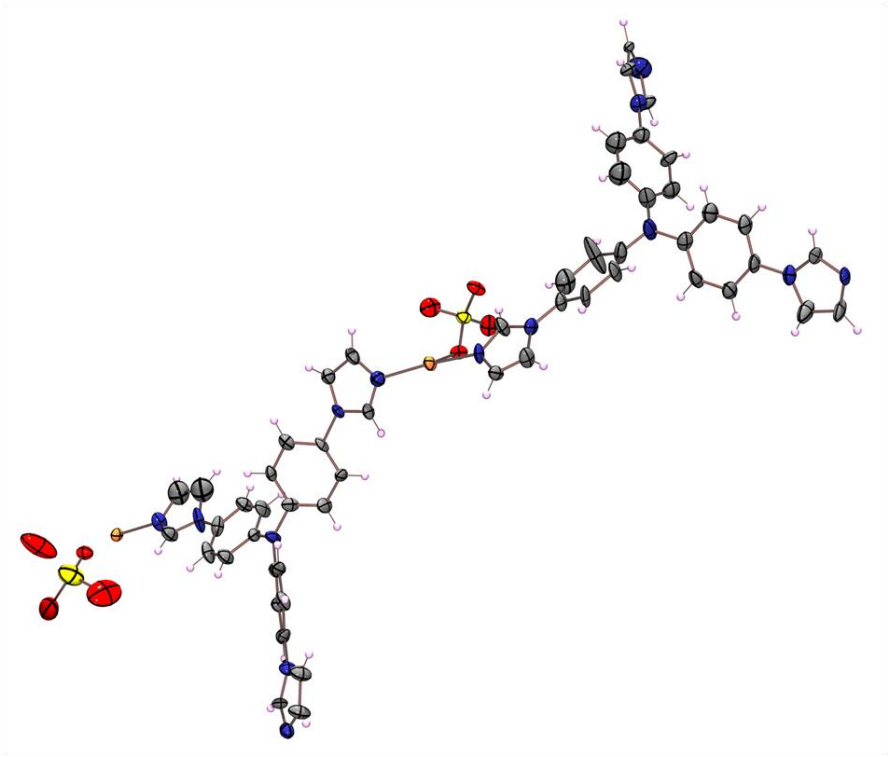

Figure S17: ORTEP diagram of **IPM-312** in thermal ellipsoids 50% probability. (Colour code: C, grey; N, blue; Cd, orange; O, red; S, yellow; H, pink)

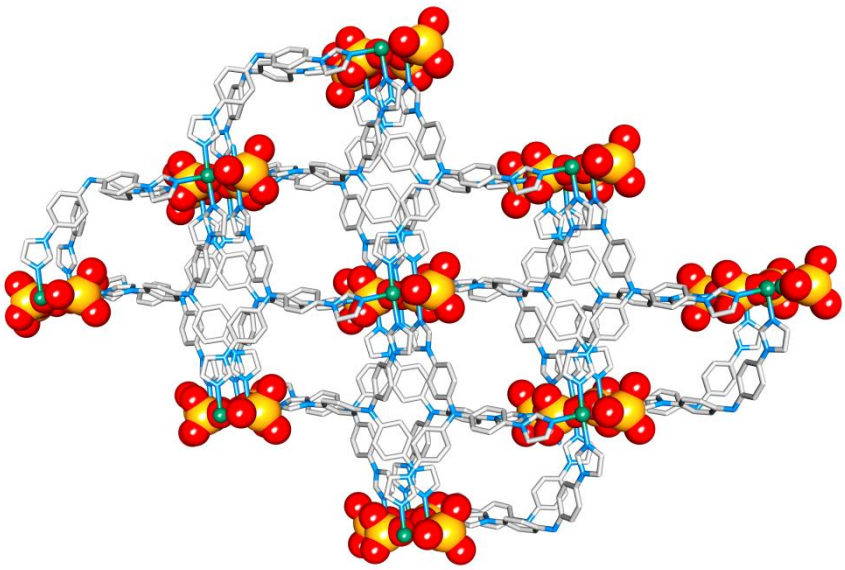

Figure S18: Figure showing packing of **IPM-312** along crystallographic *b*-axis, (Hydrogen atoms have been omitted for clarity. Colour code: C, grey; N, blue; Cd, green; O, red; S, yellow).

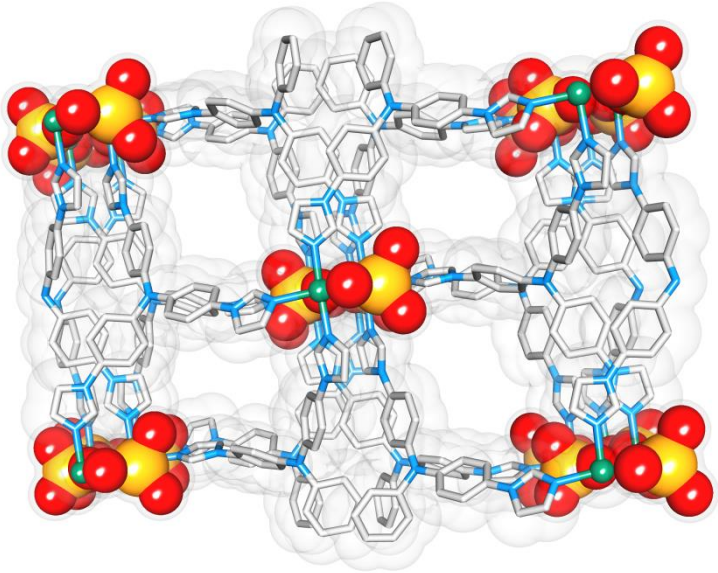

Figure S19: Figure showing packing of **IPM-312** along crystallographic *b*-axis, (Hydrogen atoms have been omitted for clarity. Colour code: C, grey; N, blue; Cd, green; O, red; S, yellow)

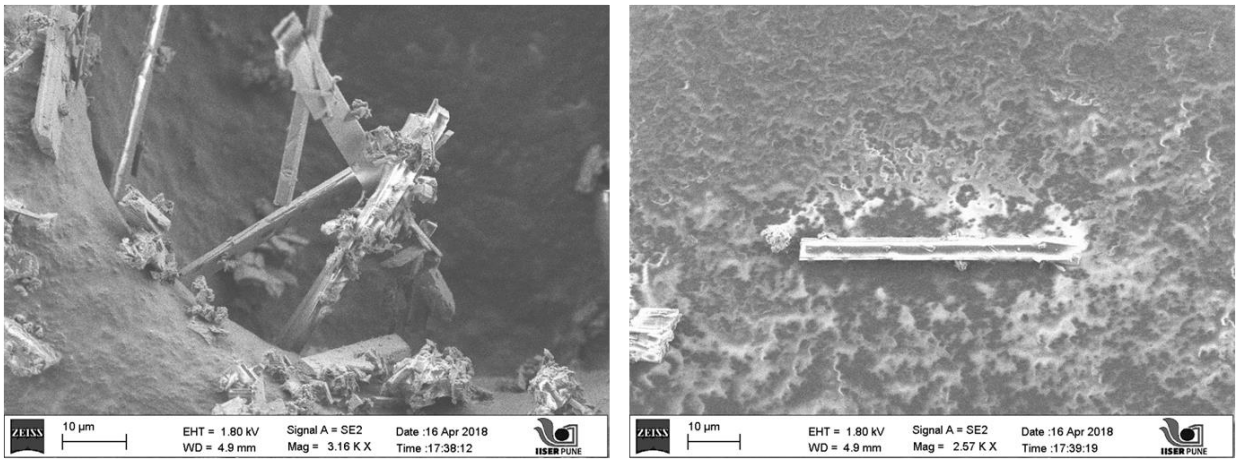

Figure S20: FESEM images for compound **IPM-312**. The images were recorded for the solid sample on carbon tape.

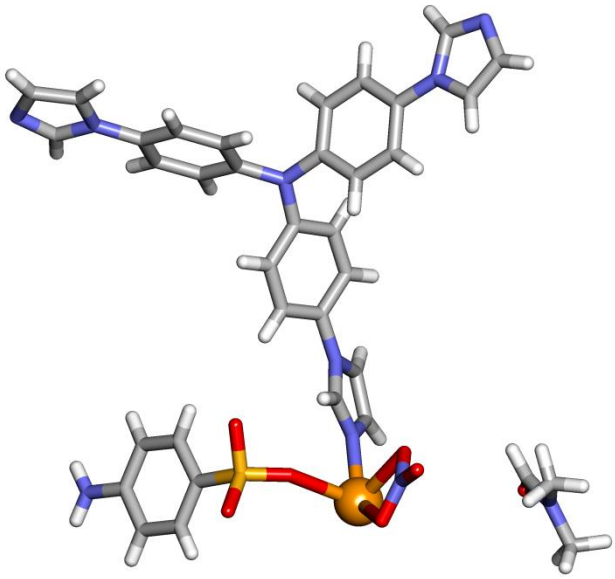

Figure S21: Asymmetric unit of **IPM-315**. (Colour code: C, grey; N, blue; Cd, orange; O, dark red; H, white; S, yellow)

