Figure S1 NMR spectra results for PIM-1 in various time-intervals with 1:64 reactants-balls mass ratio.
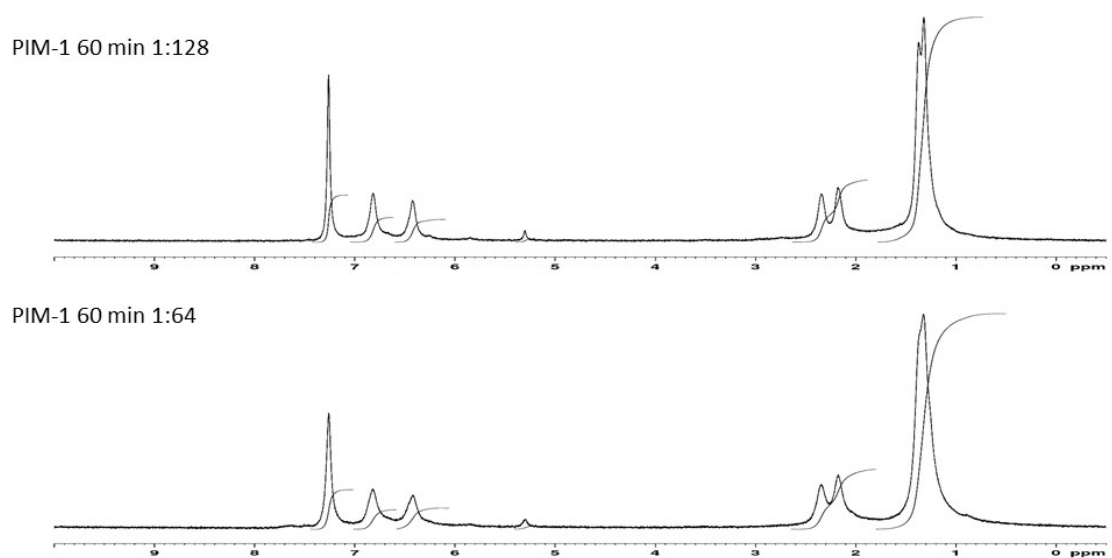

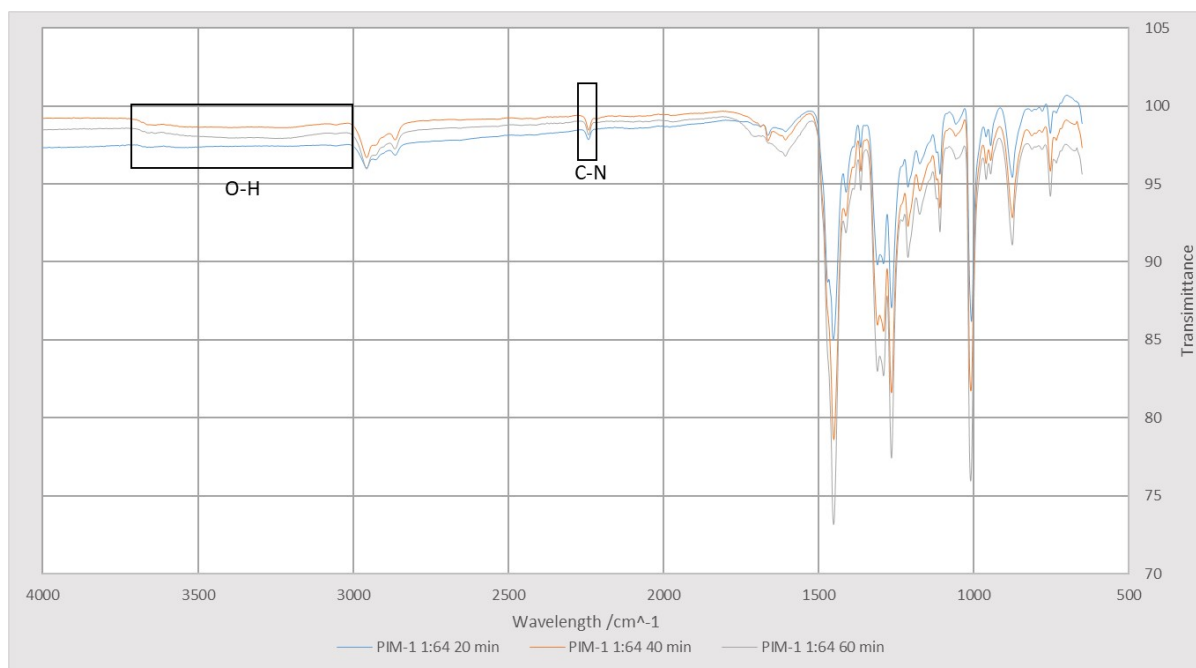**Figure S2** . NMR spectra results for PIM-1 using different reactants to balls ratio at 60 min.

