Supplementary Information

Efficient ethylene purification by a robust ethane-trapping porous organic cage

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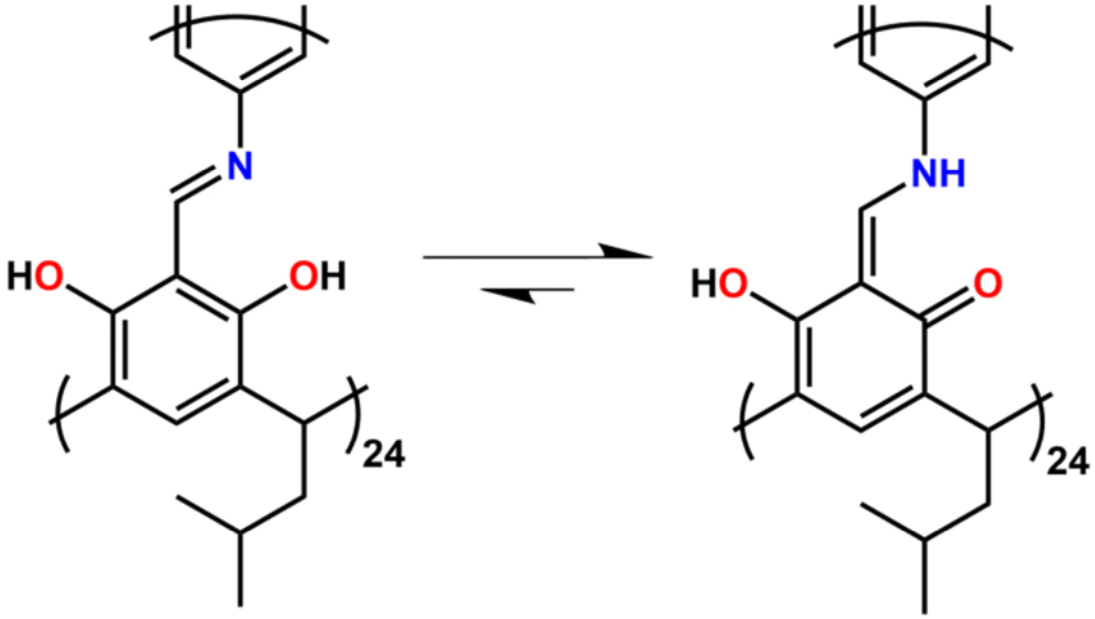
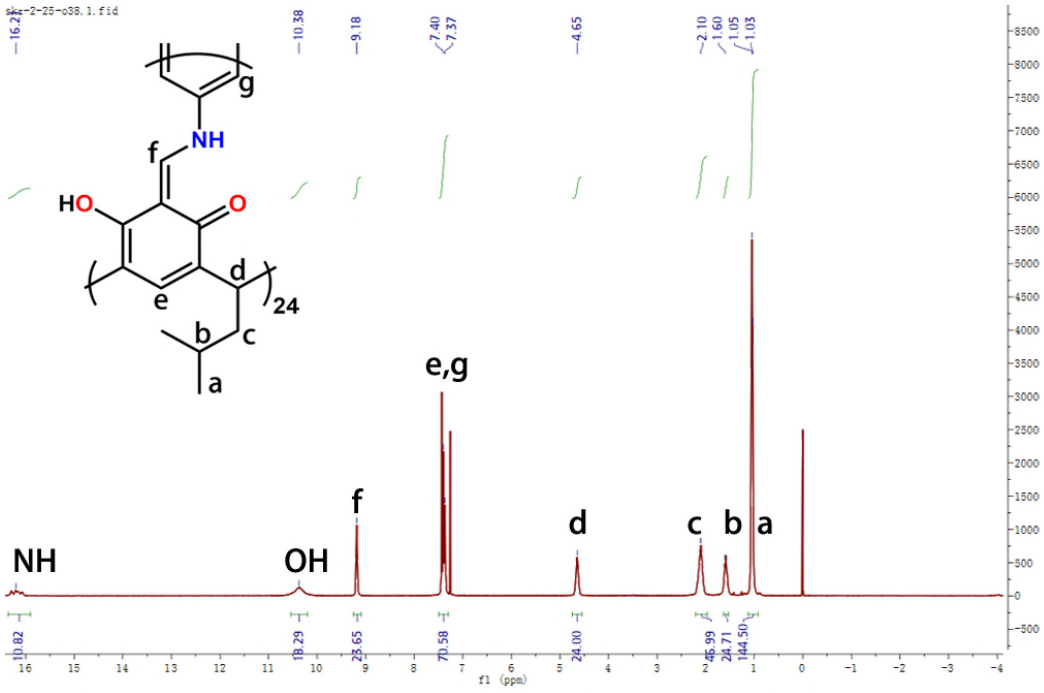
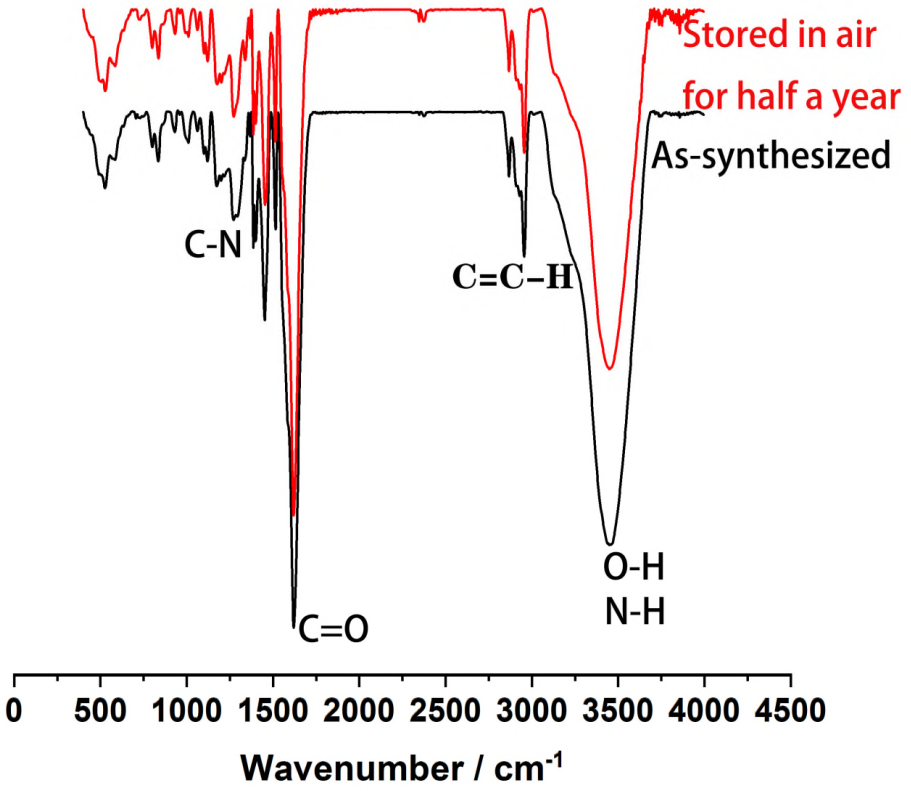