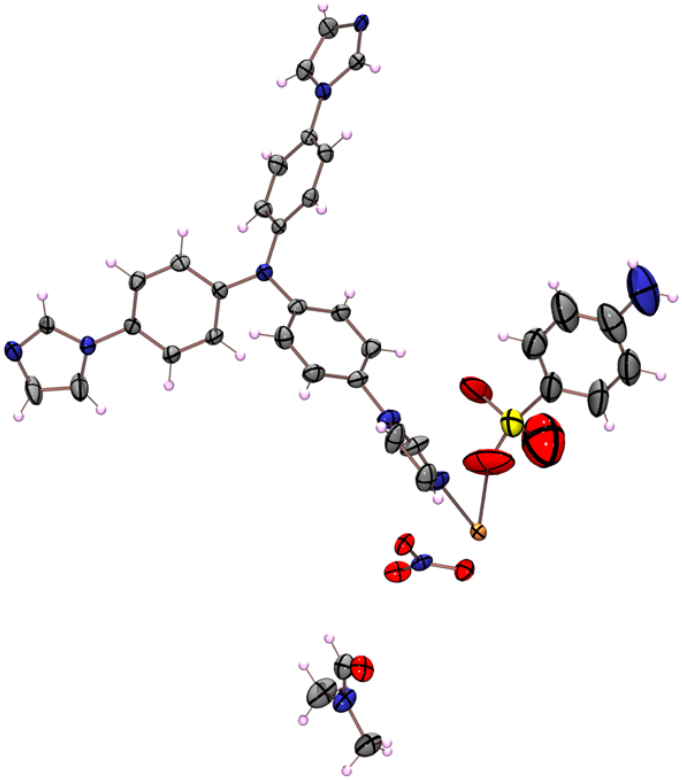

Figure S22: ORTEP diagram of **IPM-315** in thermal ellipsoids 50% probability. (Colour code: C, grey; N, blue; Cd, orange; O, red; H, pink)

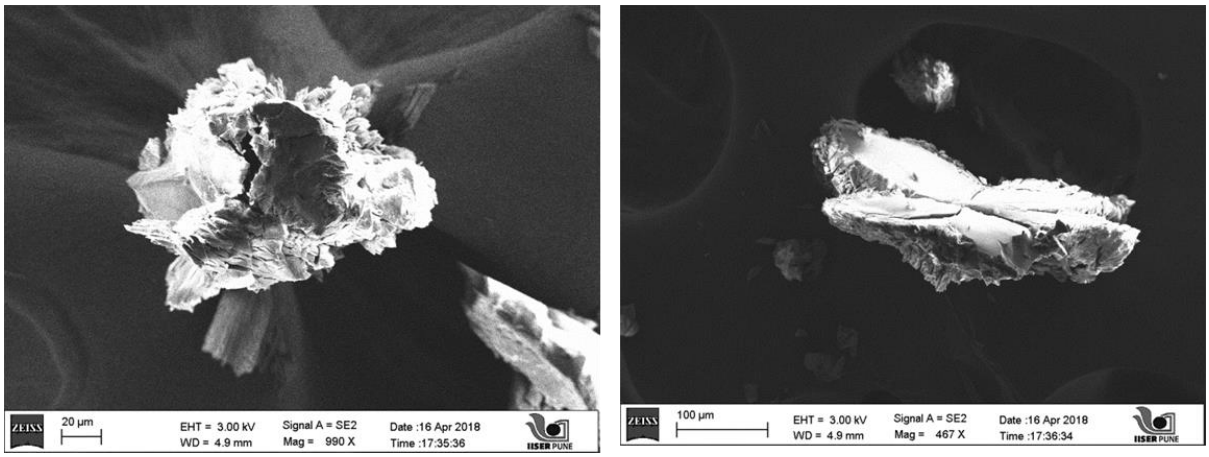

Figure S23: FESEM images for compound **IPM-315**. The images were recorded for the solid sample on carbon tape.

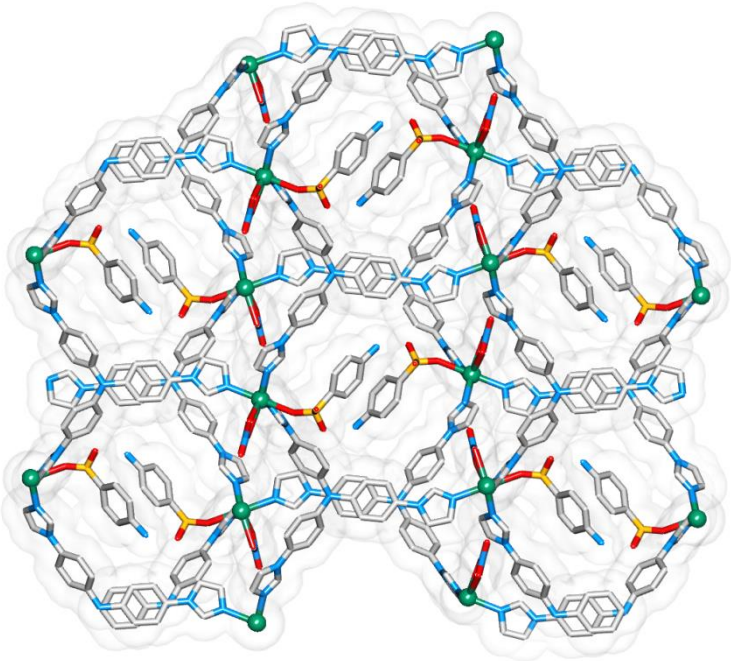

Figure S24: Figure showing packing of **IPM-315** along crystallographic *a*-axis. Guest solvent have been omitted for clarity. (Hydrogen atoms have been omitted for clarity. Colour code: C, grey; N, blue; Cd, green; O, red; S, yellow).

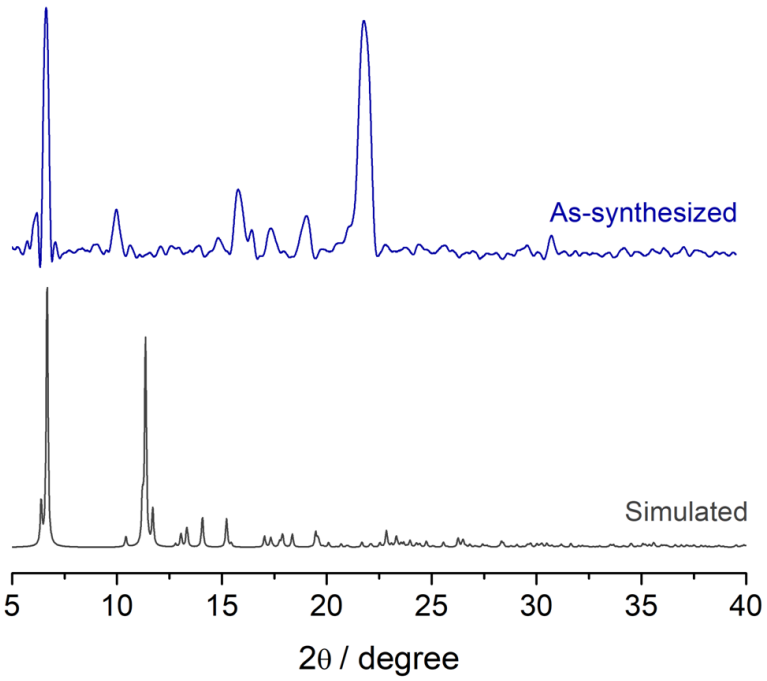

Figure S25: Powder X-ray diffraction patterns of **IPM-206**, simulated (grey), as-synthesized (blue).

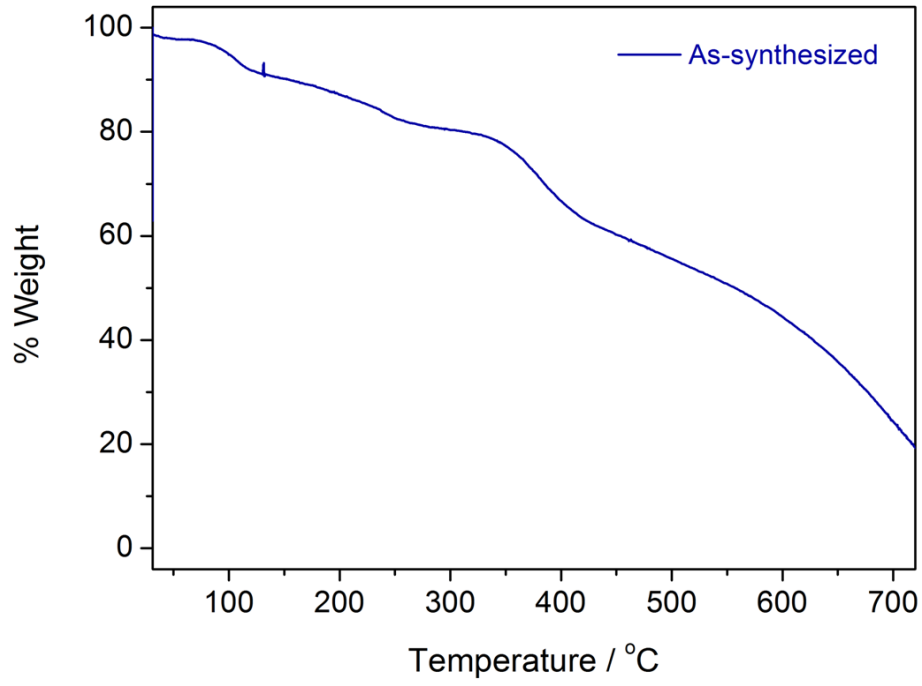

Figure S26: TGA profile for compound **IPM-206**.