Figure S3 FT-IR spectrum of PIM-1 in different time-intervals
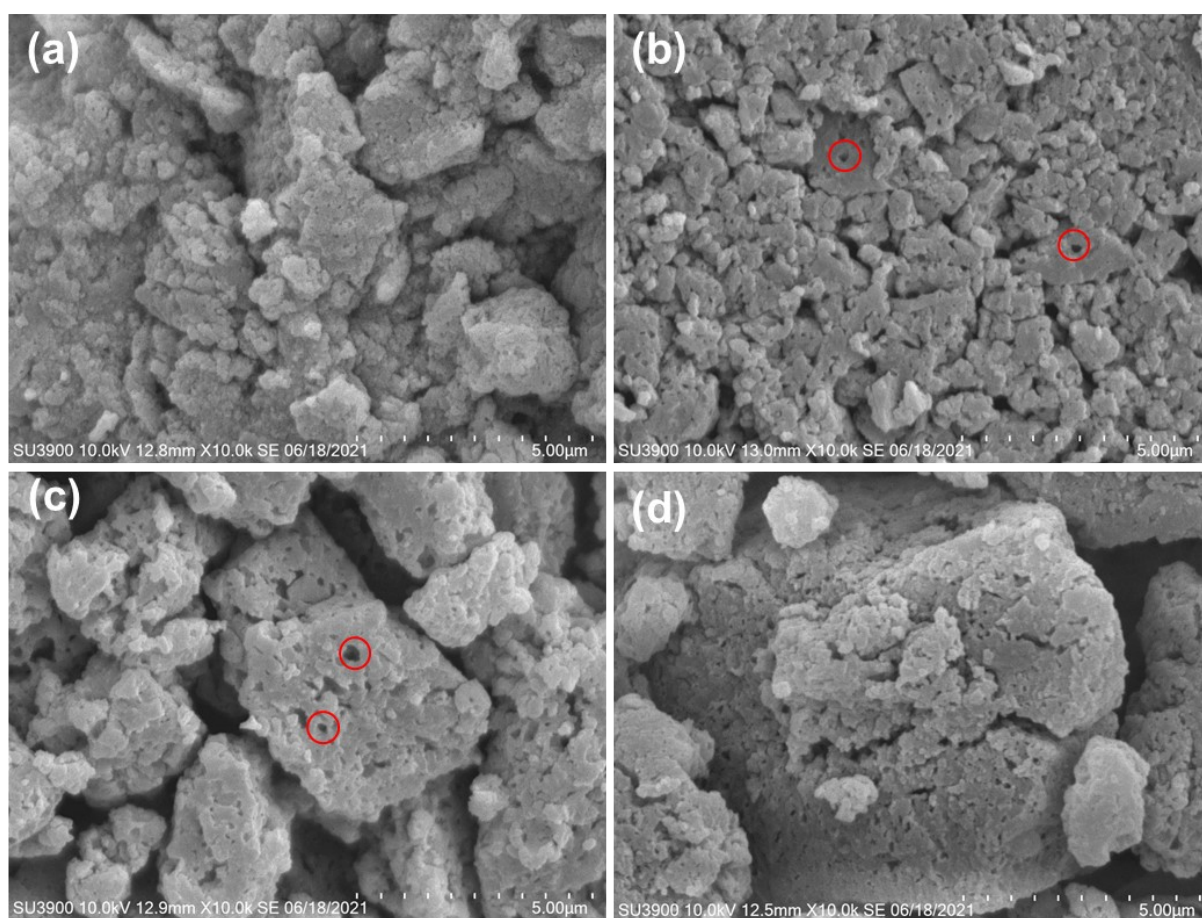

Figure S4 SEM images of PIM-1 in (a) 20 min, (b) 40 min, and (c) 60 min time-intervals with 1:64 reactants to ball mass ratio and (d) in 60 min with 1:128 reactants to ball mass ratio at 10,000x magnification.