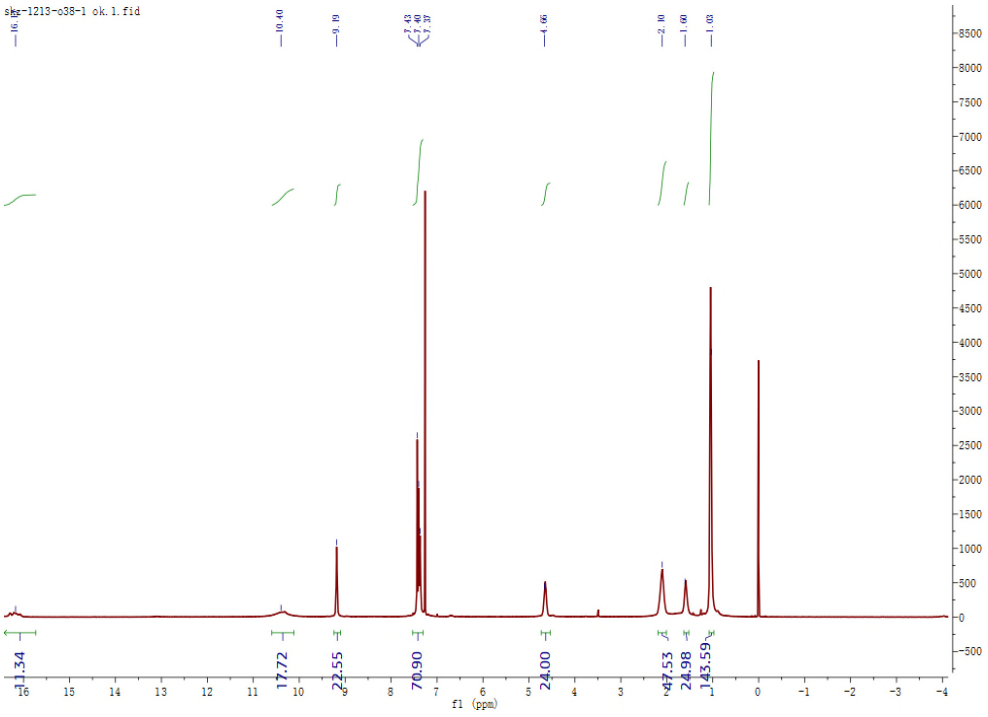
Supplementary Fig. 1 Keto–enol tautomerization within **CPOC-301**.