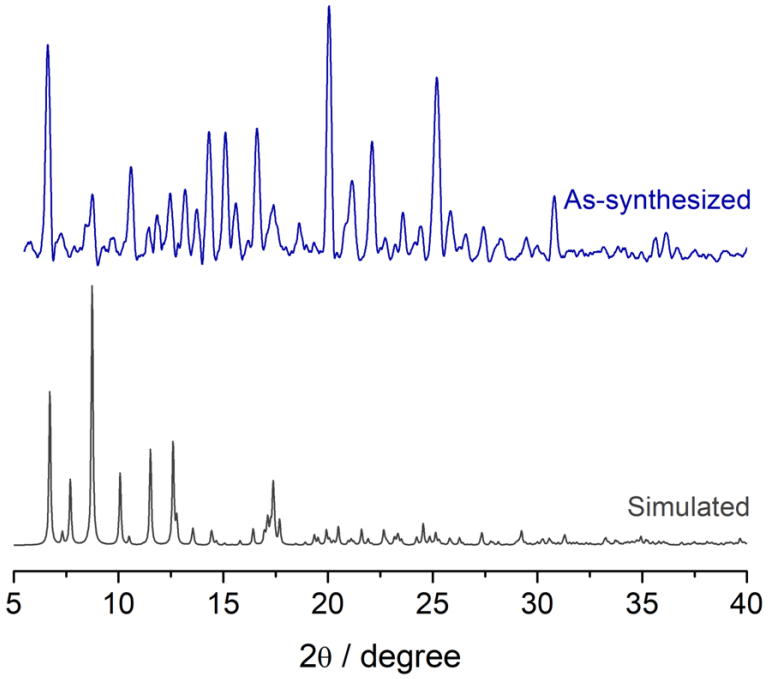

Figure S27: Powder X-ray diffraction patterns of **IPM-310**, simulated (grey), as-synthesized (blue).

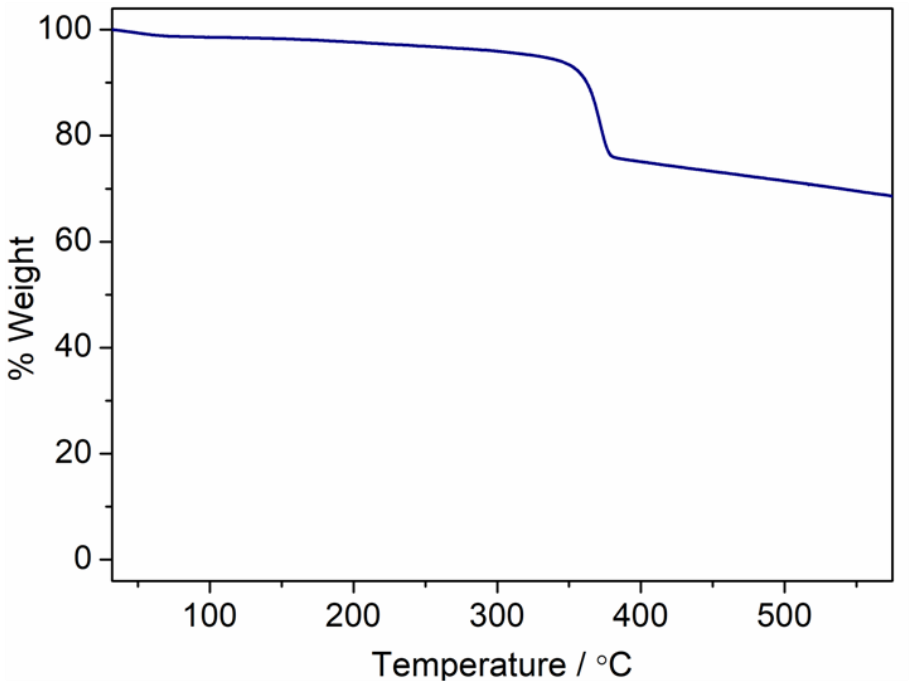

Figure S28: TGA profile for compound **IPM-310**.

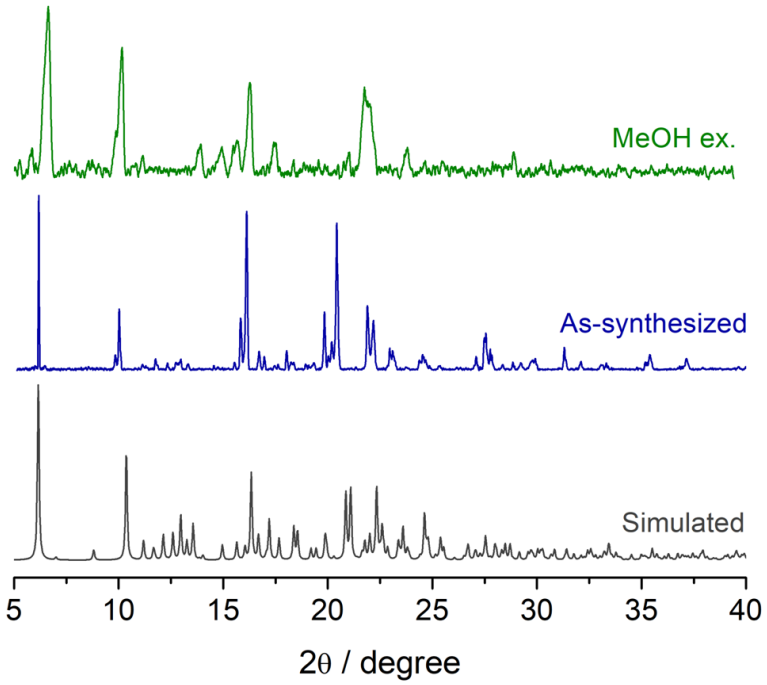

Figure S29: Powder X-ray diffraction patterns of **IPM-315**, simulated (grey), as-synthesized (blue), MeOH exchanged (green).

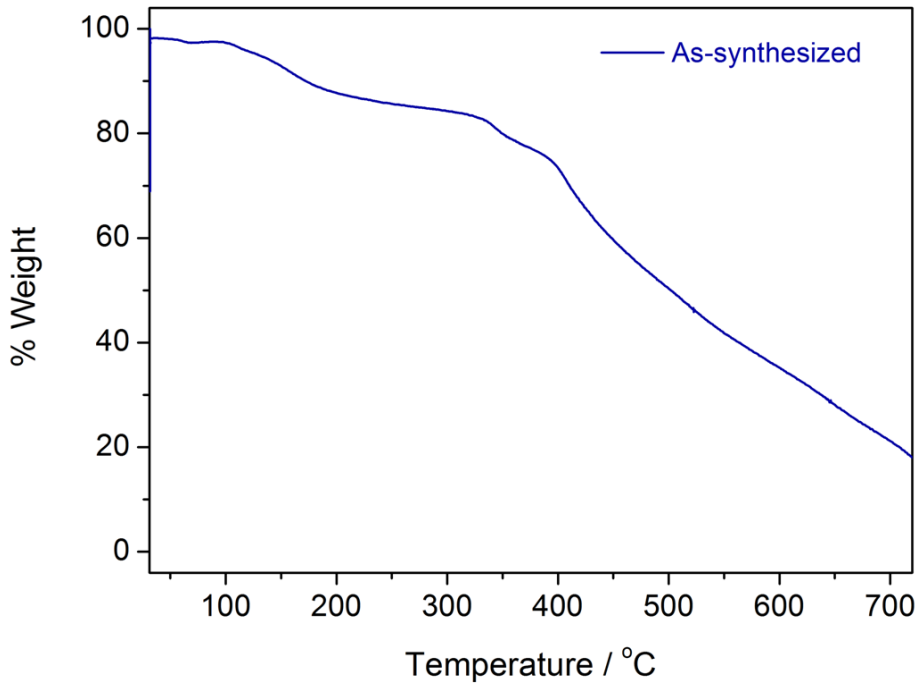

Figure S30: TGA profile for compound **IPM-315**.

