

## Supporting information

### Synergistic acid-base bifunctional covalent organic framework for efficient tandem catalysis

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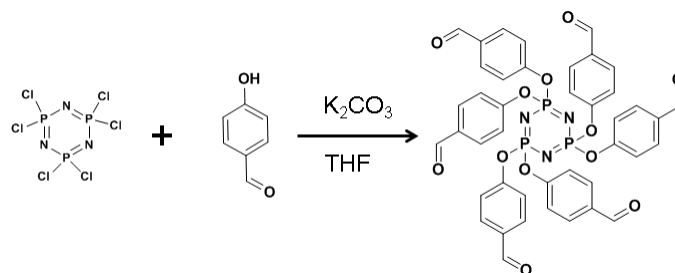
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#### I. Instruments and methods

The reagents and solvents employed were commercially available and used without further purification. The powder diffractometer (XRD) patterns were collected by a D8 ADVANCE X-ray with Cu K $\alpha$  radiation ( $\lambda = 1.5405 \text{ \AA}$ ). The total surface areas of the COFs were measured by the BET (Brunauer–Emmer–Teller) method using N<sub>2</sub> adsorption at 77 K, this was done by the Micromeritics ASAP 2000 sorption/desorption analyzer. Infrared (IR) samples were prepared as KBr pellets, and spectra were obtained in the 400–4000 cm<sup>-1</sup> range using a Perkin-Elmer 1600 FTIR spectrometer. <sup>13</sup>C NMR spectra were recorded on a MERCURY plus 400 spectrometer operating at resonance frequencies of 400 MHz. Thermogravimetric analyses (TGA) were carried out under flowing nitrogen at a heating rate of 10 °C·min<sup>-1</sup> on a TA Instrument Q5 analyzer. TEM (transmission electron microscopy) analysis was performed on a JEOL 2100 Electron Microscope at an operating voltage of 200 kV. Scanning electron microscopy (SEM) images were taken on a SUB010 scanning electron microscope with acceleration voltage of 20 kV. Gas chromatography (GC) analysis was performed on an Agilent 7890B. NH<sub>3</sub>-TPD and CO<sub>2</sub>-TPD measurements were conducted on a Quantachrome CHEMBET PULSAR TPR/TPD chemisorption analyzer (instrument no. 2021103105, Quantachrome Instruments, USA) equipped with a thermal conductivity detector (TCD) and a mass spectrometer (MS).

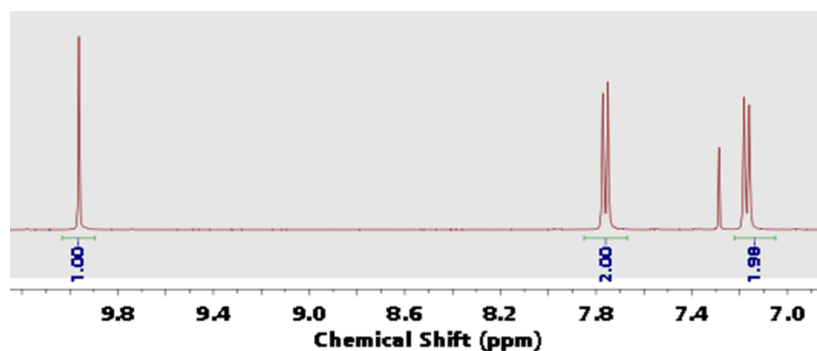
## II. Material Synthesis

### Synthesis of hexa(4-formyl-phenoxy)cyclotriphosphazene



**Fig.S1** Synthesis reaction diagram of hexa(4-formyl-phenoxy)cyclotriphosphazene (CTP).

In a round bottom flask, 2.32 g (19.0 mmol) of p-hydroxybenzaldehyde was dissolved in 100 mL dry tetrahydrofuran (THF), 3.94 g (28.5 mmol) potassium carbonate was slowly added to the system, and stirred in an ice bath for 30 min under 0°C. Then, a 50 mL solution of hexachlorocyclotriphosphazene (1.00 g; 2.9 mmol) in dry THF was slowly added, and the stirring was continued for 2 hours in an ice bath. After 2 hours, the ice bath was taken out, and the reaction was conducted at room temperature for 2 days. and the solvent was removed under reduced pressure to yield a white solid. The obtained solid was washed with dichloromethane, A white solid was obtained after removing the solvent under reduced pressure and the product was purified directly by chromatography on silica gel using dichloromethane / ethyl acetate (20:1) as the eluent to give the hexa(4-formyl-phenoxy)cyclotriphosphazene (CTP) white powder in 89% yield. <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz) δ (ppm) 9.96 (s, 6H), 7.75 (d, 12H), 7.17 (d, 12H).



**Fig. S2** <sup>1</sup>H NMR spectra of CTP in CDCl<sub>3</sub>.

### Synthesis of CTP-DABA-COF

Hexa(4-formyl-phenoxy)cyclotriphosphazene (CTP, 16.80 mg, 0.02 mmol) and 3, 5-Diaminobenzoic acid (DABA, 9.12 mg, 0.06 mmol) were dissolved in a mixed solvent system of 1, 2-dichlorobenzene/mesitylene/ethanol (1:1:1, v/v/v) with 6 M AcOH (100  $\mu$ L) as catalyst. After sonication (10 min), the sealed Pyrex vessel was heated at 90°C for 3 days and slowly cooled for 1 day. The product was washed (DMF/THF/EtOH) and dried in vacuo to obtain CTP-DABA-COF as gray powder (89% yield).

#### **Synthesis of CTP -MPD-COF**

Hexa(4-formyl-phenoxy)cyclotriphosphazene (CTP, 16.80 mg, 0.02 mmol) and m-phenylenediamine (MPD, 9.12 mg, 0.06 mmol) were dissolved in a mixed solvent system of 1, 2-dichlorobenzene/mesitylene/ethanol (1:1:1, v/v) with 6 M AcOH (100  $\mu$ L) as catalyst. After sonication (10 min), the sealed vessel was heated at 90°C for 3 days and slowly cooled for 1 day. The product was washed (DMF/THF/EtOH) and dried in vacuo to obtain CTP -MPD-COF as yellow powder (92% yield).

#### **Tandem reaction catalyzed by CTP-DABA-COF**

The catalytic reaction was performed by combining benzaldehyde dimethyl acetal (150  $\mu$ L, 1.0 mmol) and malononitrile (66.0 mg, 1.0 mmol) with CTP-DABA-COF catalyst (11.9 mg, 1.0 mol%) were placed in a 2 mL glass vessel, which was then capped and heated at 50°C under H<sub>2</sub>O (2 mL) conditions for 5 h. Upon completion, the reaction was cooled to room temperature and the conversion was quantitatively analyzed by GC. The crude product was then purified by column chromatography using petroleum ether/ethyl acetate (6:1, v/v) as the eluent.

#### **Multicomponent tandem reaction catalyzed by CTP -MPD-COF**

benzaldehyde dimethyl acetal (150  $\mu$ L, 1.0 mmol) and malononitrile (66.0 mg, 1.0 mmol), 4-hydroxy-6-methyl-2-pyrone (128.1mg, 1.00mmol) with CTP-MPD-COF catalyst (11.9 mg, 1.0 mol%) were placed in a 2 mL glass vessel, which was then capped and heated at 50°C under H<sub>2</sub>O:EtOH (1:1, 2 mL) conditions for 7 h. After the reaction was complete, the mixture was cooled to room temperature. The crude

product was then purified by column chromatography using petroleum ether/ethyl acetate (6:1, v/v) as the eluent. The conversion was then determined based on the isolated yield.

### **Stepwise catalysis comparative experiment by CTP -MPD-COF CTP-DABA-COF, CTP-MPD-COF or HCCTP**

Step 1: benzaldehyde dimethylacetal (150  $\mu$ L, 1.0 mmol) was catalyzed by **CTP-DABA-COF** (11.9 mg), **CTP-MPD-COF** (10.6 mg, 1 mol %) or **HCCTP** (3.47 mg) at 50 °C in water (2 mL).

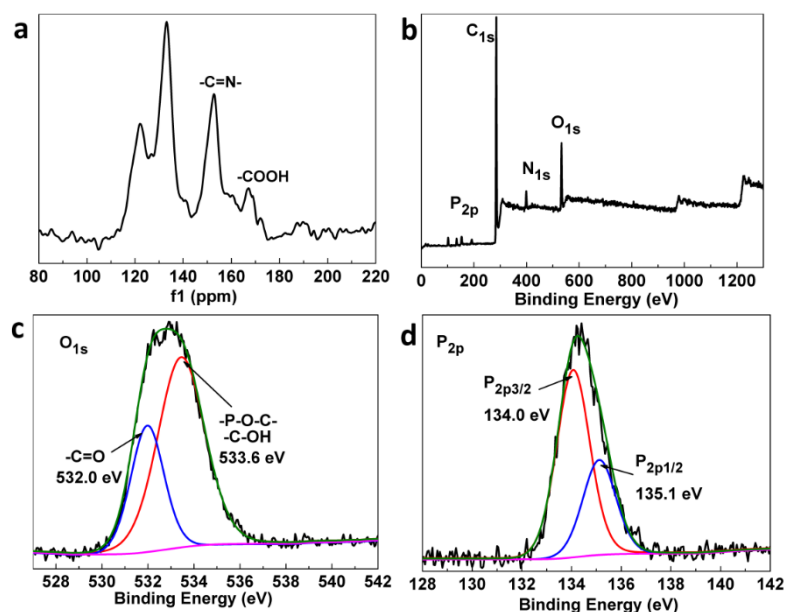
Step 2: benzaldehyde (102  $\mu$ L, 1.0 mmol) and malononitrile (0.72 g, 1.1 mmol) were catalyzed by **CTP-DABA-COF** (11.9 mg, 1 mol %), **CTP -MPD-COF** (10.6 mg) or **HCCTP** (3.47 mg) at 50°C in water (2 mL).

Step 3: benzylidenemalononitrile (154mg, 1.0 mmol) and 4-hydroxy-6-methyl-2-pyrone (128.1 mg, 1.0 mmol) were catalyzed by **CTP-DABA-COF** (11.9 mg, 1 mol %), **CTP -MPD-COF** (10.6 mg) or **HCCTP** (3.47 mg) at 50 °C in mixed solvent of EtOH (1 mL) and water (1 mL). b: Yield was determined by GC analysis and c: Yield was monitored by isolated yields.

### **Catalytic Experiments of CTP-DABA-COF at Various pH Conditions**

To minimize the interference of buffer anions on the acid-base bifunctional active sites of the COF and maintain stable pH during the reaction, different buffer systems with suitable buffering ranges and inert ion components were employed. Buffer solutions with pH values of 5, 6, 7, 8, and 9 were prepared using citrate-phosphate buffer (pH=5), phosphate buffer ( $\text{NaH}_2\text{PO}_4\text{-Na}_2\text{HPO}_4$ , pH=6, 7), and borate buffer (pH=8, 9), respectively. Each buffer solution (50 mL) was transferred into clean volumetric flasks, diluted to the mark, and shaken well for later use. The actual pH values were calibrated using a pH meter to ensure the error was within  $\pm 0.02$ . Catalytic reaction conditions: benzaldehyde dimethylacetal (150  $\mu$ L, 1.0 mmol) and malononitrile (66 mg, 1.0 mmol) were stirred for 5 h in 2 mL of buffer solutions with different pH values in the presence of CTP-DABA-COF (11.9 mg, 1 mol%). After

simple filtration and extraction, the yield was determined by gas chromatography (GC) analysis.



**Fig. S3** (a) Solid-state  $^{13}\text{C}$  CP-MAS NMR spectra, (b) survey scan XPS profile, the high resolution XPS spectra of O 1s (c) and P 2p (d) of **CTP-DABA-COF**.

### III. Simulated Structure of CTP-DABA-COF

Structural modeling of **CTP-DABA-COF** was generated using the Materials Studio (ver. 2018) suite of programs. Molecular geometry optimization was performed with MS DMol3 module. The initial lattice was created by starting with the space group P1. The a and b lattice parameters (initially 37.2204 Å) were estimated according to the center to center distance between the vertices of COF. The constructed model was geometry optimized using the Forcite module (Universal force fields, Ewald summations). Then the calculated PXRD pattern was generated with the Reflex Plus module. Finally, Pawley refinement was applied for profile fitting, producing the refined PXRD profile with the lattice parameters of  $a = b = 30.3180$  Å and  $c = 11.5320$  Å,  $\alpha = \beta = 90^\circ$  and  $\gamma = 120^\circ$ . Rwp and Rp values converged to 0.76 and 0.49 %, respectively. Reflex Module in Material Studio using data from  $2\theta = 2.0$ - $30^\circ$ . Backgrounds were first refined applying a 2nd order Chebyshev Polynomial.

**Table S1.** Simulated structure of **CTP-DABA-COF** based on AA-stacking

space group P1
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$a = b = 45.0000 \text{ \AA}, c = 5.0000 \text{ \AA},$ $\alpha = \beta = 90^\circ$ and $\gamma = 120^\circ$							
Atom	x/a	y/b	z/c	Atom	x/a	y/b	z/c
P1	0.29381	0.67686	0.46613	C130	1.00876	0.42074	0.14317
N2	0.3226	0.6667	0.28151	O131	0.98075	0.39501	0.06577
P3	0.36497	0.67666	0.39749	O132	1.03699	0.42305	0.07127
N4	0.38492	0.72195	0.46688	O133	0.61608	0.28526	0.16634
P5	0.36519	0.74788	0.52305	O134	0.65227	0.28841	0.64569
N6	0.32285	0.71636	0.64479	C135	0.64333	0.25189	0.58642
O7	0.26111	0.6836	0.27132	C136	0.58873	0.24882	0.23466
O8	0.26395	0.63806	0.67376	C137	0.55546	0.23684	0.35476
C9	0.2265	0.61355	0.62107	C138	0.52924	0.20012	0.37875
C10	0.22373	0.67089	0.33676	C139	0.53282	0.17173	0.27924
C11	0.21002	0.69244	0.41541	C140	0.56469	0.18401	0.14927
C12	0.17317	0.6809	0.42476	C141	0.59051	0.22026	0.13358
C13	0.14599	0.64716	0.34639	C142	0.66731	0.24004	0.54522
C14	0.15959	0.62655	0.25783	C143	0.65771	0.20361	0.54553
C15	0.19618	0.63835	0.25275	C144	0.62365	0.17526	0.59817
C16	0.21217	0.58436	0.44675	C145	0.60076	0.18724	0.65073
C17	0.17515	0.55981	0.42764	C146	0.61062	0.22333	0.64474
C18	0.14887	0.56117	0.58376	C147	0.61369	0.13556	0.58801
C19	0.16348	0.58904	0.76396	N148	0.58457	0.10544	0.64595
C20	0.20019	0.6134	0.7784	C149	0.57915	0.06929	0.61075
C21	0.10584	0.63549	0.37486	C150	0.50402	0.13176	0.3204
N22	0.07561	0.60724	0.30252	N151	0.50105	0.10119	0.24462
C23	0.03944	0.60083	0.36152	C152	0.47154	0.06516	0.31419
C24	0.03683	0.62534	0.51693	C153	0.60565	0.06629	0.48947
C25	0.00534	0.62216	0.59533	C154	0.6035	0.03459	0.43576
C26	-0.02606	0.59369	0.51793	C155	0.57411	0.0034	0.50428
C27	-0.02859	0.56663	0.36211	C156	0.54508	0.00147	0.62611
C28	0.00546	0.57058	0.28192	C157	0.54785	0.03565	0.67787
N29	-0.06479	0.53712	0.29893	C158	0.44517	0.06299	0.47677
C30	-0.0949	0.53375	0.39129	C159	0.41731	0.03169	0.56415
C31	0.00525	0.64944	0.76047	C160	0.41385	0.00001	0.48827
O32	-0.02287	0.64714	0.83442	C161	0.43751	-0.00307	0.32601
O33	0.03338	0.67565	0.83154	C162	0.46739	0.03084	0.23861
P34	0.6482	0.38966	0.53071	N163	0.51423	-0.03425	0.67573
N35	0.62843	0.344	0.47857	C164	0.51302	-0.06484	0.63557
P36	0.64826	0.31871	0.4036	N165	0.43059	-0.03954	0.2685
N37	0.69043	0.35089	0.28326	C166	0.40296	-0.06962	0.35241
P38	0.71947	0.39003	0.46542	C167	0.63256	0.03412	0.30033
N39	0.69057	0.40017	0.65021	O168	0.63113	0.00575	0.24656
O40	0.65212	0.42113	0.26447	O169	0.65924	0.06198	0.23386