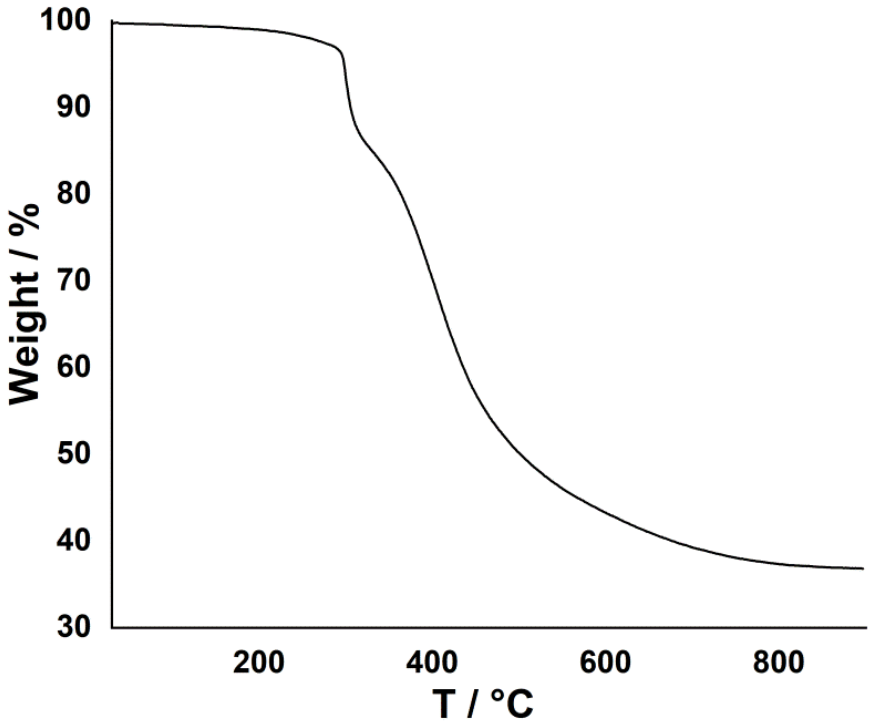
Supplementary Fig. 2 ^{1}HNMR of **CPOC-301** ($CDCl_3$, 400 MHz, 298 K). The lower integral areas at 10.38 and 16.21 ppm are due to the active hydrogen atoms.