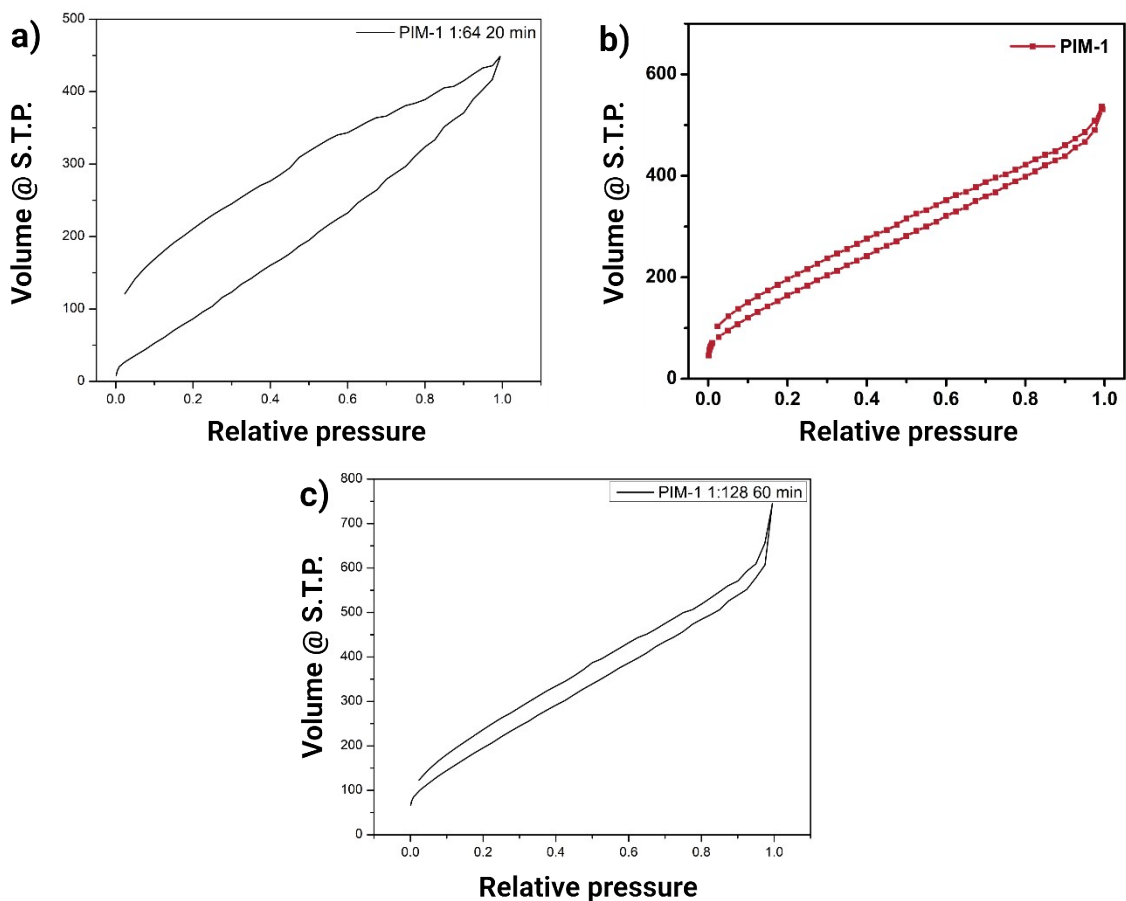
Figure S5 Adsorption-desorption isotherm of PIM-1 at (a) 20 min and (b) 60 min with 1: 64 reactants-to-ball ratio and (c) 60 min with 1:128 reactants-to-balls ratio.