O41	0.61648	0.39331	0.76364	C170	0.39095	0.03199	0.74003
C42	0.58706	0.39949	0.69119	O171	0.36558	0.004	0.8228
C43	0.64289	0.44883	0.29914	O172	0.39323	0.06023	0.8105
C44	0.66219	0.48145	0.43432	O173	1.36112	0.77626	0.26496
C45	0.65149	0.5076	0.43923	O174	1.39732	0.78324	0.75278
C46	0.62135	0.50455	0.3061	H175	0.2281	0.72025	0.47525
C47	0.60408	0.47332	0.16247	H176	0.16416	0.69907	0.49805
C48	0.61481	0.4476	0.15988	H177	0.14164	0.59925	0.18574
C49	0.55126	0.37551	0.73937	H178	0.20183	0.61809	0.16992
C50	0.52406	0.38469	0.73999	H179	0.22971	0.57924	0.31382
C51	0.52981	0.41913	0.70625	H180	0.16526	0.53752	0.28041
C52	0.56481	0.44275	0.6656	H181	0.14634	0.59337	0.90778
C53	0.59112	0.43303	0.66388	H182	0.20692	0.63398	0.9372
C54	0.49943	0.42816	0.69841	H183	0.09796	0.65317	0.47662
N55	0.49885	0.45815	0.71348	H184	0.06104	0.64939	0.58649
C56	0.46743	0.46247	0.67997	H185	-0.05127	0.59177	0.58224
C57	0.60942	0.53298	0.33257	H186	0.00467	0.54918	0.15456
N58	0.58219	0.53575	0.24116	H187	-0.09453	0.55409	0.52939
C59	0.57543	0.56548	0.29559	H188	0.02803	0.69072	0.98008
C60	0.437	0.43408	0.58595	H189	0.68693	0.48799	0.54398
C61	0.40686	0.43526	0.53187	H190	0.66737	0.53256	0.55408
C62	0.40551	0.46553	0.57094	H191	0.58031	0.46708	0.03959
C63	0.43338	0.4963	0.66411	H192	0.59779	0.4246	0.02805
C64	0.4653	0.49449	0.71838	H193	0.54242	0.34738	0.78043
C65	0.59999	0.59321	0.44665	H194	0.49612	0.36392	0.76854
C66	0.597	0.62196	0.51564	H195	0.57369	0.47103	0.63189
C67	0.56842	0.62466	0.4364	H196	0.6178	0.4563	0.63655
C68	0.54129	0.59962	0.28287	H197	0.47165	0.40675	0.67607
C69	0.54529	0.56921	0.21063	H198	0.62572	0.55751	0.45131
N70	0.42854	0.52759	0.68193	H199	0.43592	0.40854	0.5499
C71	0.39848	0.52768	0.64843	H200	0.38085	0.46589	0.52632
C72	0.38889	0.55765	0.64137	H201	0.48866	0.51903	0.79218
N73	0.51158	0.60597	0.21467	H202	0.62398	0.59325	0.52061
C74	0.50848	0.63353	0.29057	H203	0.56649	0.64806	0.4969
C75	0.47963	0.64472	0.24969	H204	0.5239	0.54837	0.08475
C76	0.44806	0.62553	0.1149	H205	0.37348	0.50247	0.61751
C77	0.42232	0.63605	0.09619	H206	0.52972	0.65519	0.4118
C78	0.42378	0.66606	0.20517	H207	0.4416	0.60033	0.01314
C79	0.45657	0.68677	0.33471	H208	0.39736	0.61939	-0.01664
C80	0.48283	0.67625	0.35687	H209	0.46322	0.71259	0.42602
C81	0.41244	0.59282	0.61366	H210	0.5071	0.69518	0.46858
C82	0.40254	0.61895	0.60098	H211	0.44108	0.60221	0.59984
C83	0.36889	0.61426	0.60246	H212	0.42306	0.6472	0.58796

C84	0.34471	0.57834	0.64007	H213	0.3162	0.5692	0.66228
C85	0.35416	0.55144	0.65264	H214	0.33175	0.52411	0.67268
O86	0.39578	0.67458	0.14941	H215	0.40356	0.38203	0.3863
O87	0.36108	0.643	0.64813	H216	0.66359	0.66609	0.91875
C88	0.37614	0.40428	0.42666	H217	0.47028	0.81085	0.63288
O89	0.3491	0.40521	0.36501	H218	0.51639	0.87386	0.60313
O90	0.37658	0.37641	0.39342	H219	0.4393	0.90415	0.72123
C91	0.62448	0.6498	0.67723	H220	0.39523	0.84545	0.73691
O92	0.62236	0.67601	0.74475	H221	0.32416	0.80704	0.52782
O93	0.65053	0.64781	0.75216	H222	0.3432	0.871	0.54389
C94	0.37048	0.81304	0.31156	H223	0.4353	0.89494	0.08757
C95	0.42548	0.81913	0.67431	H224	0.41889	0.83535	0.07871
C96	0.46135	0.83046	0.64669	H225	1.10805	0.51469	0.39139
C97	0.48853	0.86684	0.63433	H226	1.06415	0.47589	0.3257
C98	0.48302	0.89575	0.65907	H227	0.95188	0.42074	0.32888
C99	0.44815	0.88461	0.69557	H228	1.00733	0.51674	0.78936
C100	0.42173	0.84866	0.70309	H229	0.90846	0.41182	0.41987
C101	0.34985	0.82571	0.43232	H230	0.86785	0.47103	0.05733
C102	0.36025	0.86246	0.44029	H231	0.80378	0.42896	0.03607
C103	0.39146	0.89013	0.32401	H232	0.78351	0.48968	0.60306
C104	0.4104	0.87689	0.1961	H233	0.8453	0.53097	0.63858
C105	0.40003	0.84056	0.19282	H234	0.87105	0.46567	0.78521
C106	1.10855	0.53396	0.54193	H235	0.80706	0.4439	0.79723
N107	1.07856	0.5301	0.64056	H236	0.78593	0.3492	0.40639
C108	1.04237	0.50124	0.56888	H237	0.84744	0.36926	0.37716
C109	1.03989	0.4752	0.40079	H238	1.05853	0.44466	0.17882
C110	1.00852	0.44737	0.31566	H239	0.54831	0.25606	0.43704
C111	0.97699	0.44377	0.39804	H240	0.50379	0.19226	0.48213
C112	0.97427	0.46733	0.5646	H241	0.57125	0.16521	0.04982
C113	1.00827	0.49696	0.65258	H242	0.6145	0.22442	0.02391
N114	0.93799	0.46045	0.62773	H243	0.69559	0.25931	0.50969
C115	0.90794	0.43283	0.54367	H244	0.67789	0.19601	0.50189
C116	0.86765	0.42059	0.57546	H245	0.57282	0.16829	0.70133
C117	0.86478	0.50592	0.35493	H246	0.5882	0.22742	0.69468
C118	0.85045	0.47652	0.18887	H247	0.63349	0.12838	0.52045
C119	0.8138	0.45209	0.17491	H248	0.47956	0.12467	0.43658
C120	0.78718	0.45324	0.31978	H249	0.63048	0.09032	0.42926
C121	0.80125	0.48369	0.48065	H250	0.57309	-0.02197	0.46113
C122	0.83821	0.50842	0.49827	H251	0.52463	0.03523	0.77309
C123	0.85348	0.43952	0.69129	H252	0.4456	0.08738	0.54493
C124	0.81676	0.42749	0.69898	H253	0.39082	-0.02496	0.55956
C125	0.78947	0.39607	0.59433	H254	0.48751	0.02956	0.10833
C126	0.80368	0.37606	0.48781	H255	0.53711	-0.06528	0.57127

C127	0.84068	0.38799	0.47519	H256	0.38159	-0.06917	0.4715
O128	0.74977	0.42918	0.26224	H257	0.66127	0.08329	0.35912
O129	0.75188	0.38269	0.65862	H258	0.36712	0.05637	0.84278

**Table S2.** Simulated structure of **CTP-DABA-COF** based on AB-stacking

space group <i>P1</i>							
$a = 38.7971 \text{ \AA}, b = 38.2150 \text{ \AA}, c = 10.0412 \text{ \AA},$							
$\alpha = 95.6312^\circ, \beta = 94.4678^\circ, \gamma = 122.6385^\circ$							
Atom	x/a	y/b	z/c	Atom	x/a	y/b	z/c
P1	0.27859	0.65412	0.19568	C259	0.023	0.86249	0.83049
N2	0.30216	0.63571	0.28754	O260	0.04645	0.96591	0.64008
P3	0.35419	0.66355	0.29567	O261	0.07172	0.97785	0.93401
N4	0.37081	0.71453	0.3413	C262	0.00277	0.66551	0.62491
P5	0.35428	0.73332	0.22394	O263	-0.02954	0.66606	0.59939
N6	0.31424	0.69149	0.11607	O264	0.00113	0.63182	0.58787
O7	0.239	0.6121	0.07163	C265	0.35855	1.04113	0.6214
O8	0.25929	0.67641	0.30578	O266	0.35905	1.07477	0.6268
C9	0.22472	0.64704	0.36007	O267	0.39252	1.04332	0.62677
C10	0.20368	0.61308	0.04143	C268	0.07321	1.10984	0.55761
C11	0.20596	0.6511	0.04477	C269	0.05527	1.1206	0.85277
C12	0.16999	0.65095	0.02185	C270	0.09442	1.12913	0.90169
C13	0.13132	0.61293	-0.00701	C271	0.1281	1.17047	0.94434
C14	0.12879	0.57476	-0.01494	C272	0.12332	1.204	0.93928
C15	0.16492	0.57493	0.00857	C273	0.08402	1.19586	0.89677
C16	0.21969	0.6099	0.39381	C274	0.05009	1.15424	0.85471
C17	0.18347	0.58006	0.4384	C275	0.03825	1.11126	0.52392
C18	0.15179	0.58685	0.4497	C276	0.04295	1.14963	0.51199
C19	0.15696	0.62425	0.41916	C277	0.08248	1.1867	0.53179
C20	0.19346	0.65434	0.3758	C278	0.11753	1.18505	0.55865
C21	0.09439	0.6145	-0.02163	C279	0.11283	1.14662	0.57055
N22	0.05725	0.58093	-0.0361	C280	-0.1991	0.8692	1.00997
C23	0.02134	0.58295	-0.04351	N281	-0.23295	0.86852	1.00528
C24	0.0249	0.62171	-0.03682	C282	-0.27167	0.83122	1.01713
C25	-0.01008	0.62363	-0.03625	C283	-0.27576	0.79225	1.01195
C26	0.95116	0.58641	-0.04134	C284	-0.31446	0.75503	1.00742
C27	0.94703	0.54741	-0.04689	C285	0.65054	0.75692	1.00822
C28	-0.01765	0.54601	-0.04713	C286	0.65405	0.79565	1.01457
N29	0.90825	0.51007	-0.03569	C287	-0.307	0.83258	1.0176
C30	0.87439	0.50938	-0.04066	N288	0.61812	0.79762	1.00744
C31	-0.00589	0.66452	-0.02197	C289	0.58103	0.76403	0.99365
O32	0.96212	0.66605	-0.03454	C290	0.54406	0.76553	0.9794

O33	0.02977	0.69866	0.00536	C291	0.52331	0.79135	0.52333
P34	0.63103	0.39246	0.16698	C292	0.51817	0.75393	0.55353
N35	0.61267	0.34077	0.15439	C293	0.48171	0.72383	0.59709
P36	0.63897	0.32973	0.26686	C294	0.45048	0.73113	0.61334
N37	0.68165	0.37579	0.34692	C295	0.45548	0.76828	0.57985
P38	0.71083	0.40773	0.24105	C296	0.49165	0.79813	0.5351
N39	0.68061	0.41676	0.13901	C297	0.54653	0.80367	0.98692
O40	0.60235	0.39922	0.03784	C298	0.51035	0.80342	0.96379
O41	0.62894	0.41216	0.3313	C299	0.4716	0.76523	0.93172
C42	0.59036	0.40583	0.3443	C300	0.4694	0.72725	0.92881
C43	0.60879	0.4393	0.05416	C301	0.50542	0.72749	0.95136
C44	0.64711	0.47592	0.11366	O302	0.41599	0.70178	0.66802
C45	0.65141	0.51476	0.13749	O303	0.43621	0.7661	0.902
C46	0.61763	0.51765	0.10193	C304	-0.31861	0.71416	0.99346
C47	0.57968	0.48152	0.03873	O305	0.64579	0.67999	0.96643
C48	0.57542	0.44261	0.01438	O306	-0.28655	0.7127	1.00597
C49	0.55305	0.36679	0.29599	O307	0.33794	0.61509	0.66533
C50	0.51501	0.36217	0.30356	O308	0.27952	0.61566	0.83972
C51	0.51376	0.39641	0.35903	C309	0.27671	0.58039	0.8813
C52	0.55094	0.43514	0.41015	C310	0.30571	0.57375	0.60843
C53	0.589	0.43967	0.40361	C311	0.267	0.56408	0.54831
C54	0.47343	0.39134	0.35817	C312	0.23333	0.52233	0.51629
N55	0.47071	0.42353	0.3867	C313	0.23795	0.48975	0.54229
C56	0.43204	0.42017	0.3845	C314	0.27713	0.49894	0.5933
C57	0.62226	0.55816	0.13912	C315	0.31094	0.54086	0.62525
N58	0.59126	0.56214	0.11789	C316	0.31205	0.58157	0.93222
C59	0.59438	0.60083	0.15875	C317	0.30863	0.54541	0.96573
C60	0.39423	0.38101	0.37152	C318	0.26987	0.50764	0.95001
C61	0.35676	0.37858	0.36644	C319	0.23416	0.50645	0.9038
C62	0.35723	0.41564	0.37195	C320	0.23764	0.54286	0.87051
C63	0.39483	0.45491	0.38447	C321	0.26867	0.4699	0.97427
C64	0.432	0.45688	0.39231	N322	0.23476	0.43264	0.95603
C65	0.63137	0.63689	0.22908	C323	0.23568	0.39633	0.97368
C66	0.63324	0.67395	0.27248	C324	0.20029	0.44807	0.53742
C67	0.59762	0.67457	0.24617	N325	0.20074	0.41575	0.56362
C68	0.56046	0.63866	0.17638	C326	0.16306	0.37739	0.57564
C69	0.55917	0.60205	0.133	C327	0.27359	0.39961	0.99779
N70	0.39623	0.49327	0.39158	C328	0.27472	0.36409	1.00884
C71	0.36477	0.49499	0.34967	C329	0.23745	0.32488	0.99612
C72	0.36806	0.53535	0.36467	C330	0.19914	1.32077	0.97225
N73	0.5233	0.63806	0.15268	C331	0.1985	0.35666	0.95981
C74	0.52047	0.66876	0.20332	C332	0.12951	0.37821	0.61512
C75	0.48163	0.66659	0.17948	C333	0.09315	0.3413	0.63234