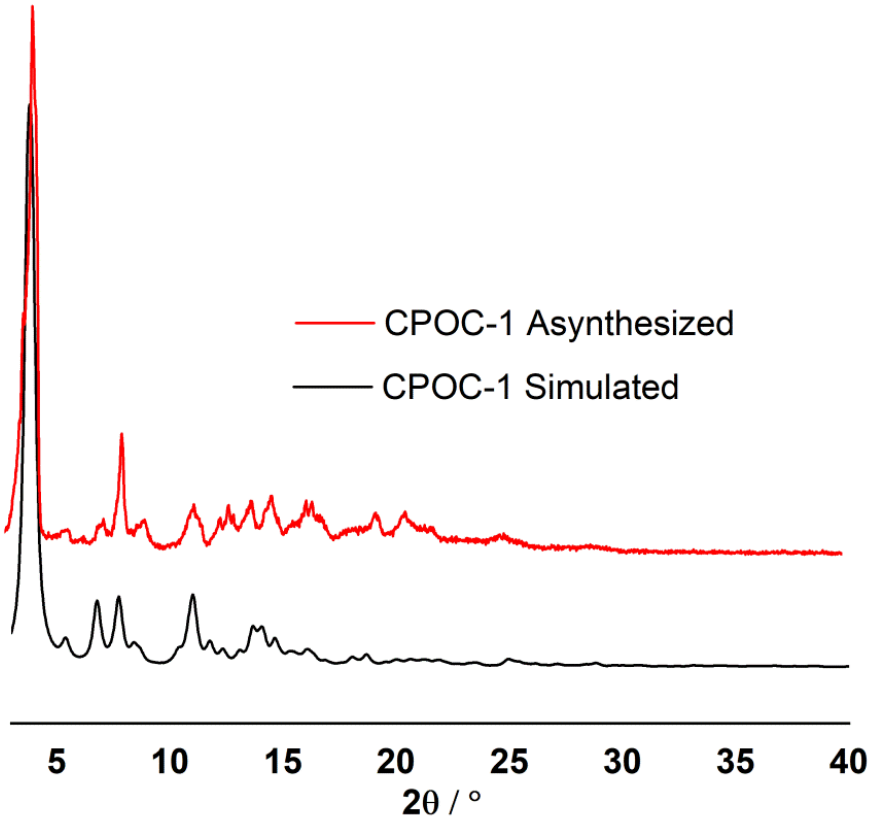
Supplementary Fig. 3 FT-IR spectra of **CPOC-301**.



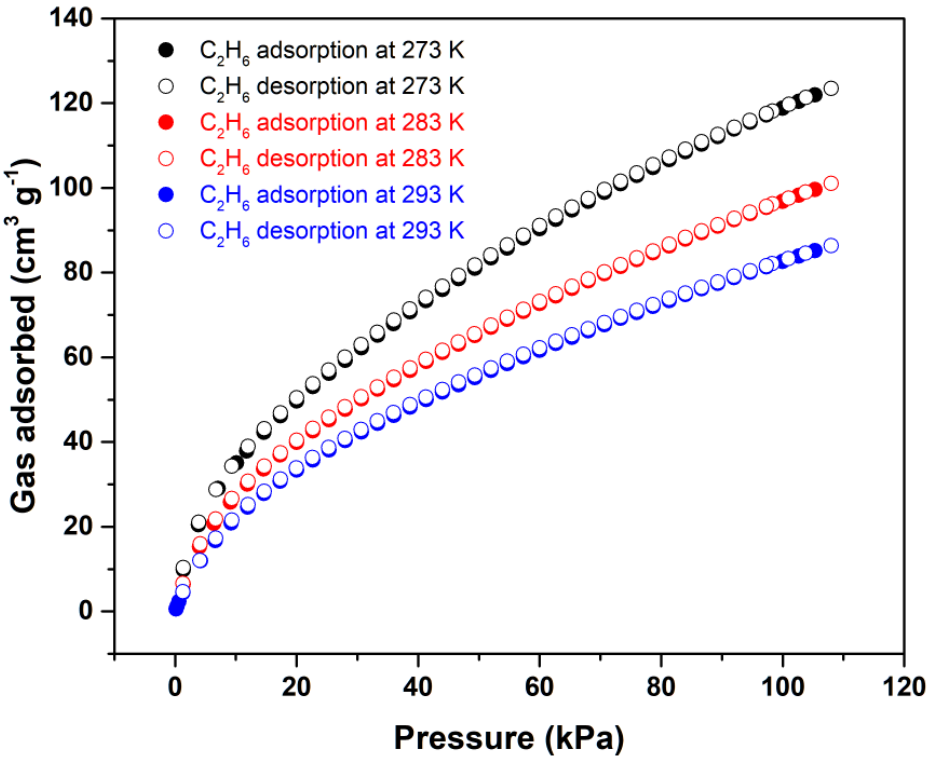
Supplementary Fig. 4 ^{1}HNMR of **CPOC-301** after storing in air for half a year ($CDCl_3$, 400 MHz, 298 K). The lower integral areas at 10.40 and 16.19 ppm are due to the active hydrogen atoms.