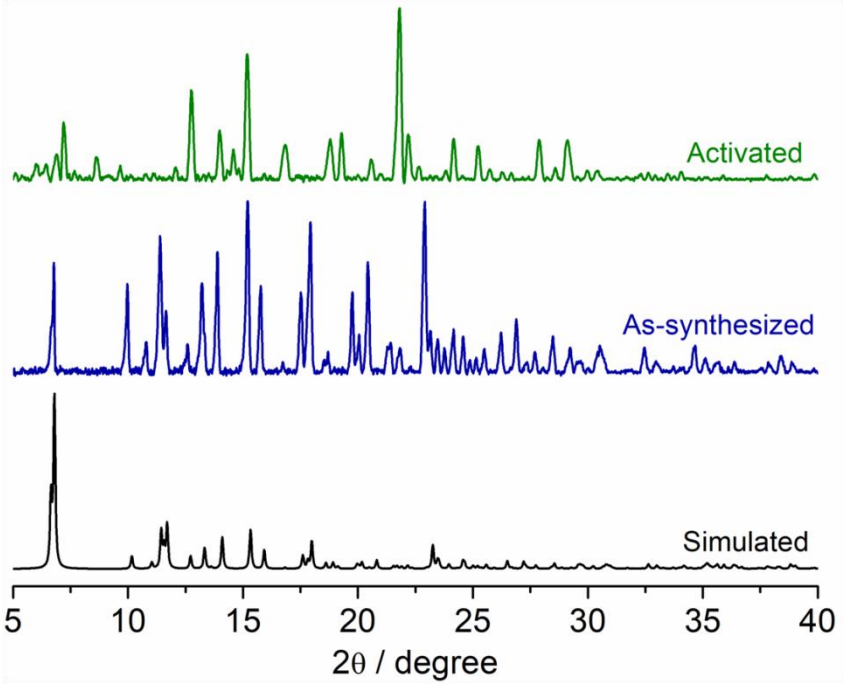

Figure S31: Powder X-ray diffraction patterns of **IPM-311**, simulated (grey), as-synthesized (blue), activated (green).

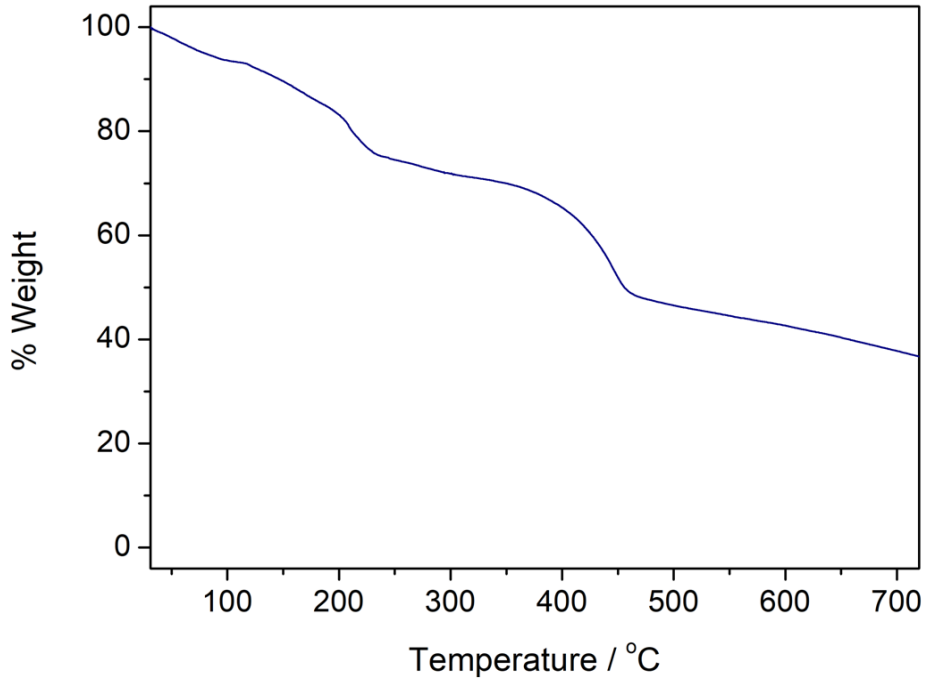

Figure S32: TGA profile for compound **IPM-311**.

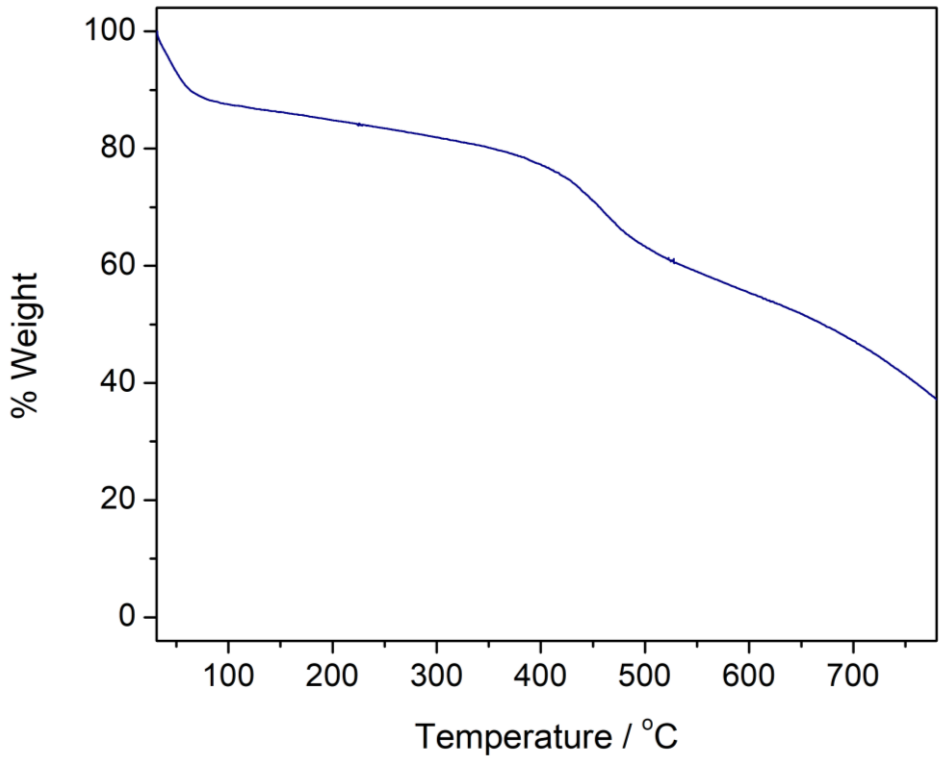

Figure S33: TGA profile for compound **IPM-312**.

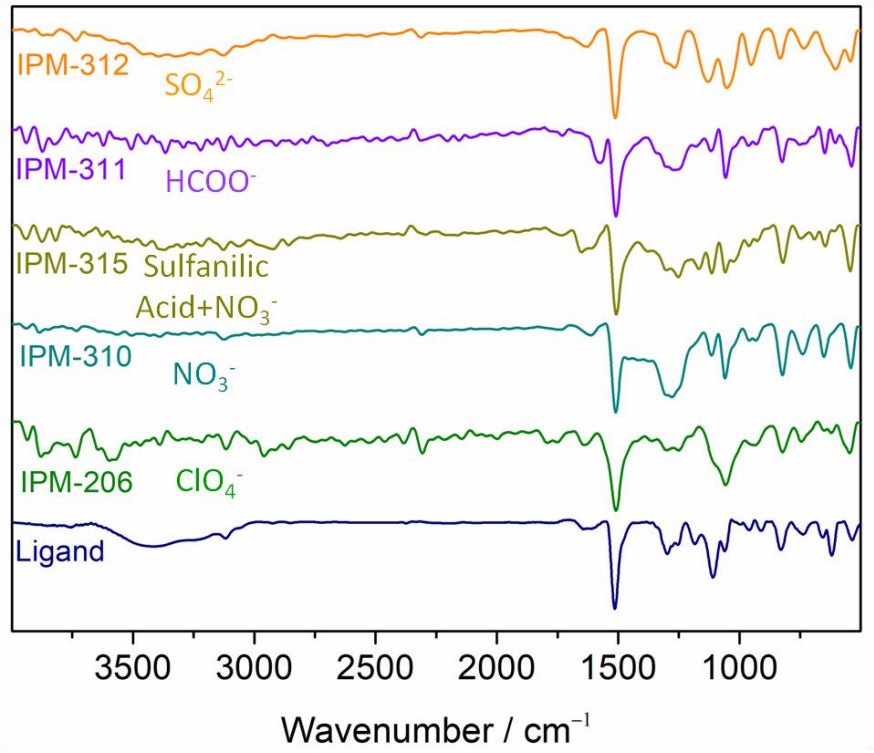

Figure S34: FT-IR profiles for ligand and all the compounds.

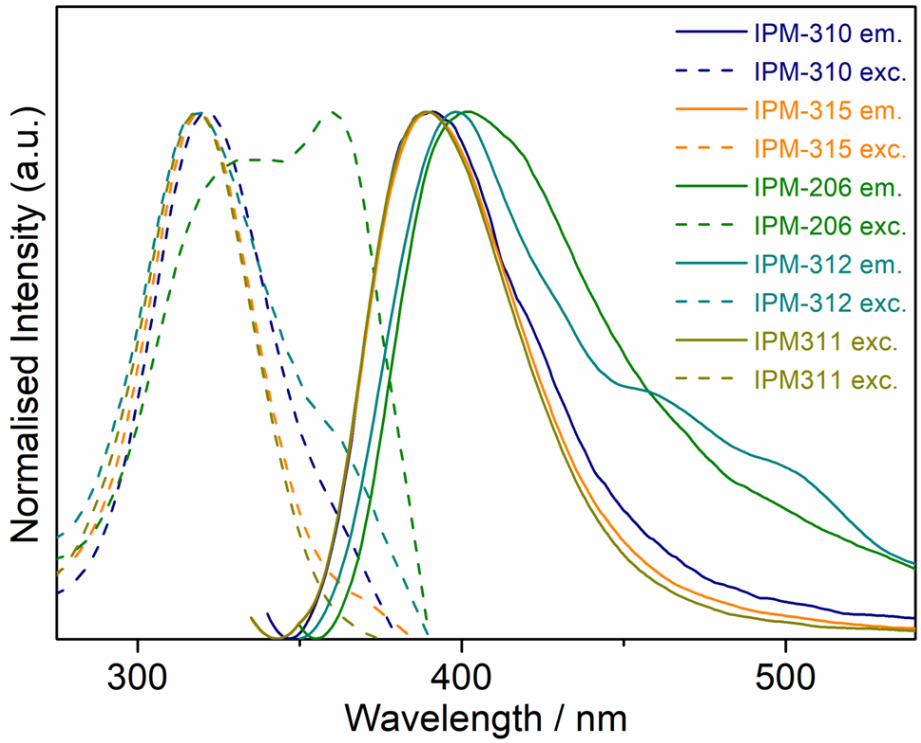

Figure S35: Excitation and emission profiles for various compounds.