C76	0.44721	0.63318	0.09035	C334	0.09025	0.30312	0.60855
C77	0.41003	0.63109	0.07373	C335	0.12357	1.30164	0.57014
C78	0.40677	0.66197	0.14697	C336	0.16025	0.33907	0.55631
C79	0.44169	0.69604	0.2332	N337	0.16099	1.28007	0.95243
C80	0.47889	0.69824	0.24913	C338	0.16083	1.24665	0.96756
C81	0.40145	0.57089	0.45028	N339	0.12114	1.26269	0.55254
C82	0.40373	0.60878	0.46753	C340	0.08583	1.22681	0.5376
C83	0.37317	0.61203	0.39832	C341	0.31461	0.36773	1.02848
C84	0.33967	0.57644	0.3119	O342	0.31554	0.33509	1.0323
C85	0.33713	0.53824	0.29566	O343	0.34847	0.4035	1.04054
O86	0.36836	0.65738	0.13619	C344	0.05905	0.34289	0.6804
O87	0.37638	0.6504	0.42551	O345	0.02415	0.3091	0.68025
C88	0.31727	0.33749	0.35512	O346	0.06453	0.37811	0.7248
O89	0.28329	0.33525	0.34996	O347	0.06925	1.07264	0.58259
O90	0.31683	0.30388	0.35012	O348	0.02203	1.07993	0.79249
C91	0.67225	0.71186	0.34436	H349	0.2374	0.6824	0.06635
O92	0.67405	0.74567	0.38146	H350	0.1721	0.68199	0.02667
O93	0.70448	0.7112	0.36933	H351	0.0973	0.54357	-0.04055
C94	0.39844	0.79777	0.09125	H352	0.16265	0.54377	0.00083
C95	0.36987	0.80467	0.36462	H353	0.24532	0.60399	0.38482
C96	0.40854	0.81415	0.42445	H354	0.17965	0.55003	0.46574
C97	0.44235	0.85584	0.45636	H355	0.13139	0.63016	0.42966
C98	0.43792	0.88856	0.43055	H356	0.19768	0.68496	0.3532
C99	0.39879	0.87956	0.37985	H357	0.0977	0.64604	-0.02052
C100	0.36484	0.8377	0.34799	H358	0.05657	0.65207	-0.03178
C101	0.3631	0.79662	0.04054	H359	0.92233	0.58742	-0.04103
C102	0.36655	0.8328	0.00715	H360	-0.02082	0.51449	-0.05031
C103	0.40531	0.87054	0.02278	H361	0.87413	0.53758	-0.06703
C104	0.44103	0.8717	0.06875	H362	0.02932	0.72087	0.0841
C105	0.43752	0.83526	0.10193	H363	0.67496	0.47399	0.14283
C106	0.11283	0.55311	0.48485	H364	0.68257	0.54424	0.1861
N107	0.0806	0.55525	0.48543	H365	0.5522	0.48383	0.00707
C108	0.04184	0.52097	0.51202	H366	0.54456	0.41349	-0.03817
C109	0.03702	0.48306	0.53589	H367	0.55369	0.33867	0.25033
C110	-0.00147	0.44874	0.55313	H368	0.48487	0.3304	0.26442
C111	0.96447	0.45234	0.54533	H369	0.55021	0.46307	0.45726
C112	0.96857	0.4899	0.52083	H370	0.61902	0.47115	0.44692
C113	0.00737	0.52403	0.50376	H371	0.44365	0.35858	0.33204
N114	0.93302	0.49238	0.50019	H372	0.65371	0.58717	0.18801
C115	0.89609	0.46072	0.50693	H373	0.39382	0.35083	0.36501
C116	0.85907	0.46156	0.47576	H374	0.32693	0.41402	0.36626
C117	0.83553	0.47334	-0.01348	H375	0.46253	0.48893	0.40523
C118	0.83321	0.43836	0.02924	H376	0.66023	0.63616	0.25131

C119	0.79728	0.40768	0.07421	H377	0.5986	0.70442	0.28148
C120	0.76372	0.41198	0.07863	H378	0.529	0.57298	0.07607
C121	0.76572	0.4462	0.0301	H379	0.33413	0.46495	0.30054
C122	0.80143	0.47669	-0.01501	H380	0.54858	0.69821	0.26792
C123	0.8615	0.49718	0.43904	H381	0.44953	0.60767	0.03132
C124	0.82525	0.4954	0.39731	H382	0.38219	0.60413	0.0002
C125	0.78638	0.45798	0.38999	H383	0.43968	0.72201	0.29044
C126	0.78417	0.42277	0.4309	H384	0.50709	0.72599	0.31926
C127	0.82032	0.4246	0.47311	H385	0.42691	0.56892	0.50624
O128	0.7303	0.38357	0.13947	H386	0.43072	0.63746	0.53863
O129	0.75097	0.45666	0.33879	H387	0.31449	0.57864	0.25486
C130	-0.00654	0.40862	0.57251	H388	0.30978	0.50946	0.226
O131	0.95934	0.3784	0.598	H389	0.28427	0.27625	0.33347
O132	0.02307	0.40372	0.56181	H390	0.72535	0.73564	0.45818
O133	0.65347	0.29824	0.17737	H391	0.41238	0.78768	0.44712
O134	0.60716	0.30564	0.39044	H392	0.47375	0.86332	0.5037
C135	0.60336	0.26844	0.41457	H393	0.39466	0.90633	0.36462
C136	0.62015	0.25754	0.11772	H394	0.33297	0.83054	0.30832
C137	0.58091	0.249	0.06999	H395	0.33125	0.76593	0.02633
C138	0.54718	0.20765	0.02801	H396	0.3376	0.83165	-0.03316
C139	0.552	0.17414	0.03256	H397	0.47285	0.90226	0.07907
C140	0.59137	0.18228	0.07387	H398	0.46667	0.83622	0.13778
C141	0.62535	0.22392	0.11524	H399	0.11144	0.52418	0.51239
C142	0.6384	0.26701	0.44636	H400	0.06473	0.48001	0.5414
C143	0.6338	0.22865	0.45783	H401	0.93284	0.42459	0.55889
C144	0.59428	0.19159	0.43947	H402	0.01076	0.55446	0.483
C145	0.55919	0.19325	0.4144	H403	0.89155	0.43078	0.53808
C146	0.56379	0.23166	0.40294	H404	0.86058	0.4349	0.02736
C147	0.59091	0.15145	0.43344	H405	0.79523	0.37902	0.10746
N148	0.55559	0.11563	0.4199	H406	0.73798	0.44918	0.02743
C149	0.55299	0.07658	0.40223	H407	0.80272	0.50443	-0.05326
C150	0.51448	0.1315	0.00499	H408	0.89303	0.52764	0.44318
N151	0.51433	0.09809	0.01994	H409	0.82724	0.52453	0.36897
C152	0.47616	0.05743	0.00081	H410	0.75272	0.39251	0.42973
C153	0.58612	0.07486	0.36314	H411	0.81814	0.39579	0.5055
C154	0.58298	0.03655	0.33919	H412	0.05094	0.42874	0.63368
C155	0.54658	-0.00022	0.35696	H413	0.57646	0.27603	0.06536
C156	0.51322	1.00084	0.39711	H414	0.51546	0.20108	-0.0103
C157	0.51626	0.03927	0.41659	H415	0.59572	0.15506	0.07378
C158	0.43786	0.0534	-0.02206	H416	0.65738	0.23035	0.14702
C159	0.40058	0.01424	-0.03423	H417	0.6707	0.29721	0.46285
C160	0.40167	-0.02132	-0.02361	H418	0.66232	0.22749	0.48226
C161	0.43956	0.98188	-0.00044	H419	0.5269	0.16327	0.40335

C162	0.47677	0.02151	0.01287	H420	0.53518	0.23298	0.38407
N163	0.47545	0.9626	0.40941	H421	0.62006	0.15086	0.44073
C164	0.4757	0.93015	0.43523	H422	0.48328	0.12637	-0.03168
N165	0.44047	0.94554	0.01682	H423	0.61605	0.105	0.35059
C166	0.40654	0.90831	-0.00121	H424	0.5436	-0.03173	0.33884
C167	0.61685	0.0347	0.29034	H425	0.48875	0.04016	0.44419
O168	0.61116	-0.00062	0.24604	H426	0.43693	0.0824	-0.03095
O169	0.65178	0.06838	0.28969	H427	0.37154	-0.05359	-0.03375
C170	0.36073	0.0107	-0.0529	H428	0.50761	0.02443	0.0336
O171	0.32683	-0.02505	-0.06512	H429	0.5064	0.93327	0.4632
O172	0.35987	0.04341	-0.05574	H430	0.3756	0.9038	-0.03756
O173	0.39562	0.76248	0.13277	H431	0.656	0.09397	0.36605
O174	0.3375	0.76337	0.30776	H432	0.39203	0.07178	-0.03719
P175	-0.03573	0.97039	0.72654	H433	-0.07767	0.9861	0.53873
N176	-0.00612	0.96083	0.82948	H434	-0.14331	0.98288	0.46528
P177	0.0437	0.98515	0.80411	H435	-0.21789	0.85086	0.52535
N178	0.06228	1.03691	0.81803	H436	-0.15231	0.85371	0.59708
P179	0.0367	1.04841	0.70432	H437	-0.06292	0.92908	0.93983
N180	-0.00586	1.00256	0.62237	H438	-0.12763	0.87399	1.0218
O181	-0.07575	0.92176	0.62696	H439	-0.18535	0.94358	0.94123
O182	-0.05532	0.99459	0.82729	H440	-0.12033	0.99921	0.86015
C183	-0.08866	0.96629	0.88873	H441	-0.21805	0.94738	0.43422
C184	-0.11125	0.92051	0.57732	H442	-0.25797	0.95471	0.41659
C185	-0.1091	0.95581	0.53762	H443	0.61008	0.89819	0.43599
C186	-0.14528	0.95406	0.49672	H444	-0.336	0.82376	0.48686
C187	-0.184	0.91707	0.49409	H445	0.56361	0.85417	0.46165
C188	-0.18638	0.88134	0.52951	H446	-0.27353	1.02964	0.45618
C189	-0.1501	0.88306	0.56998	H447	0.36098	0.79966	0.71835
C190	-0.09062	0.93212	0.93749	H448	0.36572	0.86894	0.74761
C191	-0.12625	0.90174	0.98325	H449	0.24881	0.80971	0.46678
C192	-0.16031	0.90515	0.98209	H450	0.24478	0.74133	0.43366
C193	-0.15802	0.94007	0.93909	H451	0.2357	0.65616	0.68224
C194	-0.12216	0.97065	0.89349	H452	0.16811	0.65198	0.65307
C195	-0.22103	0.91798	0.46436	H453	0.22535	0.77023	0.94076
N196	-0.25795	0.88622	0.47077	H454	0.29272	0.77408	0.97247
C197	-0.29349	0.88878	0.45167	H455	0.12608	0.67989	0.70396
C198	-0.28938	0.92652	0.4297	H456	0.34131	0.91373	0.67353
C199	-0.32341	0.93016	0.42358	H457	0.0761	0.67302	0.68864
C200	0.63808	0.89564	0.4399	H458	0.01464	0.74146	0.71834
C201	0.63324	0.85755	0.46121	H459	0.14534	0.80472	0.89537
C202	-0.3323	0.85447	0.46796	H460	0.34897	0.96486	0.60909
N203	0.59449	0.82309	0.48717	H461	0.28165	1.02762	0.61093
C204	0.56225	0.82519	0.48841	H462	0.21294	0.88989	0.56821

C205	-0.31837	0.97045	0.40716	H463	0.02047	0.7907	0.77993
O206	0.65211	0.97533	0.41984	H464	0.23161	1.0203	0.64481
O207	-0.28426	1.00088	0.38212	H465	0.12575	0.91568	0.51468
P208	0.32116	0.71477	0.6773	H466	0.05669	0.90747	0.52354
N209	0.30451	0.66378	0.63164	H467	0.12156	1.0393	0.72512
P210	0.32096	0.64495	0.74905	H468	0.19048	1.04786	0.7128
N211	0.3609	0.68675	0.85725	H469	0.12176	0.89316	0.96575
P212	0.39665	0.7241	0.77787	H470	0.12915	0.96352	1.0121
N213	0.37319	0.74256	0.68575	H471	-0.00053	0.90328	0.82451
O214	0.29909	0.72801	0.54735	H472	-0.00803	0.83316	0.7801
O215	0.3069	0.72093	0.83665	H473	-0.03174	0.60482	0.56462
C216	0.26843	0.7162	0.82565	H474	0.41572	1.06917	0.70896
C217	0.30237	0.76641	0.5746	H475	0.09884	1.10209	0.90674
C218	0.33585	0.80193	0.6613	H476	0.15976	1.17703	0.9836
C219	0.33843	0.84015	0.6778	H477	0.07969	1.22308	0.89644
C220	0.30757	0.84313	0.60878	H478	0.01812	1.14782	0.82192
C221	0.27421	0.80767	0.52281	H479	0.00595	1.08105	0.50625
C222	0.27188	0.76975	0.5053	H480	0.0145	1.1508	0.48601
C223	0.23358	0.68207	0.73935	H481	0.14985	1.21505	0.57079
C224	0.19632	0.67974	0.72317	H482	0.1414	1.14529	0.59085
C225	0.19343	0.71132	0.79264	H483	-0.1988	0.84105	1.03665
C226	0.22779	0.74479	0.88186	H484	-0.24725	0.79067	1.01141
C227	0.26503	0.74701	0.89874	H485	0.61869	0.72682	1.00369
C228	0.15455	0.70903	0.76841	H486	-0.30419	0.86393	1.02047
N229	0.15156	0.73965	0.8189	H487	0.57636	0.73187	0.99232
C230	0.11434	0.73891	0.79464	H488	0.54372	0.74802	0.54259
C231	0.31088	0.88349	0.6242	H489	0.47728	0.6931	0.6196
N232	0.27946	0.88527	0.58223	H490	0.42986	0.77419	0.58918
C233	0.28089	0.92365	0.58984	H491	0.49533	0.82814	0.50809
C234	0.07731	0.70297	0.72433	H492	0.57801	0.83488	1.01187
C235	0.04162	0.70348	0.69735	H493	0.51234	0.83444	0.97103
C236	0.04333	0.74045	0.74058	H494	0.43798	0.69593	0.90788
C237	0.08019	0.77653	0.81145	H495	0.5032	0.6964	0.94681
C238	0.11545	0.77543	0.83788	H496	-0.26315	0.7377	1.08973
C239	0.31852	0.96293	0.60316	H497	0.26302	0.59046	0.52551
C240	0.31903	1.00003	0.6093	H498	0.20188	0.5147	0.4687
C241	0.28157	0.99762	0.60401	H499	0.28141	0.47227	0.60869
C242	0.24374	0.95845	0.59022	H500	0.34286	0.54818	0.66516
C243	0.24374	0.9217	0.5818	H501	0.3439	0.61227	0.94651
N244	0.08314	0.81513	0.85238	H502	0.33758	0.54659	1.00621
C245	0.05216	0.81909	0.83	H503	0.20235	0.47588	0.89339
C246	0.05665	0.85953	0.86757	H504	0.20848	0.54187	0.83447
N247	0.20507	0.95508	0.58767	H505	0.29857	0.47237	1.01114

C248	0.20231	0.98722	0.61705	H506	0.16861	0.44284	0.50955
C249	0.16193	0.98207	0.61552	H507	0.30404	0.43163	1.00865
C250	0.12486	0.94344	0.56255	H508	0.23777	0.29554	1.00507
C251	0.08672	0.93878	0.56817	H509	0.16755	0.35347	0.93831
C252	0.08515	0.9724	0.62838	H510	0.13174	0.40933	0.6336
C253	0.12236	1.01136	0.67863	H511	0.06056	0.2726	0.62022
C254	0.16049	1.0161	0.67198	H512	0.18784	0.33827	0.52926
C255	0.09439	0.89553	0.93288	H513	0.19099	1.24967	1.00467
C256	0.09856	0.93439	0.95787	H514	0.05578	1.22571	0.52841
C257	0.06533	0.93779	0.91666	H515	0.34793	0.42652	1.11543
C258	0.02722	0.9013	0.85495	H516	0.03412	0.37358	0.73455