Table S1 Inventory inputs and outputs for both synthesis methods.

| Inputs | Unit | Provider | Quantity | | Data/ Remark |
			Mechanosynthesis	Wet Chemical Method	
TTSBI	mg	Assumptions	680.0	681.0	**Mechanosynthesis:** Calculated using concentration ratio. Wet Chemical Method: A scale factor of 0.133 is used to correspond with the product yield of mechanosynthesis.
TFTPN	mg	Assumptions	400.0	400.0	**Mechanosynthesis**: Calculated using concentration ratio. **Wet Chemical Method:** A scale factor of 0.133 is used to correspond with the product yield of mechanosynthesis.

K$_2$CO$_3$	mg	market for potassium carbonate | potassium carbonate | Cutoff, U - GLO	1200	826.67	**Mechanosynthesis:** Calculated using concentration ratio. **Wet Chemical Method**: A scale factor of 0.133 is used to correspond with the product yield of mechanosynthesis.
Toluene	ml	market for toluene, liquid | toluene, liquid | Cutoff, U - RER	-	0.6	**Wet Chemical method:** A scale factor of 0.133 is used to correspond with the product yield of mechanosynthesis.
DMSO	ml	market for dimethyl sulfoxide | dimethyl sulfoxide | Cutoff, U - GLO	-	5.3	**Wet Chemical method:** A scale factor of 0.133 is used to correspond with the product yield of mechanosynthesis.
Ethanol	ml	market for ethanol, without water, in 99.7% solution state, from ethylene | ethanol, without water, in 99.7% solution state, from ethylene | Cutoff, U - RER	85.3	85.3	**Mechanosyntheis and Wet Chemical method:** The chemicals are scaled towards 10mg of product will use up 1ml of chemicals to wash.
Methanol	ml	market for methanol | methanol | Cutoff, U - GLO	85.3	-	**Wet Chemical method:** The chemicals are scaled towards 10mg of product will use up 1ml of chemicals to wash.
De-ionised water	ml	water production, deionised | water, deionised | Cutoff, U - Europe without Switzerland	85.3	85.3	**Mechanosyntheis and Wet Chemical method:** The chemicals are scaled towards 10mg of product will use up 1ml of chemicals to wash.
Electricity for heat (silicon oil bath)	kWh	market for electricity, high voltage | electricity, high voltage | Cutoff, U - GB	-	0.4 (for 8 hours)	**Wet Chemical method:** A water bath, NE1D-4 used as the power rating reference.
Electricity for stirring	kWh	market for electricity, high voltage | electricity, high voltage | Cutoff, U - GB	-	0.8 (for 8.05 hours)	**Wet Chemical method:** A disperser, T 25 digital ULTRA-TURRAX ® used as the power rating reference.
Electricity for milling	kWh	market for electricity, high voltage | electricity, high voltage | Cutoff, U - GB	0.1 (for 15 minutes)	-	**Mechanosyntheis:** A high frequency mixer mill, MM 200 was used as the power rating reference.