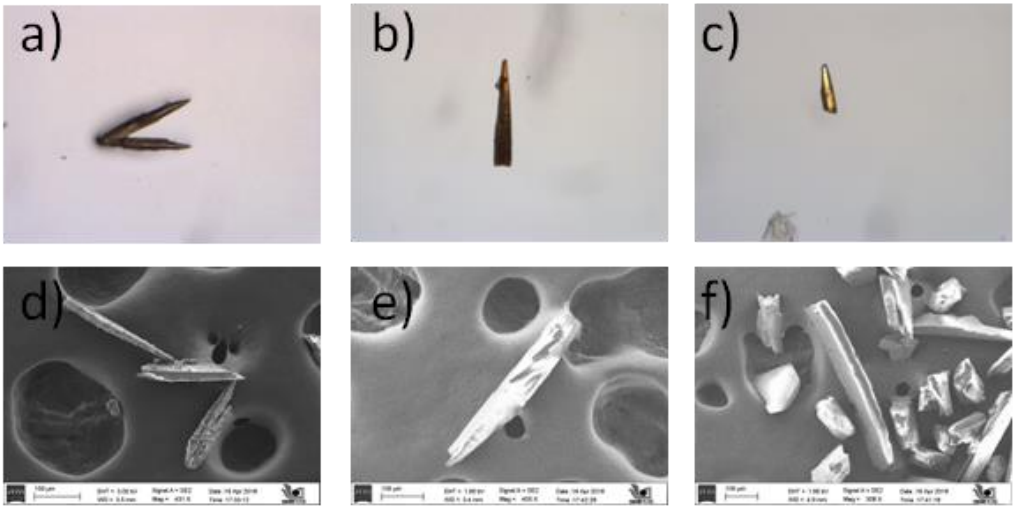

Figure S36: Naked eye images of **IPM-206**; a) As-synthesized, b) MnO_4^- exchanged, c) ReO_4^- exchanged, & SEM image of d) As-synthesized, e) MnO_4^- exchanged, f) ReO_4^- exchanged.

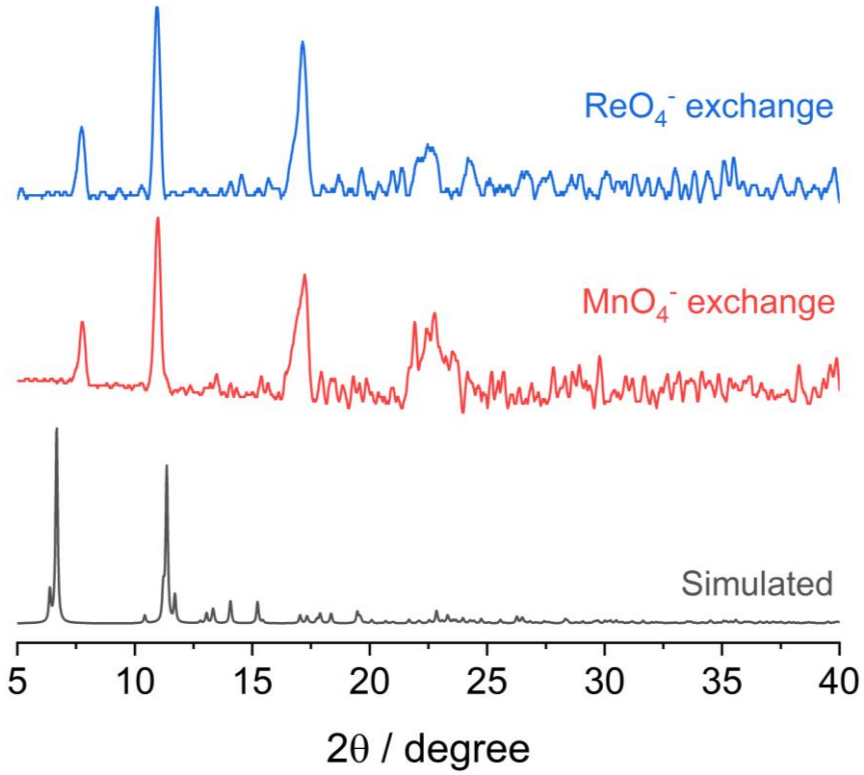

Figure S37: PXRD patterns for **IPM-206** - simulated, MnO_4^- exchanged, ReO_4^- exchanged.

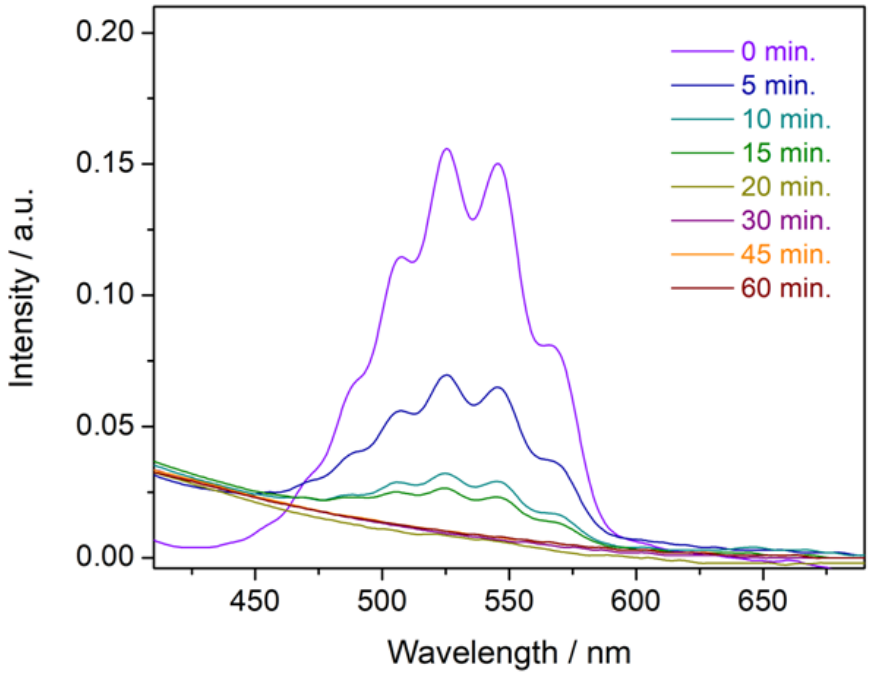

Figure S38: UV-Vis absorption spectra of MnO_4^- after addition of **IPM-206** at different intervals.

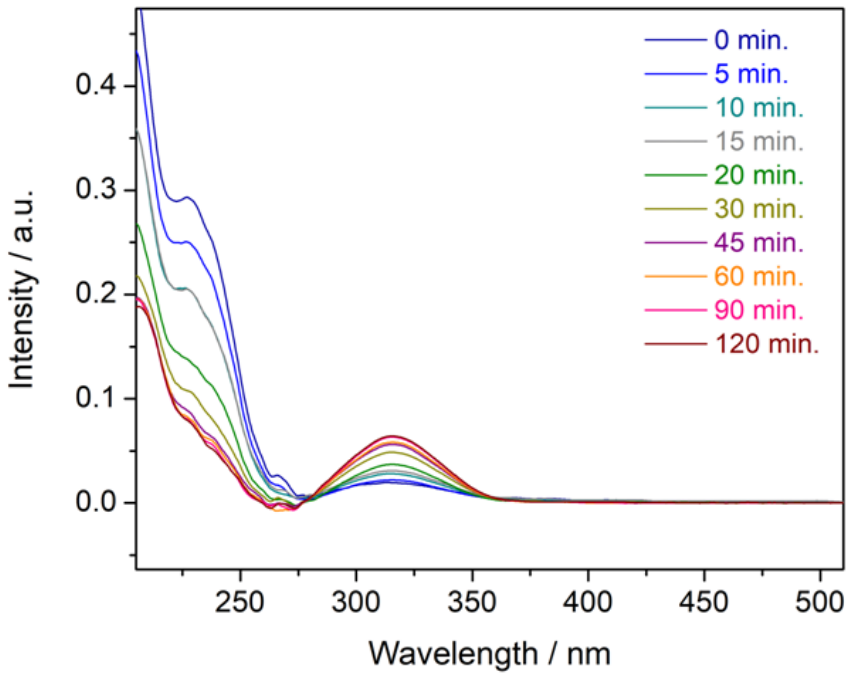

Figure S39: UV-Vis absorption spectra of ReO_4^- after addition of **IPM-206** at different intervals.