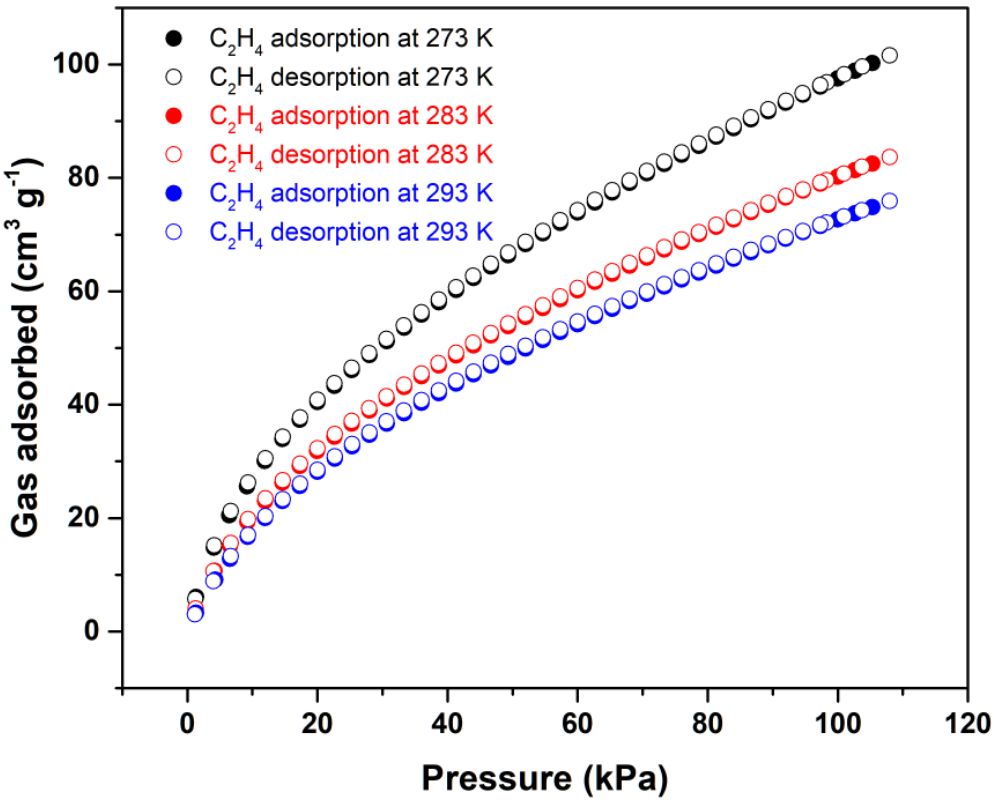
Supplementary Fig. 5 TGA curve of **CPOC-301**.



Supplementary Fig. 6 PXRD pattern of **CPOC-301**.