**Table S3.** Simulated structure of CTP-DABA-COF based on ABC-stacking

space group <i>P1</i>							
$a = b = 30.3180 \text{ \AA}, c = 11.5320 \text{ \AA}$							
$\alpha = \beta = 90^\circ$ and $\gamma = 120^\circ$							
$R_{wp} = 0.76 \%$ and $R_p = 0.49\%$							
Atom	x/a	y/b	z/c	Atom	x/a	y/b	z/c
P1	-0.07088	0.66434	-0.35216	O388	-0.65403	1.09972	-0.1056
N2	-0.03605	0.62939	-0.29332	O389	-0.86441	1.11041	-0.13387
P3	-0.00749	0.6585	-0.26287	C390	-0.85791	1.11157	-0.18082
N4	0.03873	0.71547	-0.29457	C391	-0.63341	1.15249	-0.12862
P5	-0.0395	0.74879	-0.34333	C392	-0.71865	1.18686	-0.12863
N6	-0.08324	0.7246	-0.37647	C393	-0.70115	1.24003	-0.15608
O7	0.0213	0.65256	-0.38606	C394	-0.60166	1.26217	-0.18759
O8	-0.1946	0.64486	-0.36258	C395	-0.51203	1.2273	-0.18283
C9	-0.21052	0.59644	-0.35649	C396	-0.52647	1.17388	-0.15407
C10	-0.00164	0.65972	-0.43467	C397	-0.76823	1.08567	-0.19143
C11	-0.07878	0.69851	-0.4692	C398	-0.77293	1.08132	-0.23543
C12	-0.11543	0.69991	-0.51432	C399	-0.86388	1.10374	-0.27224
C13	-0.07724	0.66293	-0.52717	C400	-0.94517	1.13485	-0.26433
C14	0.00978	0.62783	-0.495	C401	-0.94374	1.1378	-0.21917
C15	0.04714	0.62609	-0.44981	C402	-0.8722	1.09307	-0.31463
C16	-0.24758	0.59172	-0.39885	N403	-0.82074	1.05096	-0.30725
C17	-0.2448	0.54389	-0.39601	C404	-0.81918	1.02553	-0.336
C18	-0.20818	0.49889	-0.35072	C405	-0.59123	1.31746	-0.22395
C19	-0.18511	0.50348	-0.30687	N406	-0.68805	1.34452	-0.2403
C20	-0.18525	0.55125	-0.30952	C407	-0.72034	1.36801	-0.29311

C21	-0.1206	0.65972	-0.57125	C408	-0.79295	0.97259	-0.31063
N22	-0.21632	0.6839	-0.5961	C409	-0.789	0.94524	-0.33738
C23	-0.25806	0.67574	-0.63622	C410	-0.81128	0.9719	-0.39073
C24	-0.31283	0.71496	-0.6812	C411	-0.83857	1.02477	-0.41724
C25	-0.33991	0.70739	-0.72281	C412	-0.84201	1.05083	-0.38904
C26	-0.31058	0.66006	0.2811	C413	-0.78887	1.41339	-0.31782
C27	-0.26943	0.61832	0.32723	C414	-0.82695	1.43378	-0.36915
C28	-0.24448	0.62703	-0.63189	C415	-0.79399	1.40846	-0.3959
N29	-0.25731	0.56941	0.33147	C416	-0.7275	1.36302	-0.37254
C30	-0.19884	0.53074	0.36755	C417	-0.69231	1.34321	-0.32123
C31	-0.4011	0.74658	-0.77095	N418	-0.86441	1.0524	-0.47056
O32	-0.39695	0.75032	0.18638	C419	-0.97033	1.07128	-0.47906
O33	-0.47303	0.77819	-0.76283	C420	-0.98168	1.1271	-0.50651
P34	-0.35532	0.30577	0.29173	N421	-0.6995	1.33939	-0.40165
N35	-0.33281	0.24649	0.31268	C422	-0.71643	1.29193	-0.39053
P36	-0.26635	0.21739	0.36589	C423	-0.71601	1.28339	-0.43433
N37	-0.26014	0.24243	0.40128	C424	-0.77929	1.24251	-0.43383
P38	-0.32097	0.29578	0.38445	C425	-0.79296	1.23928	-0.47851
N39	-0.38133	0.32647	0.33	C426	-0.74134	1.27656	-0.52529
O40	-0.23658	0.33388	0.26267	C427	-0.66556	1.31312	-0.52436
O41	-0.4488	0.32925	0.24562	C428	-0.65458	1.31696	-0.48019
C42	-0.45511	0.33177	0.19835	C429	-1.04915	1.15006	-0.48376
C43	-0.22443	0.38559	0.24667	C430	-1.05554	1.20326	-0.50519
C44	-0.14863	0.40108	0.27353	C431	-0.99579	1.23637	-0.55116
C45	-0.13057	0.45321	0.25662	C432	-0.93497	1.21401	-0.57637
C46	-0.1899	0.49185	0.21307	C433	-0.92769	1.16055	-0.55417
C47	-0.27286	0.47541	0.18924	O434	-0.77276	1.28179	-0.57239
C48	-0.28817	0.42362	0.20456	O435	-0.99072	1.28865	-0.56755
C49	-0.39637	0.29686	0.18738	C436	-0.76528	0.88871	-0.3106
C50	-0.40567	0.302	0.13845	O437	-0.78845	0.85889	-0.32572
C51	-0.47024	0.34274	0.09837	O438	-0.71117	0.8703	-0.26374
C52	-0.52551	0.37783	0.11012	C439	-0.90432	1.47998	-0.39635
C53	-0.52056	0.37214	0.159	O440	-0.94038	1.50027	-0.44091
C54	-0.48647	0.35286	0.0459	O441	-0.93812	1.49937	-0.36591
N55	-0.43193	0.32656	0.02807	C442	-0.63355	1.46618	-0.68379
C56	-0.43944	0.3441	-0.02561	C443	-0.90207	1.518	-0.64357
C57	-0.17012	0.5467	0.19156	C444	-0.8922	1.54211	-0.61356
N58	-0.0621	0.56355	0.18202	C445	-0.91997	1.59415	-0.63451
C59	-0.04889	0.6074	0.13266	C446	-0.96183	1.62423	-0.68566
C60	-0.42755	0.31041	-0.04543	C447	-0.97154	1.59907	-0.7149
C61	-0.43008	0.329	-0.09886	C448	-0.94203	1.54729	-0.6948
C62	-0.44626	0.38197	-0.13283	C449	-0.56673	1.45054	-0.71332
C63	-0.45861	0.4168	-0.1147	C450	-0.55814	1.48216	-0.76687

C64	-0.45352	0.39691	-0.06122	C451	-0.61669	1.53032	-0.7931
C65	-0.09728	0.65543	0.12064	C452	-0.6686	1.54795	-0.76183
C66	-0.09896	0.6965	0.06968	C453	-0.67162	1.51785	-0.7084
C67	-0.04811	0.6894	0.03093	C454	-1.1282	1.36131	-0.90014
C68	-0.001	0.6416	0.04112	N455	-1.12686	1.39595	-0.94927
C69	-0.00093	0.60146	0.09265	C456	-1.13711	1.38512	-0.99015
N70	-0.46222	0.47039	-0.14971	C457	-1.14933	1.42557	-1.04163
C71	-0.46481	0.50549	-0.13605	C458	-1.15437	1.41581	-1.08291
C72	-0.38732	0.54939	-0.16375	C459	-1.1481	1.36441	-0.07187
N73	0.03645	0.63159	0.00164	C460	-1.1356	1.3231	-0.02129
C74	0.03424	0.66565	-0.04749	C461	-1.12935	1.33434	-0.98116
C75	0.05301	0.651	-0.08667	N462	-1.1239	1.27234	-0.01238
C76	0.06778	0.60057	-0.07893	C463	-1.14235	1.22842	0.02983
C77	0.07949	0.59172	-0.12044	C464	-1.09921	1.18153	0.03181
C78	0.0762	0.63305	-0.17175	C465	-0.67983	1.07739	0.16283
C79	0.06848	0.68345	-0.17951	C466	-0.6598	1.02598	0.17512
C80	0.05673	0.69186	-0.13814	C467	-0.68373	1.0091	0.14053
C81	-0.32982	0.57111	-0.13719	C468	-0.73317	1.04273	0.09199
C82	-0.24576	0.60983	-0.16135	C469	-0.76723	1.0922	0.08171
C83	-0.21776	0.62869	-0.21364	C470	-0.74233	1.10877	0.11679
C84	-0.28284	0.611	-0.24171	C471	-1.02676	1.1841	-0.00778
C85	-0.36455	0.57157	-0.21703	C472	-0.98512	1.14023	-0.00725
O86	0.07398	0.62388	-0.21291	C473	-1.01184	1.09072	0.03402
O87	-0.12652	0.66304	-0.23608	C474	-1.08702	1.08703	0.07325
C88	-0.40818	0.29491	-0.1211	C475	-1.12857	1.13148	0.07218
O89	-0.36414	0.30677	-0.16274	O476	-0.74993	1.02557	0.05739
O90	-0.443	0.24514	-0.08944	O477	-0.96299	1.04665	0.03766
C91	-0.15766	0.74676	0.0543	O478	-0.8133	0.9186	-0.01824
O92	-0.14314	0.78781	0.0149	O479	-0.99251	0.97594	-0.05092
O93	-0.24062	0.74367	0.08892	C480	-1.0659	0.94891	-0.00879
C94	0.05552	0.83501	-0.42915	C481	-0.80981	0.87961	-0.03038
C95	-0.15747	0.78228	-0.28813	C482	-0.86852	0.88135	-0.07268
C96	-0.26347	0.78168	-0.26348	C483	-0.85594	0.84068	-0.08304
C97	-0.26878	0.80355	-0.23189	C484	-0.78528	0.79659	-0.05224
C98	-0.16943	0.82687	-0.22358	C485	-0.72948	0.79602	-0.00968
C99	-0.06236	0.82377	-0.2458	C486	-0.74089	0.83608	0.00068
C100	-0.05636	0.80284	-0.27796	C487	-1.10544	0.97199	0.01963
C101	0.07385	0.81625	-0.46337	C488	-1.14027	0.94166	0.07074
C102	0.10092	0.85031	-0.51497	C489	-1.14783	0.88742	0.09379
C103	0.10943	0.90422	-0.53492	C490	-1.13168	0.8664	0.06118
C104	0.09433	0.9219	-0.49943	C491	-1.08862	0.89606	0.0111
C105	0.06823	0.88824	-0.44774	C492	-1.16781	0.85335	0.14866
C106	-0.19626	0.45088	-0.3513	N493	-1.1346	0.86944	0.18

N107	-0.13539	0.41275	-0.31531	C494	-1.10159	0.8371	0.232
C108	-0.09236	0.37034	-0.31905	C495	-0.76665	0.75343	-0.06175
C109	-0.01882	0.33309	-0.28073	N496	-0.70845	0.71396	-0.02622
C110	0.02765	0.29223	-0.28558	C497	-0.67539	0.66258	-0.01054
C111	-0.00112	0.28801	0.67112	C498	-1.10815	0.85445	0.26777
C112	-0.07752	0.32333	0.63302	C499	-1.07338	0.82313	0.31932
C113	-0.12	0.36427	-0.3614	C500	-1.03145	0.7733	0.33462
N114	-0.11656	0.31564	0.59256	C501	-1.02457	1.75404	-0.69977
C115	-0.18405	0.3478	0.55482	C502	-1.05862	0.78724	0.24892
C116	-0.25343	0.32923	0.52672	C503	-0.67352	0.63885	-0.04113
C117	-0.20619	0.4805	0.37128	C504	-0.63806	0.58698	-0.01992
C118	-0.13291	0.44009	0.40645	C505	-0.60805	0.55889	0.03283
C119	-0.13546	0.39147	0.41111	C506	-0.61128	1.5808	-0.93523
C120	-0.21517	0.38063	0.38181	C507	-0.64226	0.63311	0.04134
C121	-0.29053	0.42013	0.34728	N508	-0.98656	1.70275	-0.68301
C122	-0.28429	0.46914	0.34158	C509	-0.9955	1.67843	-0.70906
C123	-0.33855	0.36195	0.49097	N510	-0.58622	1.55094	-0.88153
C124	-0.39966	0.34767	0.4598	C511	-0.62994	1.56336	-0.84878
C125	-0.37797	0.29952	0.46358	C512	-1.07996	0.84171	0.35733
C126	-0.30186	0.26462	0.50239	O513	-1.0506	0.81883	0.40273
C127	-0.24018	0.27949	0.53297	O514	-1.12459	0.89061	0.33639
O128	-0.22101	0.33137	0.38912	C515	-0.63034	0.55915	-0.0497
O129	-0.41932	0.28917	0.42636	O516	-0.60429	0.51391	-0.03271
C130	0.10823	0.25316	-0.24566	O517	-0.6541	0.58805	-0.10103
O131	0.19659	0.23454	0.74752	O518	-0.67838	1.43027	-0.63561
O132	0.06939	0.2373	-0.19667	O519	-0.86775	1.46719	-0.62279
O133	-0.13366	0.21015	0.35194	C520	-0.16491	0.45718	-0.13825
O134	-0.31481	0.15877	0.39889	O521	-0.13033	0.50472	-0.14765
C135	-0.3097	0.12447	0.45162	O522	-0.19568	0.45218	-0.17451
C136	-0.08573	0.19426	0.3196	H523	-0.11296	0.7279	-0.46057
C137	0.03687	0.18884	0.31843	H524	-0.17792	0.7304	-0.53986
C138	0.08659	0.1673	0.29106	H525	0.0473	0.59932	-0.50432
C139	0.01768	0.15046	0.26306	H526	0.11249	0.59679	-0.42507
C140	-0.10396	0.16148	0.25987	H527	-0.27263	0.62649	-0.43556
C141	-0.15514	0.18233	0.28784	H528	-0.26853	0.54232	-0.4311
C142	-0.27761	0.07255	0.47046	H529	-0.16144	0.46911	-0.26964
C143	-0.2582	0.03952	0.52307	H530	-0.16203	0.55276	-0.27434
C144	-0.26701	0.05651	0.5594	H531	-0.06926	0.63407	-0.58068
C145	-0.31055	0.10713	0.54035	H532	-0.32964	0.7526	-0.68386
C146	-0.33293	0.14009	0.48805	H533	-0.32485	0.65426	0.24787
C147	-0.23062	0.02275	0.61295	H534	-0.21015	0.59491	-0.59541
N148	-0.21627	0.04186	0.64355	H535	-0.14473	0.53333	0.39696
C149	-0.1769	0.0162	0.69564	H536	-0.51553	0.80147	-0.79408