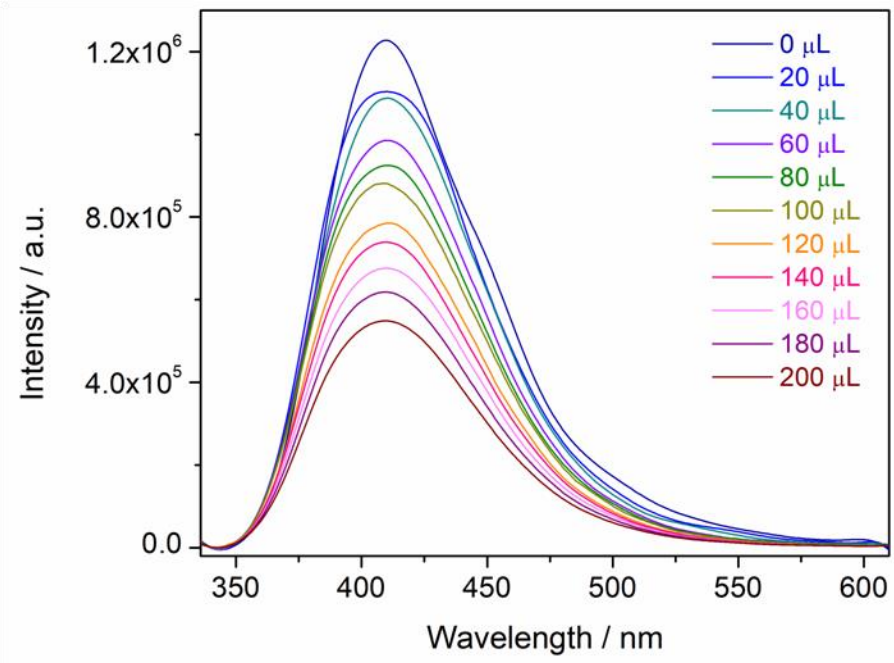

Figure S40: Fluorescence emission spectra of MnO_4^- after addition of **IPM-206** at different intervals.

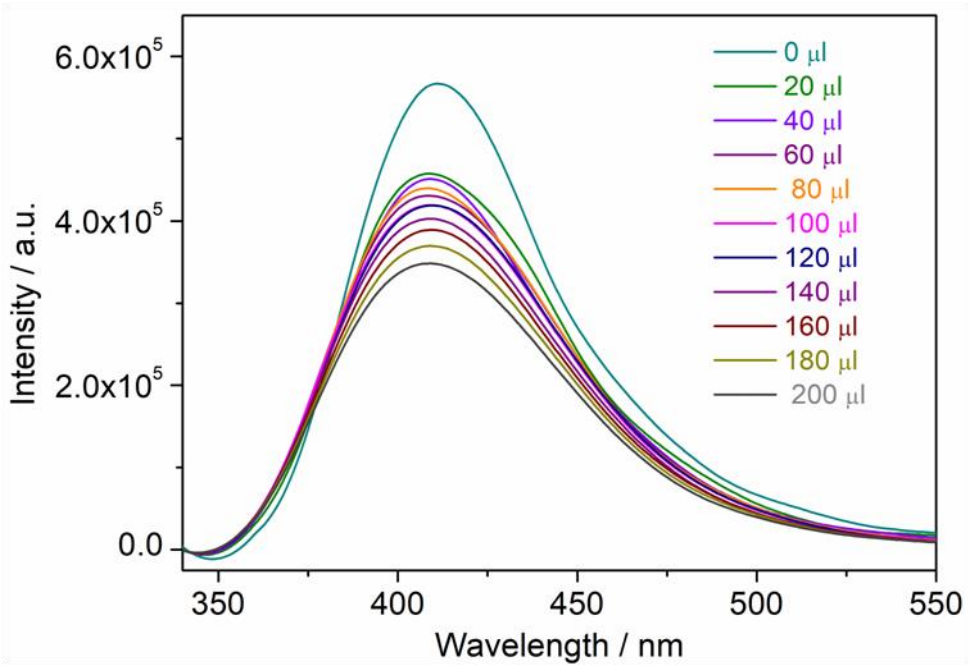

Figure S41: Fluorescence emission spectra of ReO_4^- after addition of **IPM-206** at different intervals.

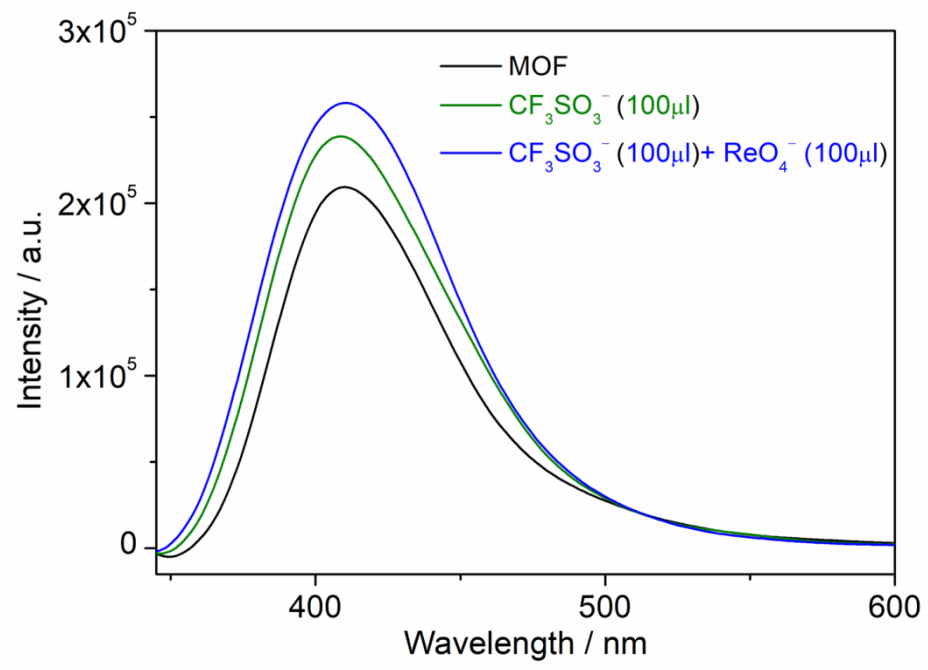

Figure S42: Fluorescence emission spectra of **IPM-206** after addition of different analytes.

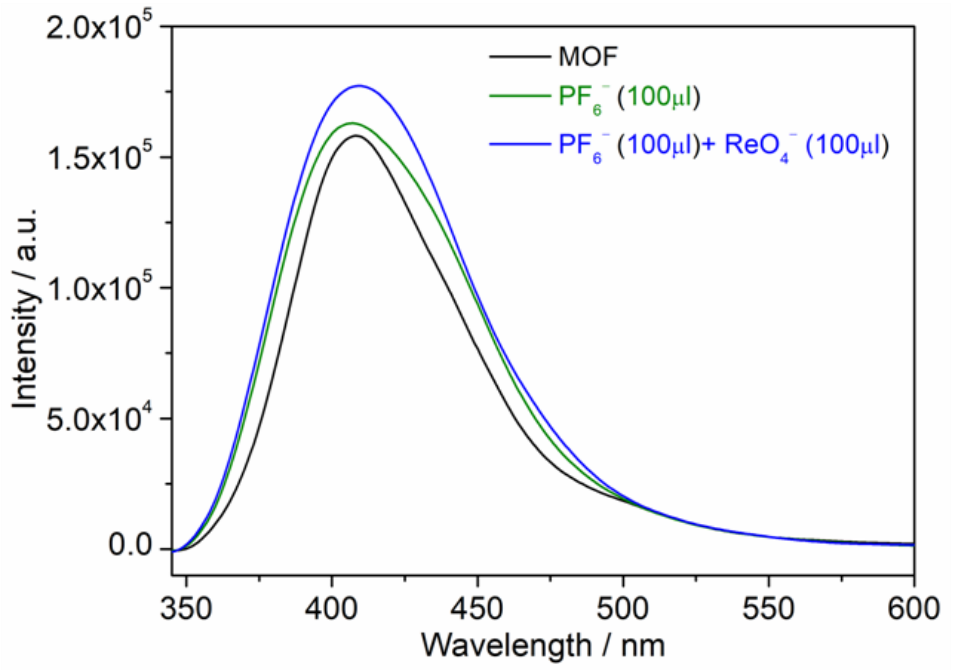

Figure S43: Fluorescence emission spectra of **IPM-206** after addition of different analytes.