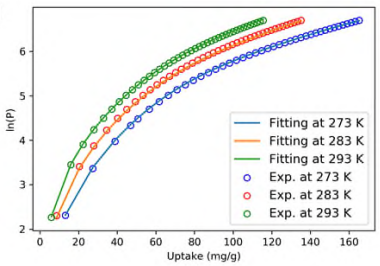


Supplementary Fig. 7 C_2H_6 adsorption/desorption isotherm of **CPOC-301** at 273, 283 and 293 K.



Supplementary Fig. 8 C_2H_4 adsorption/desorption isotherm of **CPOC-301** at 273, 283 and 293 K.

(a)

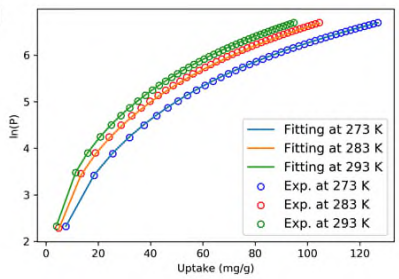


(b)

	Parameter value	Standard deviation
a0	-3895.385	177.8326
a1	23.5972	5.125331
a2	-5.132419E-2	4.952644E-2
a3	-1.312749E-3	5.581102E-4
a4	8.405202E-6	3.51366E-6
a5	-1.799377E-8	8.105978E-9
Adj. R-Square	0.9996	

Supplementary Fig. 9 (a) Virial equation fitting of the C_2H_6 adsorption isotherm of **CPOC-301** at 273, 283 and 293 K. (b) Relevant fitting parameters for C_2H_6.

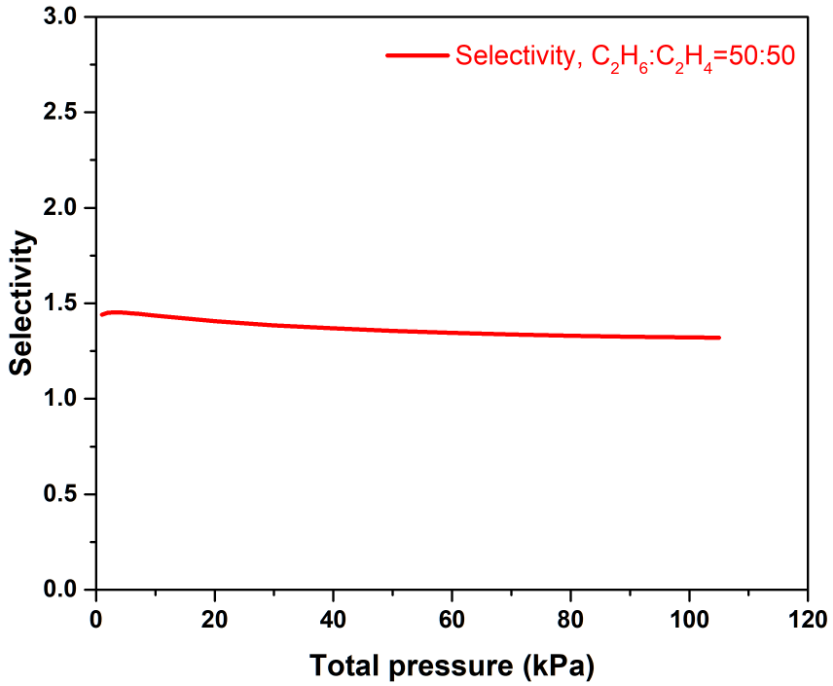
(a)



(b)

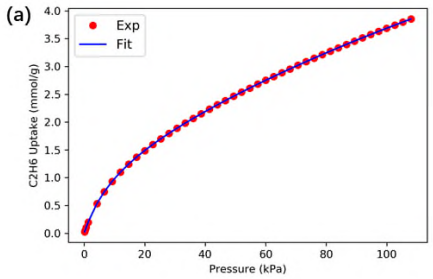
	Parameter value	Standard deviation
a0	-2888.351	140.9872
a1	13.41196	5.204910
a2	-1.88417E-2	6.563444E-2
a3	-1.055152E-3	1.000175E-3
a4	7.665586E-6	8.280272E-6
a5	-1.921508E-8	2.505110E-8
Adj. R-Square	0.9997	

Supplementary Fig. 10 (a) Virial equation fitting of the C_2H_4 adsorption isotherm of **CPOC-301** at 273, 283 and 293 K. (b) Relevant fitting parameters for C_2H_4.