C150	0.07582	0.12261	0.24081	H537	-0.10045	0.37126	0.30745
N151	0.01353	0.09293	0.22952	H538	-0.06806	0.464	0.27789
C152	0.05332	0.04165	0.24821	H539	-0.3238	0.50367	0.15542
C153	-0.16649	0.04355	0.72245	H540	-0.34699	0.41338	0.18176
C154	-0.12968	0.01932	0.77428	H541	-0.34413	0.26476	0.21753
C155	-0.09969	-0.03311	0.79937	H542	-0.35995	0.27352	0.13131
C156	-0.11234	0.93799	-0.22541	H543	-0.57503	0.41118	0.08011
C157	-0.14989	-0.03672	0.72286	H544	-0.56664	0.40016	0.16679
C158	0.06014	0.01898	0.21685	H545	-0.54522	0.38586	0.02186
C159	0.09685	-0.03251	0.23714	H546	-0.24659	0.57095	0.17049
C160	0.12581	-0.06125	0.28982	H547	-0.4109	0.26918	-0.01776
C161	0.11645	0.9593	-0.67718	H548	-0.445	0.39743	-0.17509
C162	0.08146	0.01107	0.30077	H549	-0.45641	0.42419	-0.04657
N163	-0.08996	0.88456	-0.19974	H550	-0.13677	0.65898	0.15249
C164	-0.17774	0.85452	-0.19516	H551	-0.05084	0.72226	-0.00908
N165	0.13433	0.92716	-0.62334	H552	0.03131	0.56303	0.10158
C166	0.13038	0.94194	-0.58904	H553	-0.49618	0.49847	-0.09808
C167	-0.12538	0.04681	0.80436	H554	0.01176	0.70676	-0.06267
O168	-0.07021	0.03567	0.8433	H555	0.06683	0.56681	-0.03935
O169	-0.19834	0.08894	0.78384	H556	0.08853	0.55188	-0.1134
C170	0.10408	-0.05887	0.20602	H557	0.07125	0.71784	-0.21841
O171	0.13841	-0.10248	0.22002	H558	0.0473	0.73244	-0.14729
O172	0.06475	-0.02947	0.15648	H559	-0.34679	0.5552	-0.09557
O173	0.02432	0.80327	-0.37831	H560	-0.1978	0.62473	-0.13926
O174	-0.15374	0.7628	-0.32133	H561	-0.2696	0.6278	-0.28354
P175	-0.42569	0.98021	-1.00576	H562	-0.40906	0.55692	-0.24008
N176	-0.39687	0.93975	-0.9476	H563	-0.48574	0.24064	-0.05961
P177	-0.43122	0.95537	-0.90627	H564	-0.25746	0.70854	0.11508
N178	-0.42533	1.01391	-0.92109	H565	-0.34361	0.76461	-0.27006
P179	-0.41833	1.05492	-0.98032	H566	-0.3551	0.80402	-0.21512
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O182	-0.54408	0.96162	-1.02107	H569	0.06799	0.77448	-0.44994
C183	-0.53139	0.9219	-1.03166	H570	0.11281	0.83378	-0.54055
C184	-0.35126	0.99429	-1.09537	H571	0.0998	0.96365	-0.51267
C185	-0.41221	1.04073	-1.12658	H572	0.05306	0.90327	-0.42112
C186	-0.44596	1.05469	-1.1766	H573	-0.22921	0.45219	-0.38673
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C188	-0.36128	0.97654	-1.16636	H575	0.03349	0.25535	0.66759
C189	-0.32225	0.96332	-1.11699	H576	-0.18012	0.39215	-0.39097
C190	-0.4625	0.87807	-0.99993	H577	-0.20246	0.38786	0.54564
C191	-0.43894	0.84171	-1.01445	H578	-0.07093	0.44636	0.43132
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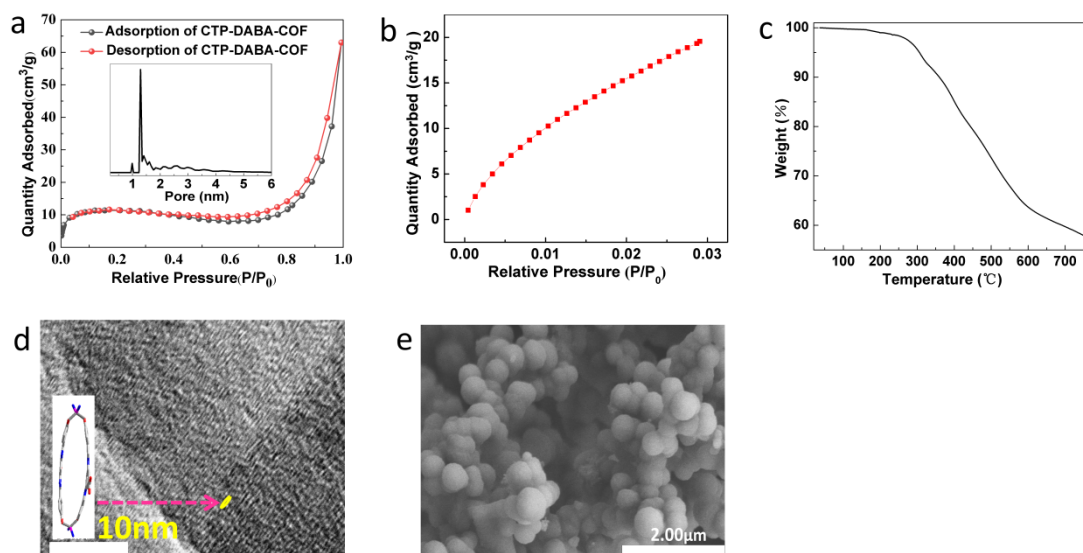
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C195	-0.46638	1.03945	-1.25002	H582	-0.35293	0.40134	0.48459
N196	-0.45716	1.00888	-1.26924	H583	-0.45697	0.37647	0.42886
C197	-0.491	1.01991	-1.31942	H584	-0.28778	0.22582	0.50729
C198	-0.5331	1.06855	-1.35763	H585	-0.17692	0.25181	0.56148
C199	-0.56455	1.07855	-1.40722	H586	-0.00802	0.25055	-0.19703
C200	-0.5545	1.03869	-0.41849	H587	0.09556	0.20035	0.34036
C201	-0.51477	0.98966	-0.38149	H588	0.18271	0.16089	0.29444
C202	-0.48304	0.98085	-1.33232	H589	-0.16211	0.15122	0.23668
N203	-0.51311	0.95026	-0.39387	H590	-0.25119	0.18886	0.28469
C204	-0.42879	0.91733	-0.38368	H591	-0.26162	0.05771	0.44375
C205	-0.60833	1.1299	-1.44782	H592	-0.22792	-0.00021	0.53538
O206	-0.62999	1.14474	-0.49325	H593	-0.32397	0.12256	0.56678
O207	-0.62658	1.16206	-1.42871	H594	-0.3683	0.17892	0.47583
P208	-0.6667	0.70363	-0.46944	H595	-0.21126	-0.01792	0.62458
N209	-0.66665	0.64275	-0.44284	H596	0.1715	0.11695	0.24856
P210	-0.64381	0.61358	-0.38276	H597	-0.18802	0.08517	0.70095
N211	-0.60384	0.6444	-0.35581	H598	-0.07132	-0.05279	0.84022
P212	-0.64017	0.70262	-0.38201	H599	-0.15887	-0.05983	0.70358
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O214	-0.5336	0.7212	-0.48886	H601	0.15324	-0.10207	0.30677
O215	-0.73951	0.72982	-0.5225	H602	0.07067	0.02834	0.32565
C216	-0.72776	0.72418	-0.56535	H603	-0.26844	0.86057	-0.1856
C217	-0.47454	0.76513	-0.49706	H604	0.12779	0.98292	-0.59909
C218	-0.53361	0.81032	-0.50648	H605	-0.25254	0.08666	0.76027
C219	-0.4719	0.85058	-0.50662	H606	0.05068	0.00561	0.14791
C220	-0.34793	0.85015	-0.50078	H607	-0.43464	1.06695	-1.11188
C221	-0.29019	0.80572	-0.49502	H608	-0.49412	1.09159	-1.19891
C222	-0.35144	0.76414	-0.49258	H609	-0.34203	0.94924	-1.18018
C223	-0.68189	0.67896	-0.56235	H610	-0.27507	0.9264	-1.09304
C224	-0.67105	0.67497	-0.6066	H611	-0.4234	0.87116	-0.96325
C225	-0.70251	0.71591	-0.65585	H612	-0.38261	0.80877	-0.9883
C226	-0.74566	0.76139	-0.65821	H613	-0.59323	0.89558	-1.12795
C227	-0.75986	0.76537	-0.61409	H614	-0.63295	0.96111	-1.10299
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C230	-0.65764	0.67172	-0.75016	H617	-0.57819	1.04551	-0.45725
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C234	-0.56527	0.64784	-0.76168	H621	-0.63034	0.81387	-0.51129
C235	-0.54961	0.65523	-0.81162	H622	-0.52689	0.88213	-0.50894

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C238	-0.74266	0.69816	-0.78832	H625	-0.65577	0.64547	-0.52504
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C240	-0.58988	1.01079	-0.58318	H627	-0.77112	0.79507	-0.69576
C241	-0.599	0.99699	-0.62167	H628	-0.79522	0.8014	-0.61731
C242	-0.51429	0.96567	-0.627	H629	-0.71552	0.75018	-0.73926
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N247	-0.51953	0.95272	-0.66637	H634	-0.48644	0.9997	-0.51664
C248	-0.47333	0.91108	-0.66309	H635	-0.67385	1.01103	-0.64891
C249	-0.43673	0.91235	-0.71044	H636	-0.34807	0.92669	-0.59832
C250	-0.40558	0.86777	-0.71261	H637	-0.93481	0.79702	-0.90657
C251	-0.3759	0.87068	-0.75929	H638	-0.44799	0.87661	-0.62607
C252	-0.37963	0.91786	-0.80632	H639	-0.40639	0.82945	-0.67708
C253	-0.4019	0.96289	-0.80417	H640	-0.34928	0.83541	-0.75954
C254	-0.4279	0.95946	-0.75728	H641	-0.39969	1.00182	-0.83862
C255	-0.82182	0.85716	-0.87829	H642	-0.44567	0.99602	-0.75835
C256	-0.75323	0.89602	-0.87906	H643	-0.91826	0.86211	-0.87897
C257	-0.63013	0.89534	-0.88278	H644	-0.79786	0.92923	-0.87986
C258	-0.5776	0.85143	-0.87987	H645	-0.48076	0.84868	-0.88176
C259	-0.64724	0.81222	-0.87809	H646	-0.59918	0.78136	-0.8804
O260	-0.36428	0.91889	-0.85265	H647	-0.45072	0.57733	-0.75527
O261	-0.56539	0.93779	-0.8908	H648	-0.72431	1.07527	-0.53856
C262	-0.44357	0.63523	-0.82565	H649	-0.4097	1.11901	-0.91906
O263	-0.39531	0.65232	-0.86752	H650	-0.47967	1.18603	-0.89993
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C265	-0.68045	1.04524	-0.57994	H652	-0.66465	1.17062	-1.04283
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O267	-0.66317	1.05289	-0.53905	H654	-0.17499	1.11356	-1.14989
C268	-0.24926	1.11237	-1.03904	H655	-0.21348	1.24161	-1.12048
C269	-0.53237	1.14086	-0.98277	H656	-0.26598	1.18025	-1.03054
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C275	-0.21727	1.09469	-1.07297	H662	-0.64349	0.88569	-0.40372
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C277	-0.19737	1.18348	-1.14411	H664	-0.31349	0.76444	-0.37585
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N281	-0.39407	0.76839	-1.04437	H668	-0.55604	0.64269	-0.27679
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C286	-0.40732	0.67634	-0.09399	H673	-0.4231	0.40607	-0.31049
C287	-0.4115	0.72196	-1.09181	H674	-0.45994	0.47935	-0.29889
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C289	-0.5441	0.7051	-0.16234	H676	-0.66892	0.51678	-0.18348
C290	-0.58915	0.70488	-0.20753	H677	-1.00927	0.48077	-0.22391
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C295	-0.38572	0.79136	-0.38102	H682	-0.76511	0.32052	0.09006
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C301	-0.54945	0.6702	-0.22318	H688	-0.19461	1.26223	-1.20922
O302	-0.52056	0.7324	-0.3858	H689	-0.85811	0.46634	0.09429
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O307	-0.55376	0.56705	-0.36581	H694	-0.61313	1.29896	-0.63022
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C319	-0.9224	0.4997	-0.23413	H706	-0.77288	1.26491	-0.15595
C320	-0.8962	0.53092	-0.2862	H707	-0.42884	1.24221	-0.20408
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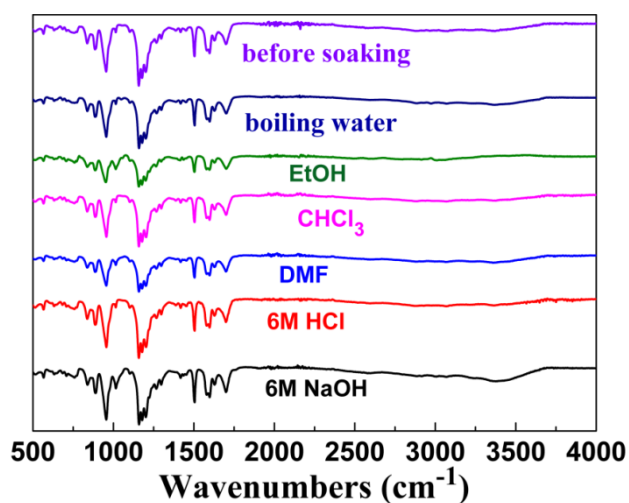
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C324	-0.4647	0.39786	-0.39693	H711	-1.01754	1.15441	-0.29203
N325	-0.41883	0.35826	-0.35704	H712	-1.01381	1.15884	-0.21181
C326	-0.38381	0.30788	-0.3424	H713	-0.92827	1.11777	-0.34843
C327	-0.82043	0.43975	-0.01434	H714	-0.5091	1.32859	-0.24694
C328	-0.80553	0.40164	0.03757	H715	-0.77844	0.95335	-0.26848
C329	-0.77956	0.35091	0.04945	H716	-0.80738	0.95132	-0.4128
C330	-0.76828	1.33816	-0.98966	H717	-0.86239	1.09252	-0.40932
C331	-0.78543	0.37707	-0.0409	H718	-0.81347	1.43245	-0.29559
C332	-0.41078	0.28214	-0.36963	H719	-0.82251	1.42388	-0.43638
C333	-0.37144	0.23143	-0.35163	H720	-0.64192	1.30674	-0.30245
C334	-0.30299	0.20759	-0.30658	H721	-1.04317	1.05103	-0.45189
C335	-0.27637	1.23192	-1.27809	H722	-0.74832	1.26093	-0.35252
C336	-0.31925	0.282	-0.29662	H723	-0.82648	1.21421	-0.3985
N337	-0.73533	1.2892	-0.98118	H724	-0.84699	1.20783	-0.47697
C338	-0.65973	1.25624	-0.94877	H725	-0.62383	1.34215	-0.5608
N339	-0.21525	1.20483	-1.23093	H726	-0.60224	1.3496	-0.4833
C340	-0.19124	1.22114	-1.19888	H727	-1.09256	1.12581	-0.44608
C341	-0.81331	0.41388	0.07991	H728	-1.10045	1.21946	-0.48386
O342	-0.79389	0.38508	0.12584	H729	-0.88868	1.23811	-0.61336
O343	-0.84529	0.46376	0.06361	H730	-0.87507	1.14455	-0.57401
C344	-0.3984	0.20152	-0.37794	H731	-0.69106	0.89792	-0.25745
O345	-0.35634	0.16033	-0.36898	H732	-0.99635	1.52626	-0.38381
O346	-0.48112	0.22402	-0.41571	H733	-0.86037	1.51982	-0.5732
O347	-0.28817	1.07887	-0.98973	H734	-0.9087	1.61162	-0.60974
O348	-0.50122	1.1032	-0.99401	H735	-1.00405	1.62035	-0.75514
P349	-0.85074	1.38944	-0.70108	H736	-0.95134	1.52925	-0.71916
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P353	-0.82106	1.42345	-0.63476	H740	-0.71371	1.53374	-0.6861
N354	-0.8527	1.43671	-0.69141	H741	-1.15141	1.32028	-0.88502
O355	-0.71709	1.37965	-0.71067	H742	-1.15563	1.46528	-1.04815
O356	-0.91409	1.40509	-0.75486	H743	-1.15139	1.35584	-0.10385
C357	-0.96682	1.39391	-0.78962	H744	-1.11564	1.30195	-0.9416
C358	-0.688	1.33356	-0.70767	H745	-1.18334	1.22506	0.065
C359	-0.71548	1.3255	-0.74878	H746	-0.6221	0.99762	0.21275
C360	-0.68818	1.279	-0.74596	H747	-0.66436	0.96846	0.15256
C361	-0.63022	1.23903	-0.70266	H748	-0.8054	1.12005	0.04402
C362	-0.6091	1.24641	-0.66024	H749	-0.76586	1.14885	0.10586
C363	-0.63594	1.29315	-0.66289	H750	-1.00126	1.22171	-0.04122
C364	-0.98603	1.34278	-0.7781	H751	-0.9317	1.14603	-0.0405

C365	-1.04059	1.33328	-0.81422	H752	-1.11389	1.04858	0.10503
C366	-1.07784	1.37372	-0.86291	H753	-1.18652	1.12672	0.104
C367	-1.06275	1.42473	-0.87261	H754	-0.92358	0.91526	-0.09794
C368	-1.00721	1.43476	-0.83709	H755	-0.90349	0.84383	-0.11678
C369	-0.59465	1.1949	-0.70712	H756	-0.67078	0.76411	0.01646
N370	-0.52737	1.1584	-0.67283	H757	-0.68949	0.83515	0.03234
C371	-0.47814	1.12285	-0.68579	H758	-1.09615	1.01403	0.00328
C372	-0.36945	1.09827	-0.66567	H759	-1.15578	0.96079	0.09368
C373	-0.3179	1.06551	-0.68114	H760	-1.14101	0.82446	0.07693
C374	-0.37677	1.05835	0.28167	H761	-1.06508	0.87725	-0.01147
C375	-0.48716	1.08081	0.26191	H762	-1.19025	0.81265	0.16143
C376	-0.53671	1.11166	-0.7203	H763	-0.80712	0.7545	-0.09594
N377	-0.54888	1.07151	0.22655	H764	-1.1411	0.89402	0.254
C378	-0.63669	1.09639	0.19604	H765	-1.00309	0.748	0.37505
C379	-0.20606	1.0364	-0.65835	H766	-1.05082	0.77435	0.22038
O380	-0.17285	0.997	0.34302	H767	-0.70112	0.66236	-0.0818
O381	-0.13556	1.05806	-0.63728	H768	-0.58235	0.51777	0.05048
P382	-0.78168	1.07375	-0.08529	H769	-0.64379	0.6525	0.06447
N383	-0.78786	1.01825	-0.07964	H770	-1.032	1.69618	-0.74861
P384	-0.85827	0.97515	-0.03217	H771	-0.6867	1.59757	-0.86072
N385	-0.86325	0.97898	0.01863	H772	-1.1247	0.9014	0.3621
P386	-0.84744	1.03269	0.01553	H773	-0.67268	0.62358	-0.1126
N387	-0.81521	1.0812	-0.03809	H774	-0.10345	0.5045	-0.11713



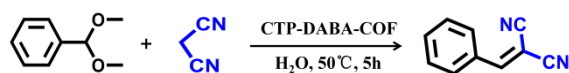
**Fig. S4** (a) N<sub>2</sub> adsorption-desorption isotherms at 77 K, the pore width distributions (inset), (b) CO<sub>2</sub> adsorption isotherms at 298 K, (c) TGA trace, (d) The lattice exhibits a wavy alignment as observed by transmission electron microscopy (TEM) and (e)

SEM image of CTP-DABA-COF.