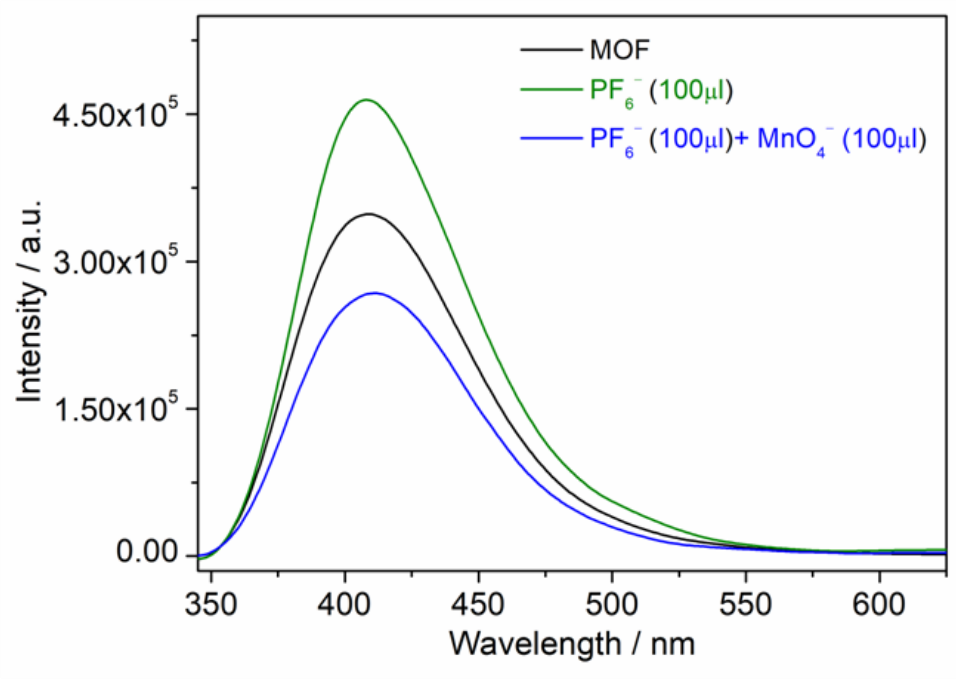

Figure S44: Fluorescence emission spectra of **IPM-206** after addition of different analytes.

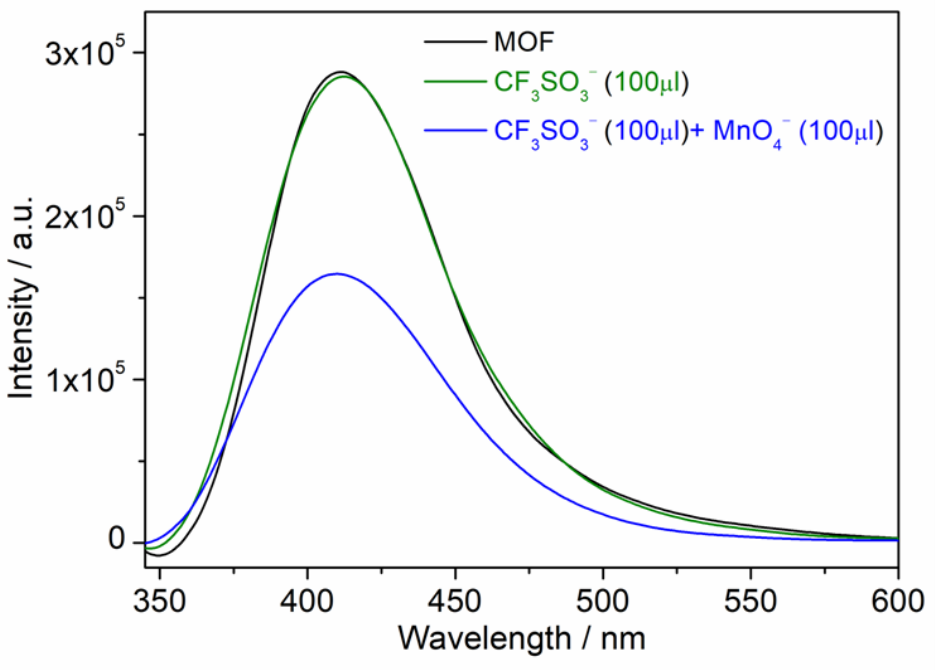

Figure S45: Fluorescence emission spectra of **IPM-206** after addition of different analytes.

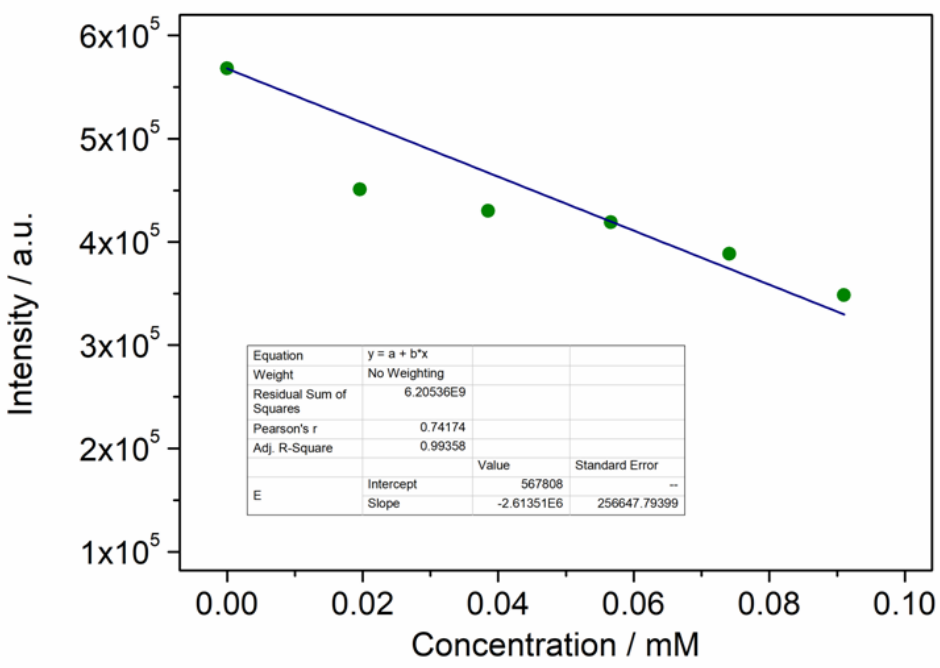

Figure S46: Linear region in the Fluorescence emission spectra after addition of $ReO4^-$ to **IPM-206** at λ_{em}= 410nm ($\lambda_{exc.}$= 325nm) (R^2 = 99.35%).

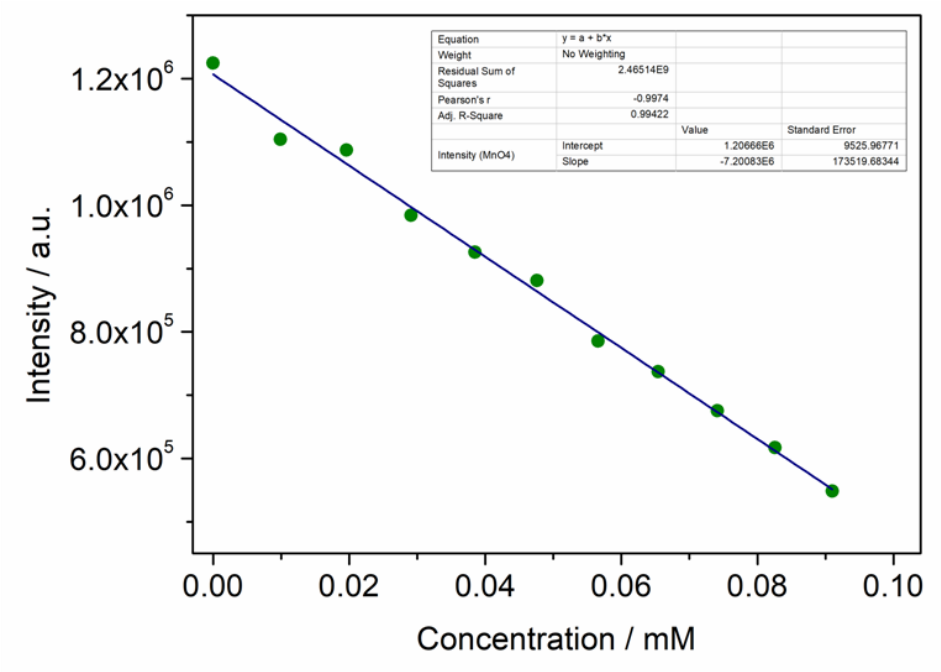

Figure S47: Linear region in the Fluorescence emission spectra after addition of $MnO4^-$ to **IPM-206** at λ_{em}= 410nm ($\lambda_{exc.}$= 325nm) (R^2 = 99.42%).

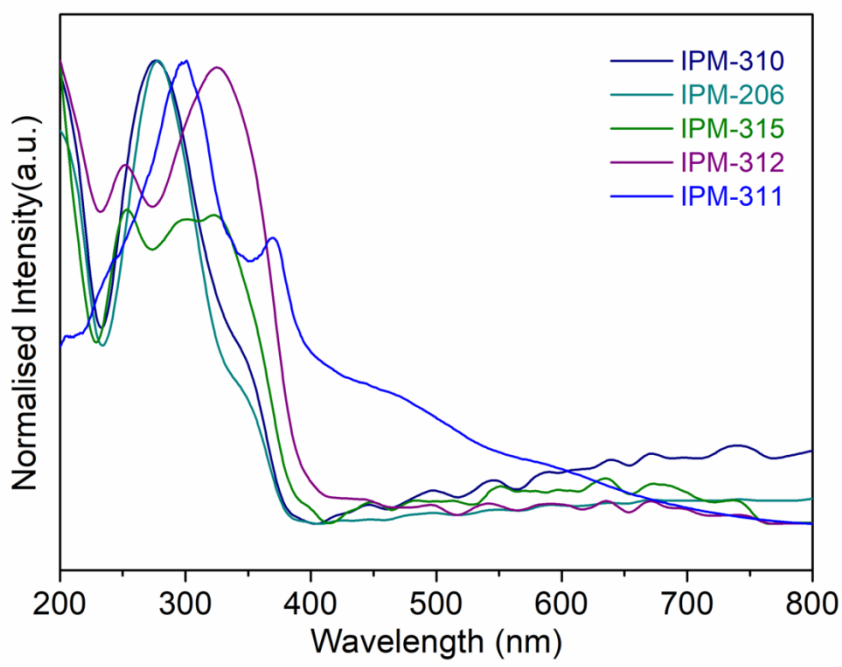

Figure S48: Solid State UV-Vis absorption profiles for **IPM-310** (Blue), **IPM-206** (cyan), **IPM-315** (green), **IPM-312** (violet) and **IPM-311** (bright blue).