Supplementary Fig. 11 Selectivity of **CPOC-301** predicted by the IAST method for an equimolar C_2H_6/C_2H_4 mixture at 293 K.

(a)

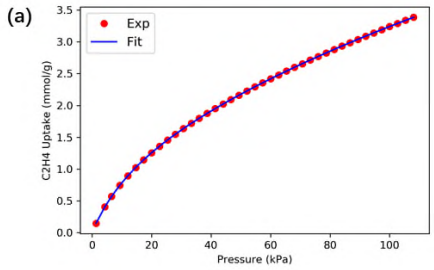


(b)

	Parameter value	Standard deviation
A1	8.201807	0.3796967
A2	1.844211	0.05399933
B1	1.080576E-3	1.026994E-4
B2	8.819491E-2	1.896082E-3
C1	1.24567	0.02814527
C2	0.967183	3.641178E-3
Adj. R-Square	0.999999	

Supplementary Fig. 12 Dual-site Langmuir-Freundlich fitting of the C_2H_6 adsorption isotherm of **CPOC-301** at 293 K. (b) Relevant fitting parameters for C_2H_6.

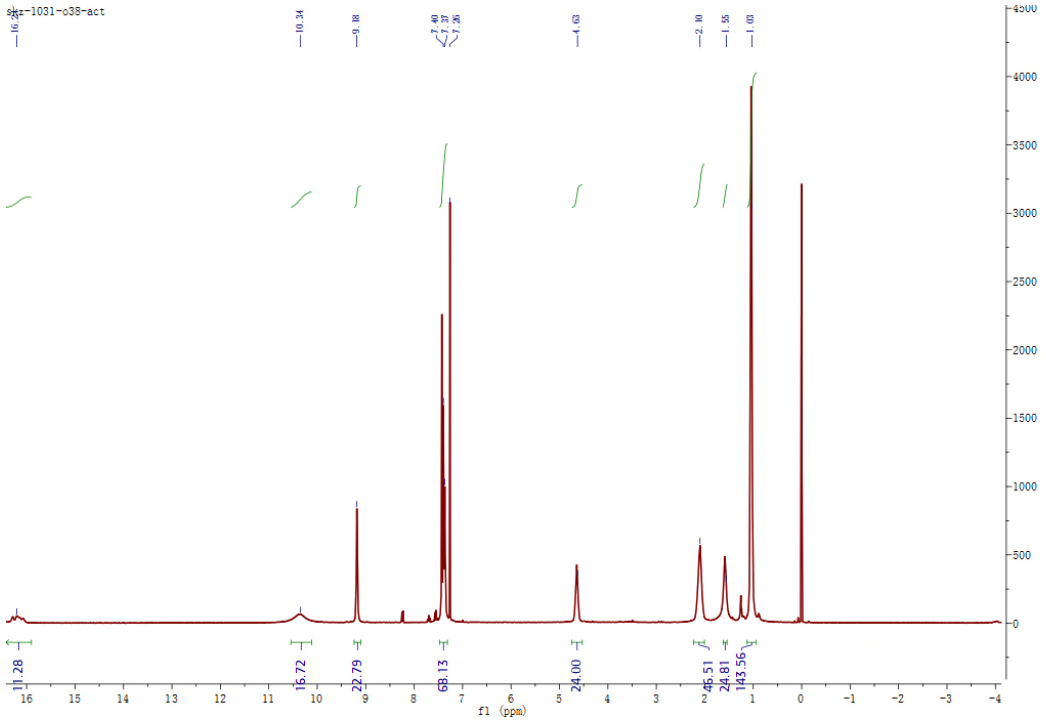
(a)