**Fig. S5** CTP-DABA-COF was treated in different solvents for 3 days.

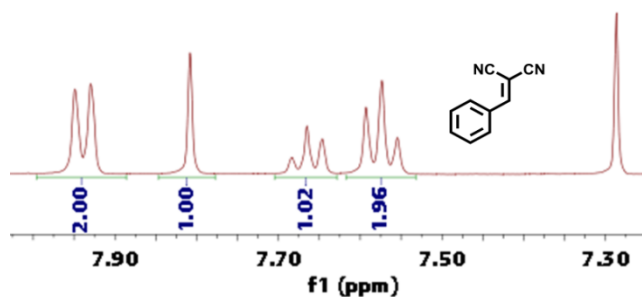
**Table S4.** Optimization of the one-pot tandem deacetalization-Knoevenagel condensation conditions. <sup>a</sup>



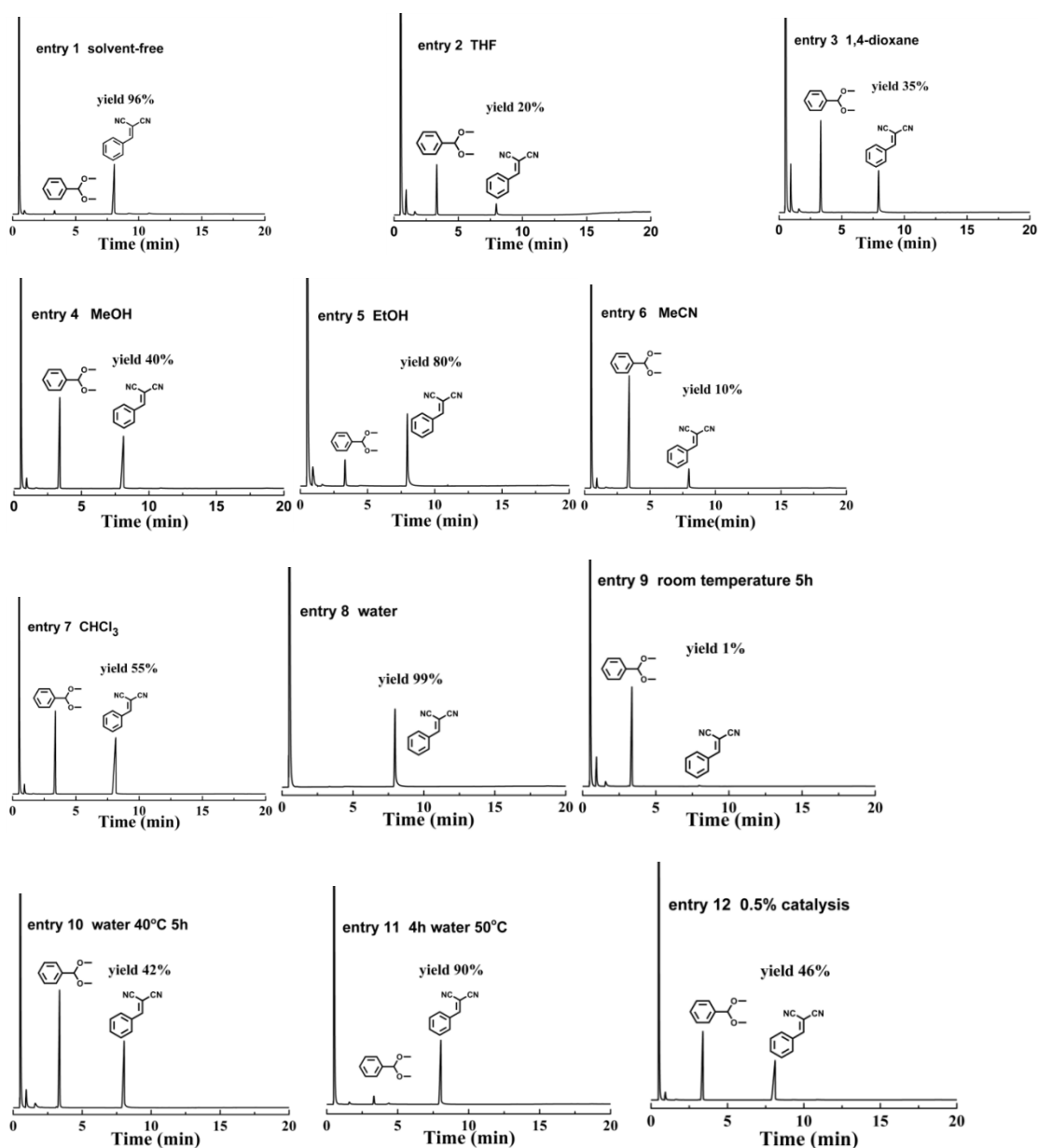
Entry	Catalyst	Solvent	Time	Temperature	Yield <sup>b</sup>
1	1.0 mol%	solvent-free	5h	50°C	96%
2	1.0 mol%	THF	5h	50°C	20%
3	1.0 mol%	1,4-dioxane	5h	50°C	35%
4	1.0 mol%	MeOH	5h	50°C	40%
5	1.0 mol%	EtOH	5h	50°C	80%
6	1.0 mol%	MeCN	5h	50°C	10%
7	1.0 mol%	CHCl <sub>3</sub>	5h	50°C	55%
8	1.0 mol%	H <sub>2</sub> O	5h	50°C	99%
9	1.0 mol%	H <sub>2</sub> O	5h	rt	1%
10	1.0 mol%	H <sub>2</sub> O	5h	40°C	42%
11	1.0 mol%	H <sub>2</sub> O	4h	50°C	90%
12	0.5 mol%	H <sub>2</sub> O	5h	50°C	46%
13	No Catalysis	H <sub>2</sub> O	5h	50°C	1%

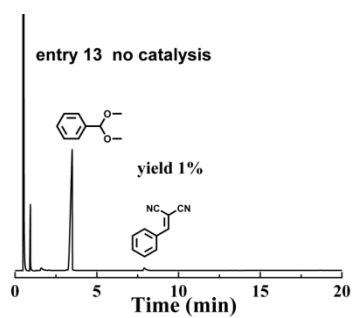
<sup>a</sup> Reaction conditions: benzaldehyde dimethylacetal (150 $\mu$ L, 1.0 mmol) and malononitrile (66 mg, 1.0 mmol) in the presence of CTP-DABA-COF (11.9 mg, 1 mol %), the mixture was stirred for 5h at different solvent (2 mL).

<sup>b</sup> Yield was determined by GC analysis.

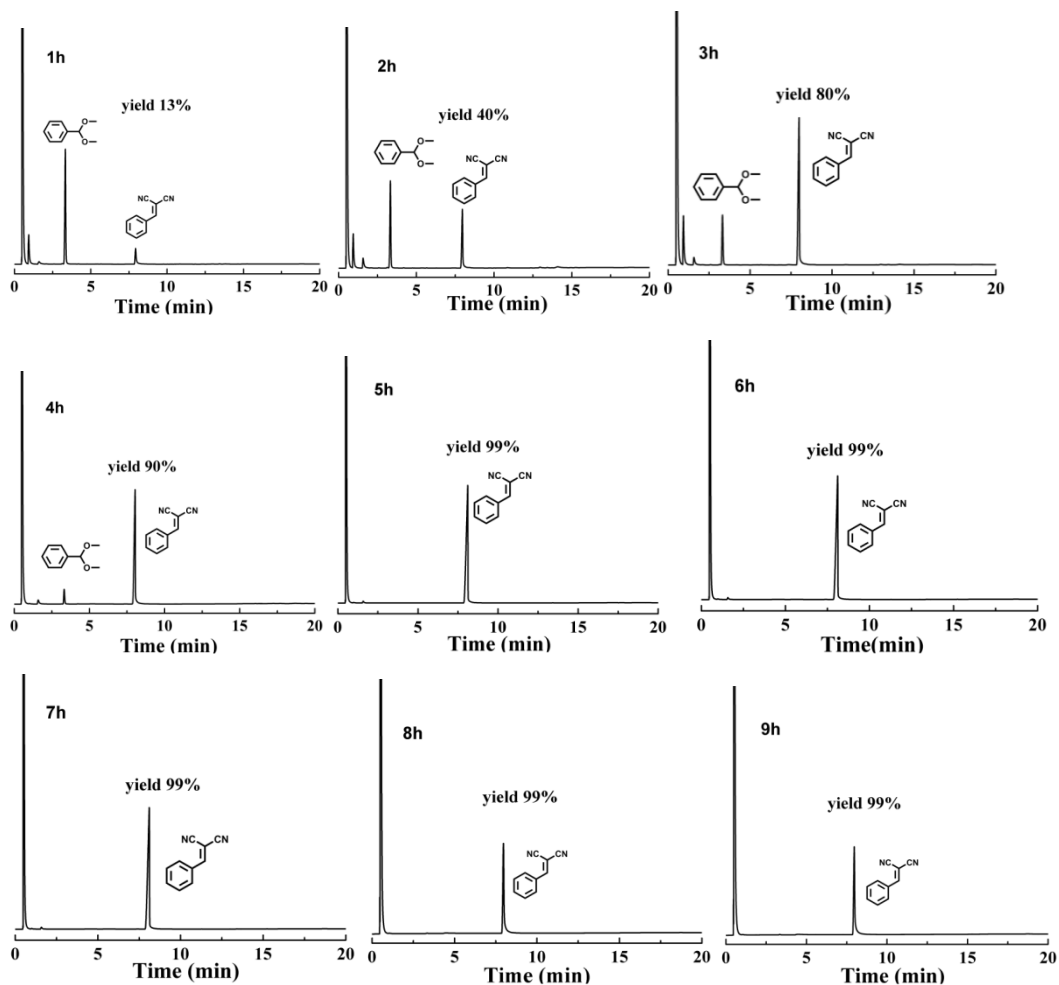


**Fig. S6** <sup>1</sup>H NMR spectra of catalytic product benzylidenemalononitrile in CDCl<sub>3</sub>.

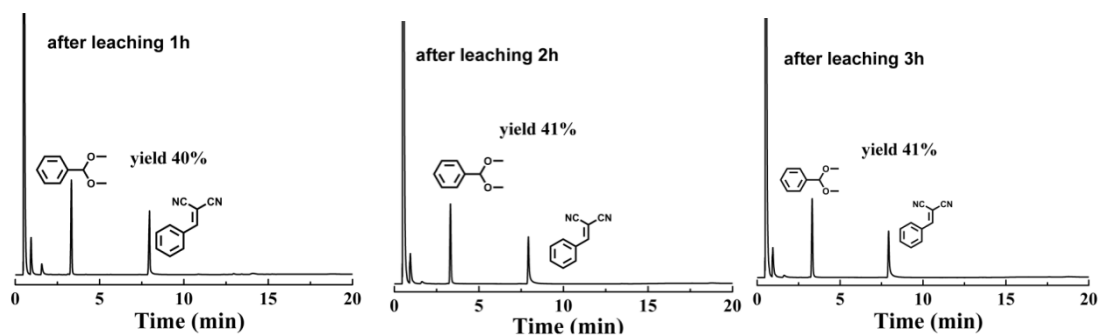




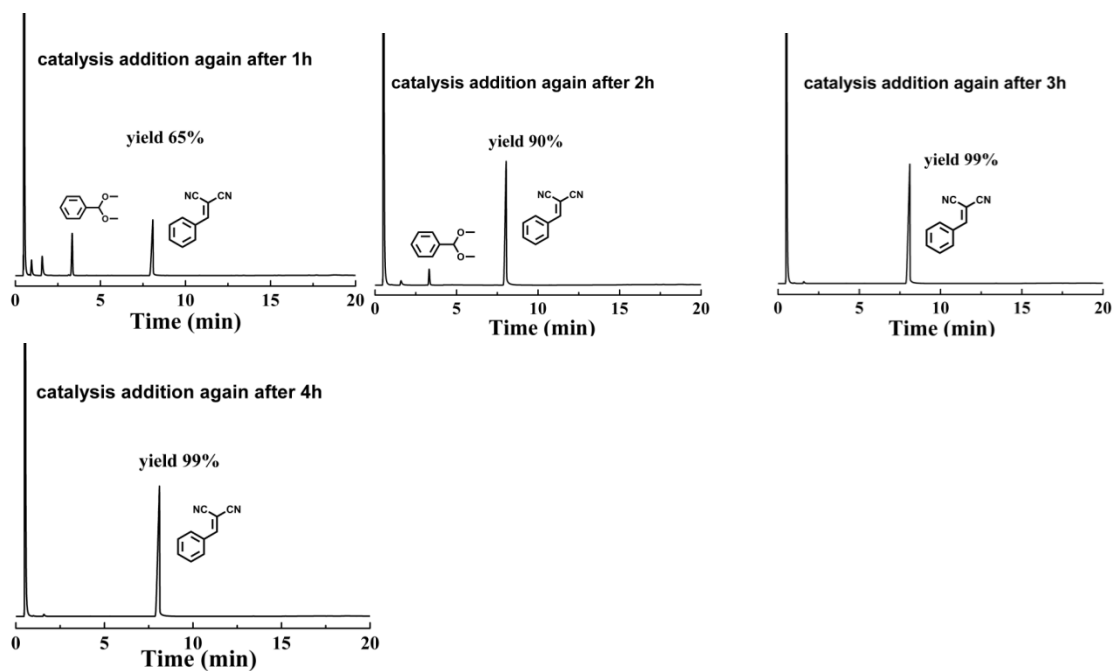
**Fig. S7** The GC of the deacetalization-Knoevenagel condensation.



