



Figure S1 XRD pattern of L-Cys-PCN-222 synthesized under the different reaction temperature when the molar ratio of PCN-222 to L-Cys was 1 : 10.

Table S1 Binding ratio of  $Zr_6$  to L-Cys in L-Cys-PCN-222 synthesized at the different molar ratio of PCN-222 to L-Cys when the synthesis temperature of L-Cys-PCN-222 was 60 °C.

Molar ratio of PCN-222 to L-Cys	Element	Peak BE	Atomic %	Binding ratio of $Zr_6$ to L-Cys
1 : 1	C	291.08	67.46	1 : 2.0
	O	536.08	22.7	
	Zr	188.08	2.84	
	N	407.58	6.06	
	S	174.98	0.94	
1 : 5	C	291.58	68.71	1 : 3.4
	O	536.58	21.57	
	Zr	191.08	2.62	
	N	410.08	5.61	
	S	174.58	1.5	
1 : 10	C	283.82	70.05	1 : 3.8
	O	530.8	19.2	
	Zr	182.32	3.14	
	N	398.74	5.65	
	S	162.89	1.97	
1 : 15	C	286	69.9	1 : 3.8
	O	535.8	19.3	
	Zr	189	3.19	
	N	401	5.7	
	S	165	2	