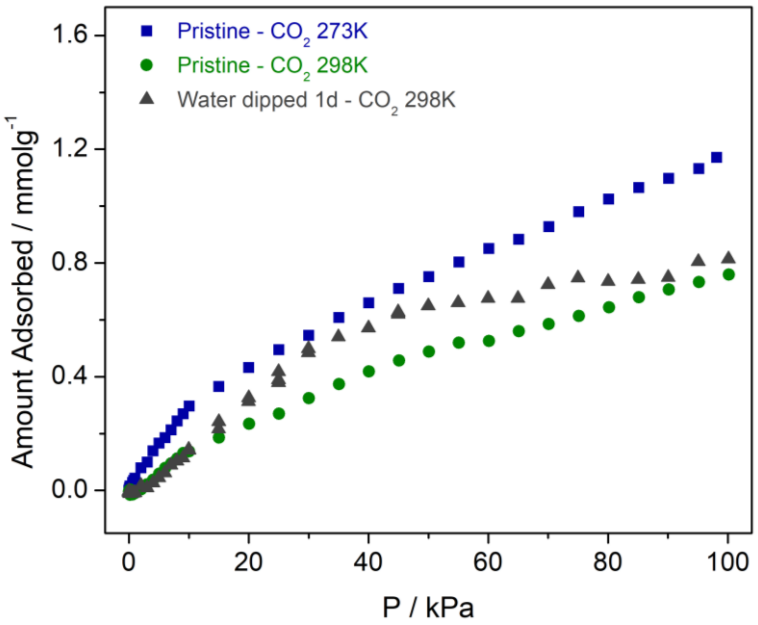

Figure S49: CO_2 adsorption isotherm for **IPM-312** after dipping in water.

Table 1. Crystal data and structure refinement for **IPM-206**.

Identification code	IPM-206 (CCDC 1846341)	
Empirical formula	C_{54} H_{42} Cd N_{14}	
Formula weight	999.41	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	*C*2/*c*	
Unit cell dimensions	a = 30.2102(19) Å	α= 90°
	b = 8.9486(6) Å	β= 118.440(2)°
	c = 31.4489(17) Å	γ = 90°
Volume	7475.8(8) $Å^3$	
Z	4	
Density (calculated)	0.888 Mg/m^3	
Absorption coefficient	0.326 mm^{-1}	
F(000)	2048	
Crystal size	0.14 x 0.12 x 0.10 mm^3	
Theta range for data collection	2.402 to 28.344°.	
Index ranges	-40<=h<=40, -11<=k<=11, -41<=l<=38	
Reflections collected	113594	
Independent reflections	9296 [R(int) = 0.0974]	
Completeness to theta = 28.42°	100.0 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9296 / 0 / 313	
Goodness-of-fit on F^2	1.100	
Final R indices [I>2sigma(I)]	R_1 = 0.0482, wR_2 = 0.1128	
R indices (all data)	R_1 = 0.0885, wR_2 = 0.1307	
Largest diff. peak and hole	0.450 and -0.392 e.$Å^{-3}$	

Table 2. Crystal data and structure refinement for **IPM-310**.

Identification code	IPM-310 (CCDC 1846342)	
Empirical formula	C_{27} H_{21} N_9 Cd O_6	
Formula weight	679.93	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	*P*-1	
Unit cell dimensions	a = 11.984(4) Å	α= 73.727(10)°
	b = 12.573(4) Å	β= 73.273 (10)°
	c = 14.220(5) Å	γ = 84.150 (12)°
Volume	1969.1(11) $Å^3$	
Z	2	
Density (calculated)	1.147 Mg/m^3	
Absorption coefficient	0.597 mm^{-1}	
F(000)	684	
Crystal size	0.12 x 0.11 x 0.10 mm^3	
Theta range for data collection	2.421 to 28.396°.	
Index ranges	-15<=h<=14, -16<=k<=16, -18<=l<=18	
Reflections collected	39207	
Independent reflections	9768 [R(int) = 0.0540]	
Completeness to theta = 28.42°	99.9 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9768 / 0 / 388	
Goodness-of-fit on F^2	1.035	
Final R indices [I>2sigma(I)]	R_1 = 0.0430, wR_2 = 0.1054	
R indices (all data)	R_1 = 0.0642, wR_2 = 0.1160	
Largest diff. peak and hole	1.922 and -0.636 $e.Å^{-3}$	

Table 3. Crystal data and structure refinement for **IPM-315**.

Identification code	IPM-315 (CCDC 1846347)	
Empirical formula	C_{36} H_{34} N_{10} Cd O_7 S	
Formula weight	863.19	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 8.9284(4) Å	α= 90°.
	b = 14.0416(7) Å	β= 90°.
	c = 28.6683(14) Å	γ = 90°.
Volume	3594.1(3) $Å^3$	
Z	4	
Density (calculated)	1.595 Mg/m^3	
Absorption coefficient	0.731 mm^{-1}	
F(000)	1760	
Crystal size	0.12 x 0.10 x 0.08 mm^3	
Theta range for data collection	2.389 to 28.362°.	
Index ranges	-11<=h<=11, -18<=k<=18, -38<=l<=38	
Reflections collected	89134	
Independent reflections	8957 [R(int) = 0.1167]	
Completeness to theta = 28.42°	99.9 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8957 / 6 / 498	
Goodness-of-fit on F^2	1.035	
Final R indices [I>2sigma(I)]	R_1 = 0.0616, wR_2 = 0.1437	
R indices (all data)	R_1 = 0.1019, wR_2 = 0.1608	
Largest diff. peak and hole	1.713 and -1.366 $e.Å^{-3}$	

Table 4. Crystal data and structure refinement for **IPM-311**.

Identification code	IPM-311 (CCDC 1846344)	
Empirical formula	C_{29} H_{23} N_7 Cd O_4	
Formula weight	645.94	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	*C*2	
Unit cell dimensions	a = 26.535(2) Å	α= 90°
	b = 15.453(2) Å	β= 101.627(4)°
	c = 8.8765(9) Å	γ = 90°
Volume	3565(7) $Å^3$	
Z	4	
Density (calculated)	1.203 Mg/m^3	
Absorption coefficient	0.650 mm^{-1}	
F(000)	1304	
Crystal size	0.18 x 0.16 x 0.14 mm^3	
Theta range for data collection	2.343 to 28.280°.	
Index ranges	-34<=h<=35, -20<=k<=20, -10<=l<=11	
Reflections collected	43878	
Independent reflections	8814 [R(int) = 0.1057]	
Completeness to theta = 28.42°	99.9 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8814 / 7 / 371	
Goodness-of-fit on F^2	0.981	
Final R indices [I>2sigma(I)]	R_1 = 0.0504, wR_2 = 0.0968	
R indices (all data)	R_1 = 0.1214, wR_2 = 0.1167	
Largest diff. peak and hole	0.546 and -0.448 e.$Å^{-3}$	

Table 5. Crystal data and structure refinement for **IPM-312**.

Identification code	IPM-312 (CCDC 1846346)	
Empirical formula	$C_{54}\ H_{42}\ N_{14}Cd_2\ O_8\ S_2$	
Formula weight	1303.93	
Temperature	150(2) K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	*P*-1	
Unit cell dimensions	a = 15.9617(11) Å	α= 113.108(4)°
	b = 16.1208(11) Å	β= 113.283(4)°
	c = 16.3842(11) Å	γ = 99.327(5)°
Volume	3301.3(4) $Å^3$	
Z	2	
Density (calculated)	1.312 Mg/m^3	
Absorption coefficient	6.220 mm^{-1}	
F(000)	1312	
Crystal size	0.15 x 0.12 x 0.10 mm^3	
Theta range for data collection	3.216 to 67.393°.	
Index ranges	-18<=h<=19, -19<=k<=19, -16<=l<=19	
Reflections collected	24186	
Independent reflections	11522 [R(int) = 0.0704]	
Completeness to theta = 28.42°	97.0 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11522 / 36 / 721	
Goodness-of-fit on F^2	0.936	
Final R indices [I>2sigma(I)]	R_1 = 0.0800, wR_2 = 0.2361	
R indices (all data)	R_1 = 0.1170, wR_2 = 0.2652	
Largest diff. peak and hole	3.778 and -2.110e.$Å^{-3}$	