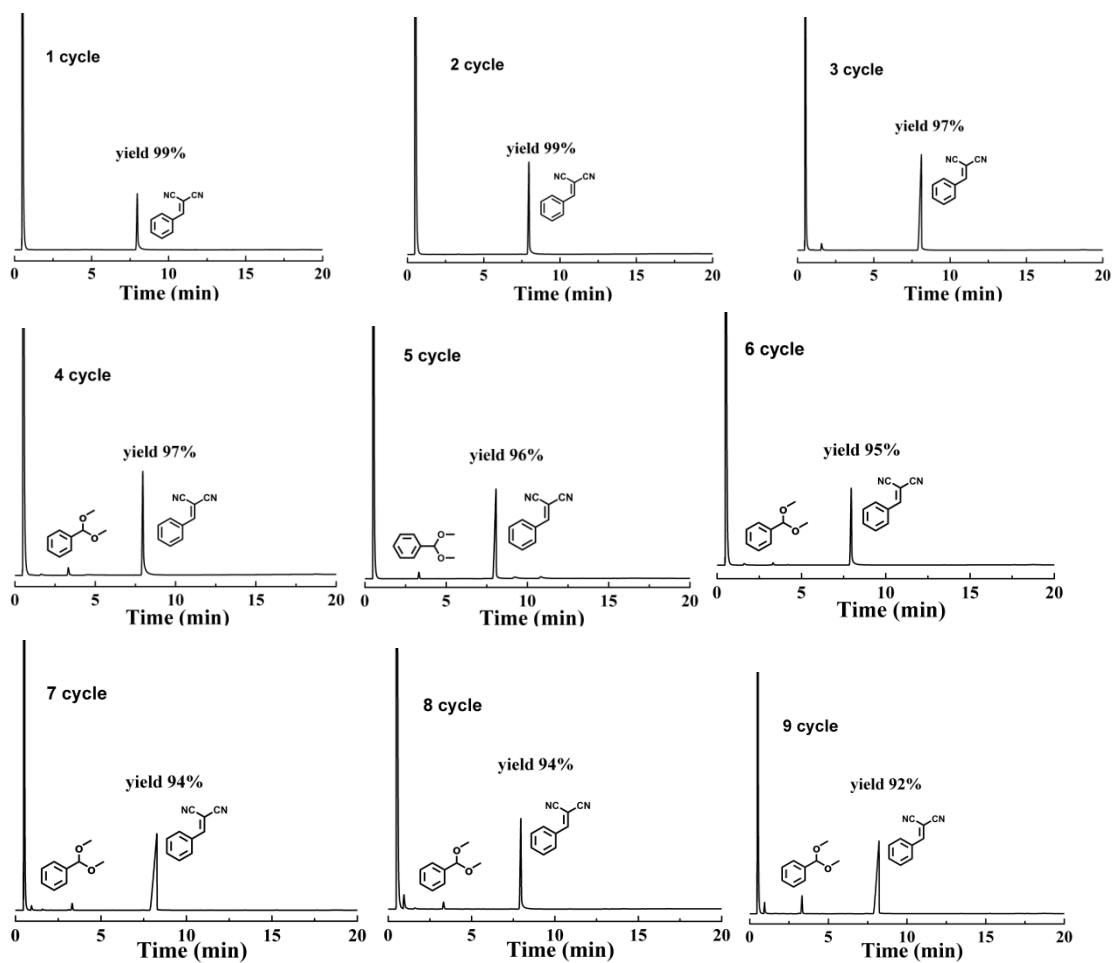
**Fig. S8** The GC of relationship between catalytic yield and time.

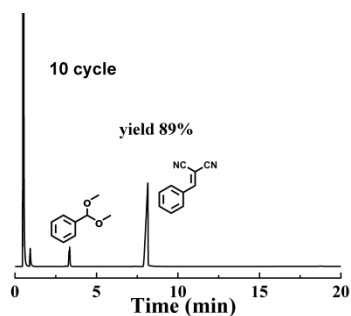


**Fig. S9** The GC of CTP-DABA-COF leaching test.

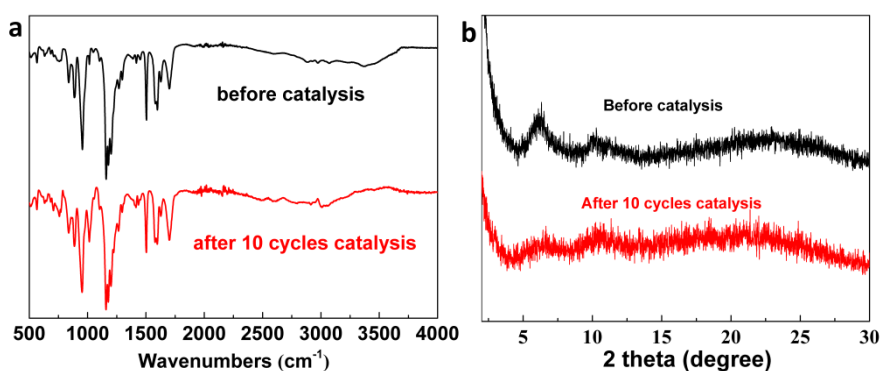


**Fig. S10** The GC of CTP-DABA-COF addition again.





**Fig. S11** The GC of CTP-DABA-COF recycling catalytic test.



**Fig. S12** The FT-IR and PXRD of CTP-DABA-COF after using ten runs.

**Table S5.** Comparison of CTP-DABA-COF with the reported catalysts for one-pot cascade deacetalization–Knoevenagel condensation.

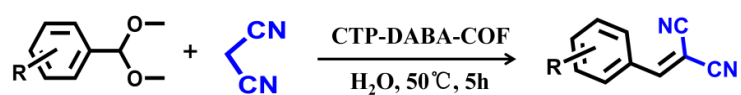
Catalyst	Conditions	Recycle	Yield	Ref.
MCM-41-P1	MeCN, toluene / 80 °C / 5h	3	90	1
HisAA-220	MeCN / 80 °C / 4h	5	77	2
MIL-101(Cr)@CS	MeCN / 80 °C / 12 h	5	99	3
Pd@N-ZDC@PTA-mSiO <sub>2</sub>	DMF / 80 °C / 24 h	5	>99	4
[Zn <sub>2</sub> (L) <sub>2</sub> (H <sub>2</sub> O) <sub>4</sub> ]·2(H <sub>2</sub> O)·6(DMF)	DMF / 80 °C / 3h	5	93.5	5
PCN-905-SO <sub>2</sub>	Toluene / 90 °C / 1 h.	1	95.5	6
Zr <sub>12</sub> BDC-NH <sub>2</sub>	CDCl <sub>3</sub> / 55 °C / 24 h.	3	91.8	7
PCN-222-Co@TpPa-1	DMSO-d <sub>6</sub> / 50 °C / 10 h.	5	99.3	8

Yb-BDC-NH <sub>2</sub>	DMSO-d <sub>6</sub> / 50 °C / 24 h	4	97	<b>9</b>
[Zn <sub>24</sub> (BDPO) <sub>12</sub> (DMF) <sub>12</sub> ]·6DMF·52H <sub>2</sub> O	Toluene / 90 °C / 3 h	5	99	<b>10</b>
BNP-2.1	Toluene / 80 °C / 24 h	4	98.5	<b>11</b>
3D DL-COF-1	CDCl <sub>3</sub> / r t / 20 h	3	98	<b>12</b>
MIL-101-AB-0.32	DMF, 1,2,4-trichlorobenzene/ 363 K	3	99	<b>13</b>
Pickering Emulsion Droplets	Water, toluene / 60 °C / 19 h	4	75	<b>14</b>
2,3-DhaTph	Toluene / 80 °C / 1 h	5	96	<b>15</b>
PPAF-SO <sub>3</sub> H-NH <sub>2</sub>	Toluene / 90 °C / 1 h	7	87	<b>16</b>
LZSM-5-AT-OH <sup>-</sup>	MeCN / 353 K / 15 h	10	91.2	<b>17</b>
PPAF-SO <sub>3</sub> H-NH <sub>2</sub>	Toluene / 90 °C / 1 h	8	100	<b>18</b>
SAB	Ethyl acetate / 50 °C / 12 h	4	99	<b>19</b>
Ti <sup>4+</sup> -mont/HT	Toluene / 80 °C / 1 h	0	93	<b>20</b>
TAPB-DMTP-PA-COF	Solvent-free, 75 °C, 5h	15	99	<b>21</b>
[NaZn(btc)(H <sub>2</sub> O) <sub>3</sub> ].1.5H <sub>2</sub> O	DMF / 80 °C / 1 h	2	99	<b>22</b>
MIL-101(Cr)@MOF-867	DMSO/ 353 K / 12 h	5	99.9	<b>23</b>
L-TPS/AP/SBA-15	H <sub>2</sub> O/toluene 100 °C / 3 h	1	100	<b>24</b>
CP 1	DMF / 80 °C / 2 h	6	99	<b>25</b>
ZIF-8	H <sub>2</sub> O/toluene / 353 K / 6 h	5	95	<b>26</b>
UiO-66-NH <sub>2</sub>	H <sub>2</sub> O/toluene / 353 K / 6 h	1	94	<b>26</b>
MIL-101-NH <sub>2</sub>	H <sub>2</sub> O/toluene / 353 K / 6 h	1	93	<b>26</b>

NUC-130	DMSO / 55 °C / 5 h.	5	99	<b>27</b>
NUC-53	DMSO/ 70 °C / 6 h	5	98	<b>28</b>
AF-SN1/2	water/ 25 °C/ 2.5-5 h	10	95	<b>29</b>
PANF-EC3/2	water/ 25°C-80°C / 6 h	10	97	<b>30</b>
1-Tb	water/ 60°C / 6 h	1	98	<b>31</b>
1-Yb	water/ 60°C / 6 h	5	97	<b>31</b>
ZIF-90@ZIF-67	H <sub>2</sub> O/toluene /353 K / 12 h	5	99.9	<b>32</b>
MIL-101(Cr)@PMF	H <sub>2</sub> O /353 K / 12 h	5	99.9	<b>33</b>
NUC-51a	DMSO/ 70°C / 4 h	5	99.9	<b>34</b>
SSICG-14	solvent-free / 70°C / 4 h	5	99	<b>35</b>
NUC-55	DMSO / 70°C / 6 h	5	99.33	<b>36</b>
YS-CLPS-SO <sub>3</sub> H@ZIF-8	H <sub>2</sub> O / acetonitrile / 80 °C / 12 h.	10	94	<b>37</b>
PCN-222-Co@TpPa-1	DMSO / 50 °C / 10 h.	5	99.3	<b>38</b>
SO <sub>3</sub> H-AEPTMS@MCM-41	Ethyl cyanoacetate, H <sub>2</sub> O / 80 °C / 1 h.	5	94.9	<b>39</b>
Ca-Zr/Ti-HMS-T	Toluene / 90 °C / 9 h.	10	99.9	<b>40</b>
0.5NH <sub>2</sub> /0.5SO <sub>3</sub> H- C <sub>12</sub> /JMSNs	Toluene, H <sub>2</sub> O/ 80 °C / 3 h.	5	100	<b>41</b>
SO <sub>3</sub> H-NH <sub>2</sub> -HMS-2x	ethyl cyanoacetate / 80 °C / 5 h.	3	95.2	<b>42</b>
HMS-Al@MS-NH <sub>2</sub>	Toluene, ethyl cyanoacetate / 110 °C / 2 h.	4	100	<b>43</b>

<b>CTP-DABA-COF</b>	<b>deacetalization–Knoevenagel condensation:</b> H <sub>2</sub> O / 50°C / 5 h	10	99	<b>This work</b>
<b>CTP-DABA-COF</b>	<b>Multicomponent tandem:</b> H <sub>2</sub> O, EtOH / 50°C / 7 h	5	96	<b>This work</b>

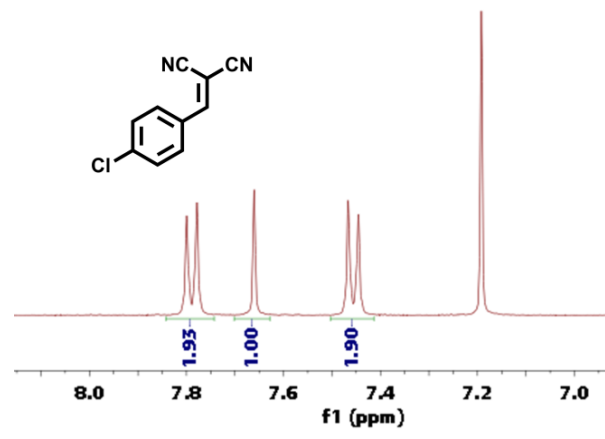
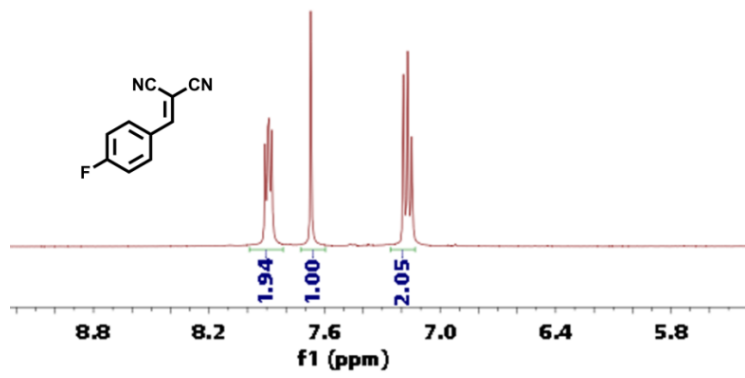
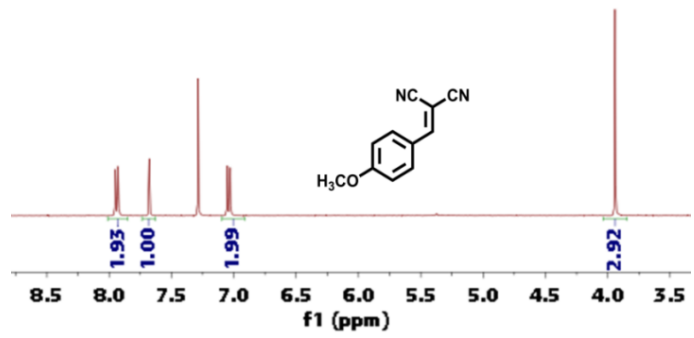
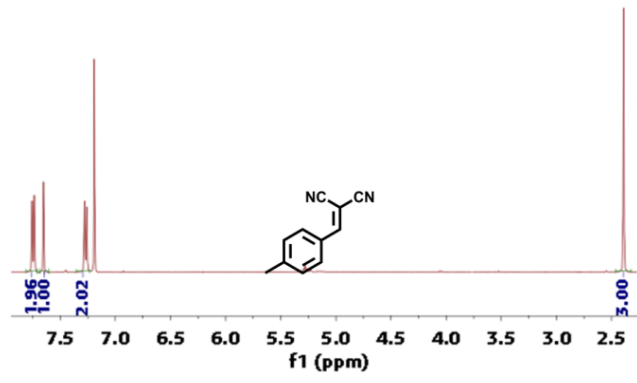
**Table S6.** The deacetalization–Knoevenagel reactions among various benzaldehyde dimethyl acetals catalysed by **CTP-DABA-COF**.



Entry	R	Catalyst	Temperature	Time	Yield
1	4-Me	1.0 mol%	50°C	5 h	99%
2	4-OMe	1.0 mol%	50°C	5 h	99%
3	4-F	1.0 mol%	50°C	5 h	99%
4	4-Cl	1.0 mol%	50°C	5 h	98%
5	4-Br	1.0 mol%	50°C	5 h	99%
6	2-Me	1.0 mol%	50°C	5 h	99%
7	2-F	1.0 mol%	50°C	5 h	96%
8	2-Cl	1.0 mol%	50°C	5 h	99%
9	3-Br	1.0 mol%	50°C	5 h	99%

<sup>a</sup> Reaction conditions: benzaldehyde dimethylacetal (150  $\mu$ L, 1.0 mmol) and malononitrile (66 mg, 1.0 mmol) in the presence of **CTP-DABA-COF** (11.9 mg, 1 mol %), the mixture was stirred for 5 h at H<sub>2</sub>O (2 mL).

<sup>b</sup> Yield was determined by GC analysis.