Electricity for	kWh	market for	1.65 (for 90	1.65 (for 60	**Mechanosyntheis and Wet Chemical**

| centrifugation		electricity, high voltage | electricity, high voltage | Cutoff, U - GB	minutes)	minutes)	method: Eppendorf – centrifuge 5810R was used as the power rating reference.
Electricity for heat (oven for drying)	kWh	market for electricity, high voltage | electricity, high voltage | Cutoff, U - GB	0.75 (for 24 hours)	0.75 (for 24 hours)	**Mechanosyntheis and Wet Chemical method:** A digital oven, GENLAB – MINO/40/TDIG was used as the power rating reference.
Output					
PIM-1	mg	-	834.96	793.569	**Mechanosynthesis:** A product of 853.0mg with the yield (98%) considered **Wet Chemical Method:** A product of 853.0mg (scale factor of 0.1333) with the yield (93%) considered.
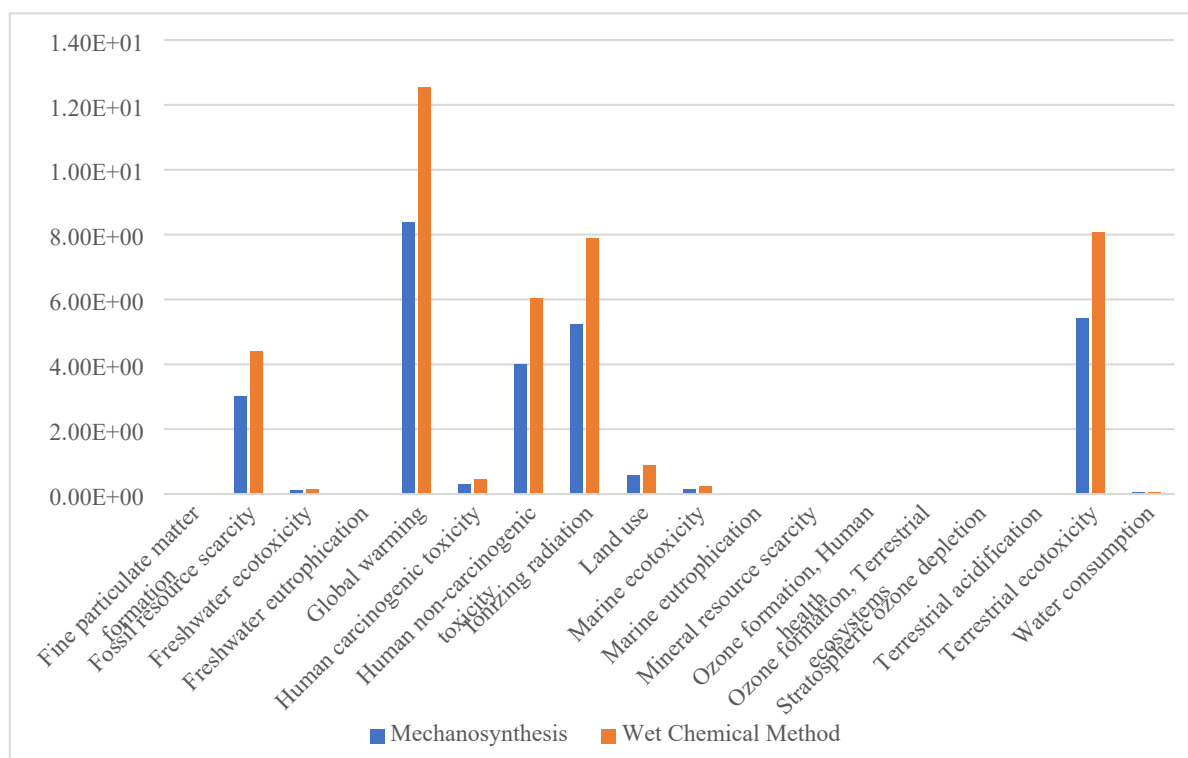
Figure S6 Normalised ReCiPe (2016) Midpoint (H) analysis result