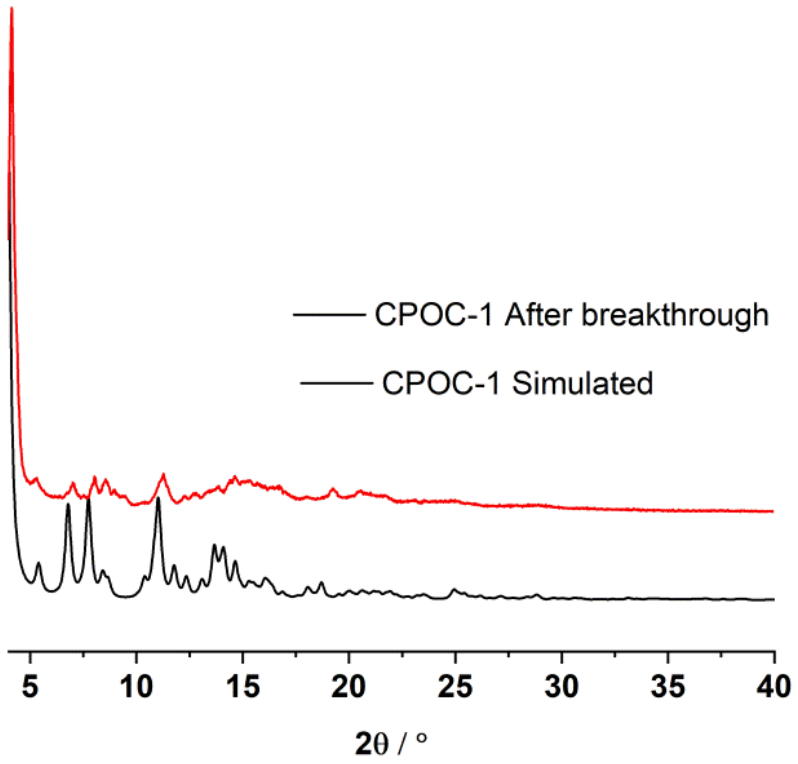
(b)

	Parameter value	Standard deviation
A1	5.518558	0.4165471
A2	2.388309	0.1088176
B1	4.205926E-4	9.145121E-5
B2	4.813541E-2	1.754617E-3
C1	1.441421	5.467777E-2
C2	0.9528982	4.886881E-3
Adj. R-Square	0.999999	

Supplementary Fig. 13 Dual-site Langmuir-Freundlich fitting of the C_2H_4 adsorption isotherm of **CPOC-301** at 293 K. (b) Relevant fitting parameters for C_2H_4.

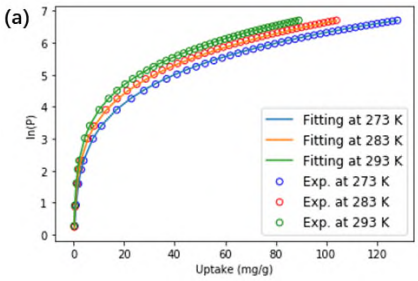


Supplementary Fig. 14 ^{1}HNMR of **CPOC-301** after breakthrough experiments ($CDCl_3$, 400 MHz, 298 K). The lower integral areas at 10.34 and 16.21 ppm are due to the active hydrogen atoms.



Supplementary Fig. 15 PXRD of **CPOC-301** after breakthrough experiments.

(a)



(b)

	Parameter value	Standard deviation
a0	-2431.677	64.59064
a1	7.11924	3.139478
a2	-5.18376E-2	4.08447E-2
a3	-3.821604E-4	6.343808E-4
a4	3.735269E-6	5.643884E-6
a5	-1.380009E-8	1.141135E-8
Adj. R-Square	0.9999	

Supplementary Fig. 16 (a) Virial equation fitting of the C_2H_2 adsorption isotherm of **CPOC-301** at 273, 283 and 293 K. (b) Relevant fitting parameters for C_2H_2.