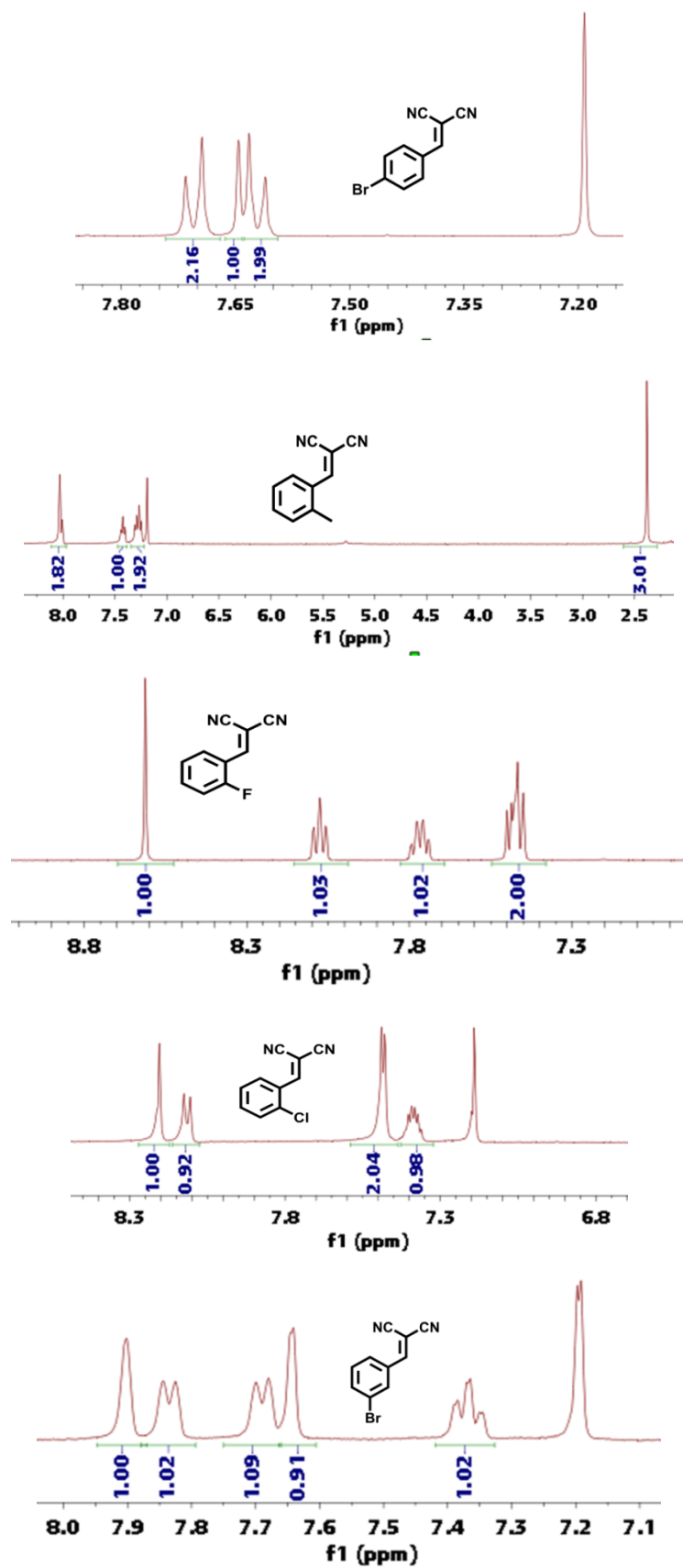
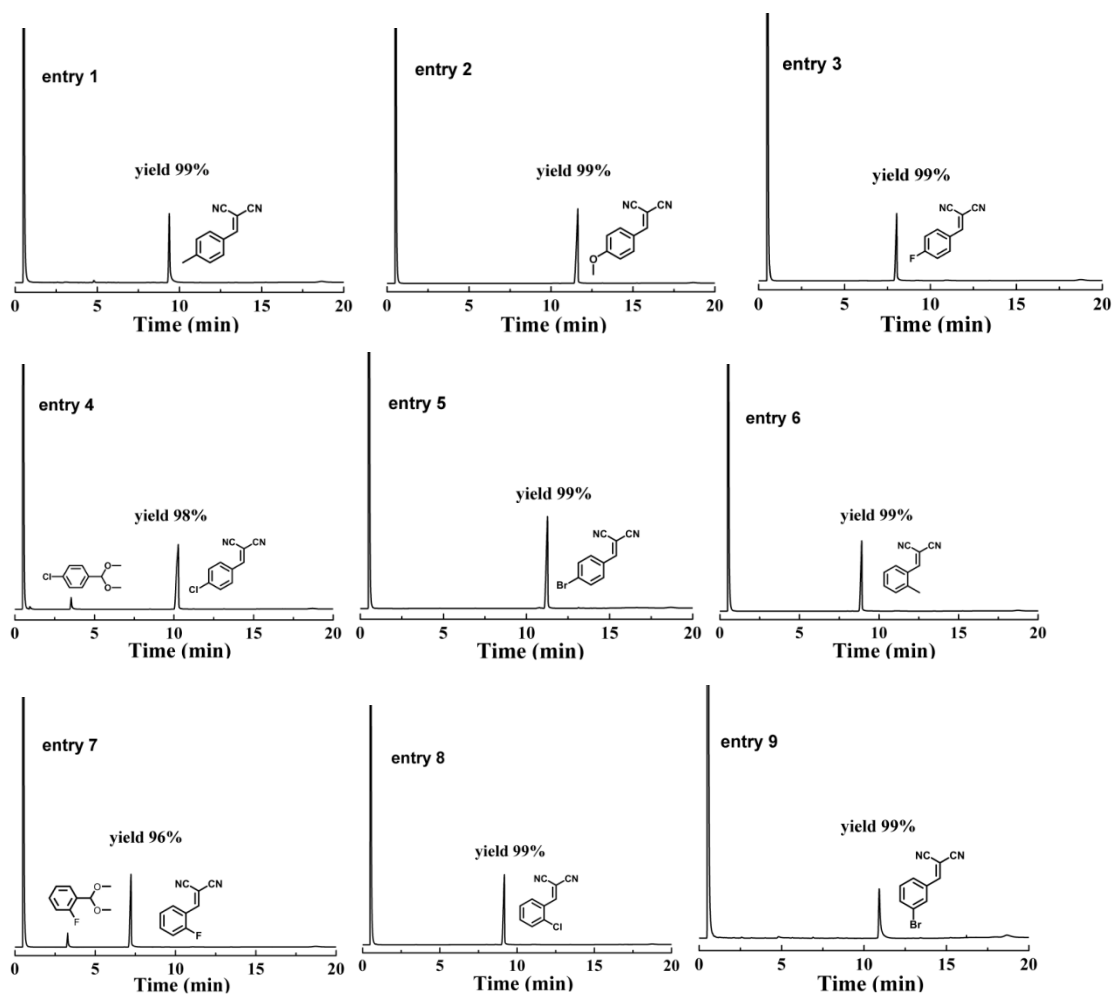
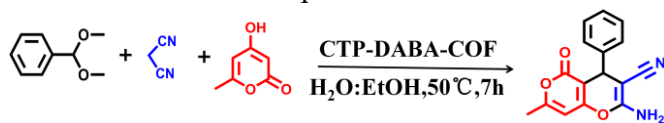


Fig. S13  $^1\text{H}$  NMR spectra of catalytic product various benzylidenemalononitrile.



**Fig. S14** GC analysis: the scope of the catalytic system was explored by performing the reactions of various substituted benzylidenemalononitrile.

**Table S7.** Optimization of the multicomponent tandem reactions conditions. <sup>a</sup>

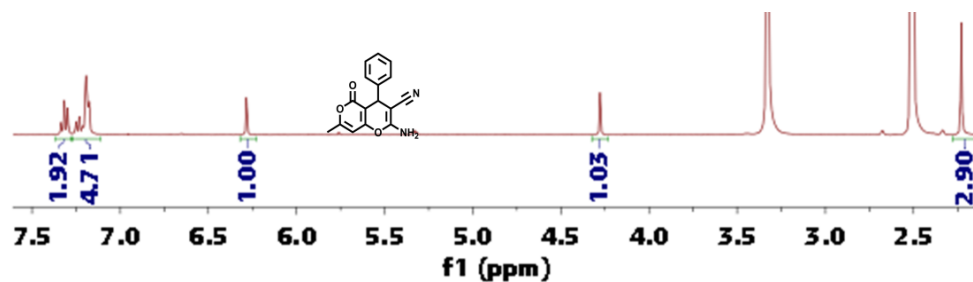


Entry	Catalyst	Solvent	Time	Temperature	Yield <sup>b</sup>
1	1.0mol%	solvent-free	7h	50°C	70%
2	1.0mol%	THF	7h	50°C	35%
3	1.0mol%	1,4-dioxane	7h	50°C	33%
5	1.0mol%	EtOH	7h	50°C	82%
6	1.0mol%	MeCN	7h	50°C	30%
7	1.0mol%	H <sub>2</sub> O	7h	50°C	65%
8	1.0mol%	H <sub>2</sub> O:EtOH=1:1	7h	50°C	96%
9	1.0mol%	H <sub>2</sub> O:EtOH=1:1	7h	60°C	96%

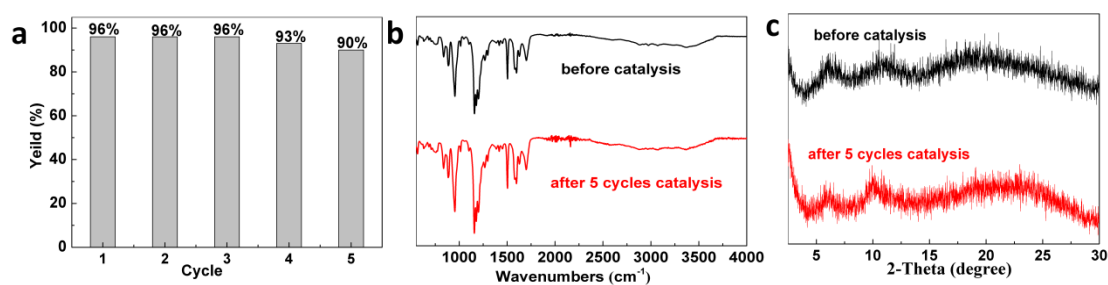
10	0.5mol%	H <sub>2</sub> O:EtOH=1:1	7h	60°C	58%
11	No Catalysis	H <sub>2</sub> O:EtOH=1:1	7h	50°C	1%

a Reaction conditions: benzaldehyde dimethylacetal (150  $\mu$ L, 1.0 mmol) and malononitrile (66 mg, 1.0 mmol) in the presence of **CTP-DABA-COF** (11.9 mg, 1 mol %), the mixture was stirred for 7 h at H<sub>2</sub>O (2 mL).

b Reaction was monitored by isolated yields.

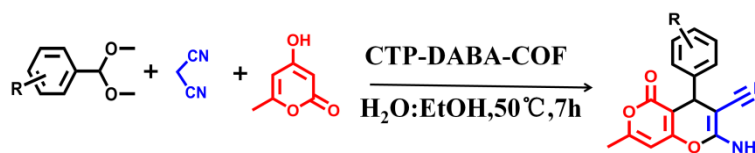


**Fig. S15** <sup>1</sup>H NMR spectra of 2-amino-7-methyl-5-oxo-4-phenyl-4H-pyrano[3,2-c]pyran-3-carbonitrile in DMSO-d<sub>6</sub>.



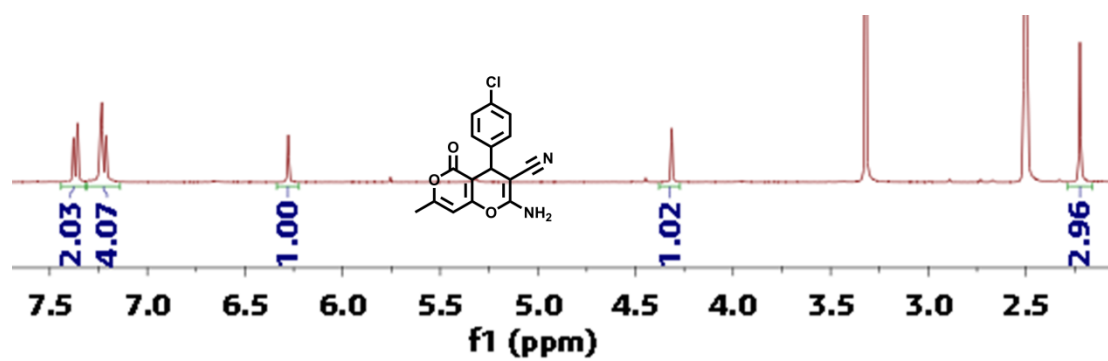
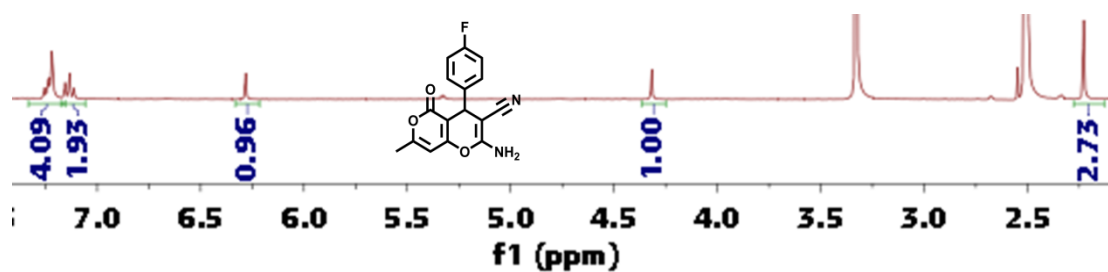
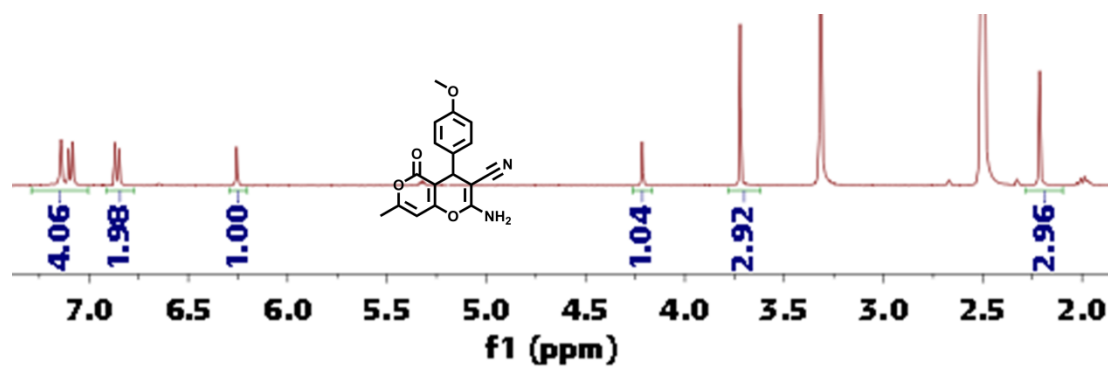
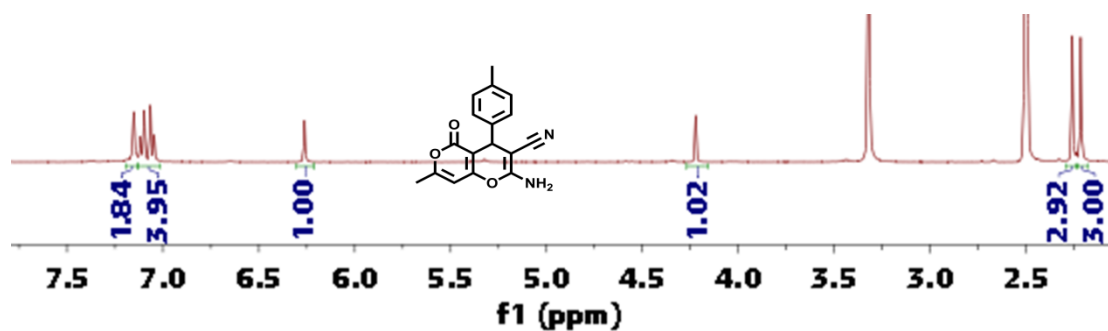
**Fig. S16** The FT-IR (b) and PXRD (c) of **CTP-DABA-COF** after five runs.

**Table S8.** The multicomponent tandem reactions among various benzaldehyde dimethyl acetals catalysed by **CTP-DABA-COF**.



Entry	R	Solvent	Temperature	Time	Yield
1	4-Me	H <sub>2</sub> O:EtOH=1:1	50°C	7 h	96%
2	4-OMe	H <sub>2</sub> O:EtOH=1:1	50°C	7 h	96%
3	4-F	H <sub>2</sub> O:EtOH=1:1	50°C	7 h	95%
4	4-Cl	H <sub>2</sub> O:EtOH=1:1	50°C	7 h	92%
5	4-Br	H <sub>2</sub> O:EtOH=1:1	50°C	7 h	90%

6	2-Me	H <sub>2</sub> O:EtOH=1:1	50°C	7 h	95%
7	2-F	H <sub>2</sub> O:EtOH=1:1	50°C	7 h	89%
8	2-Cl	H <sub>2</sub> O:EtOH=1:1	50°C	7 h	90%
9	3-Br	H <sub>2</sub> O:EtOH=1:1	50°C	7 h	90%



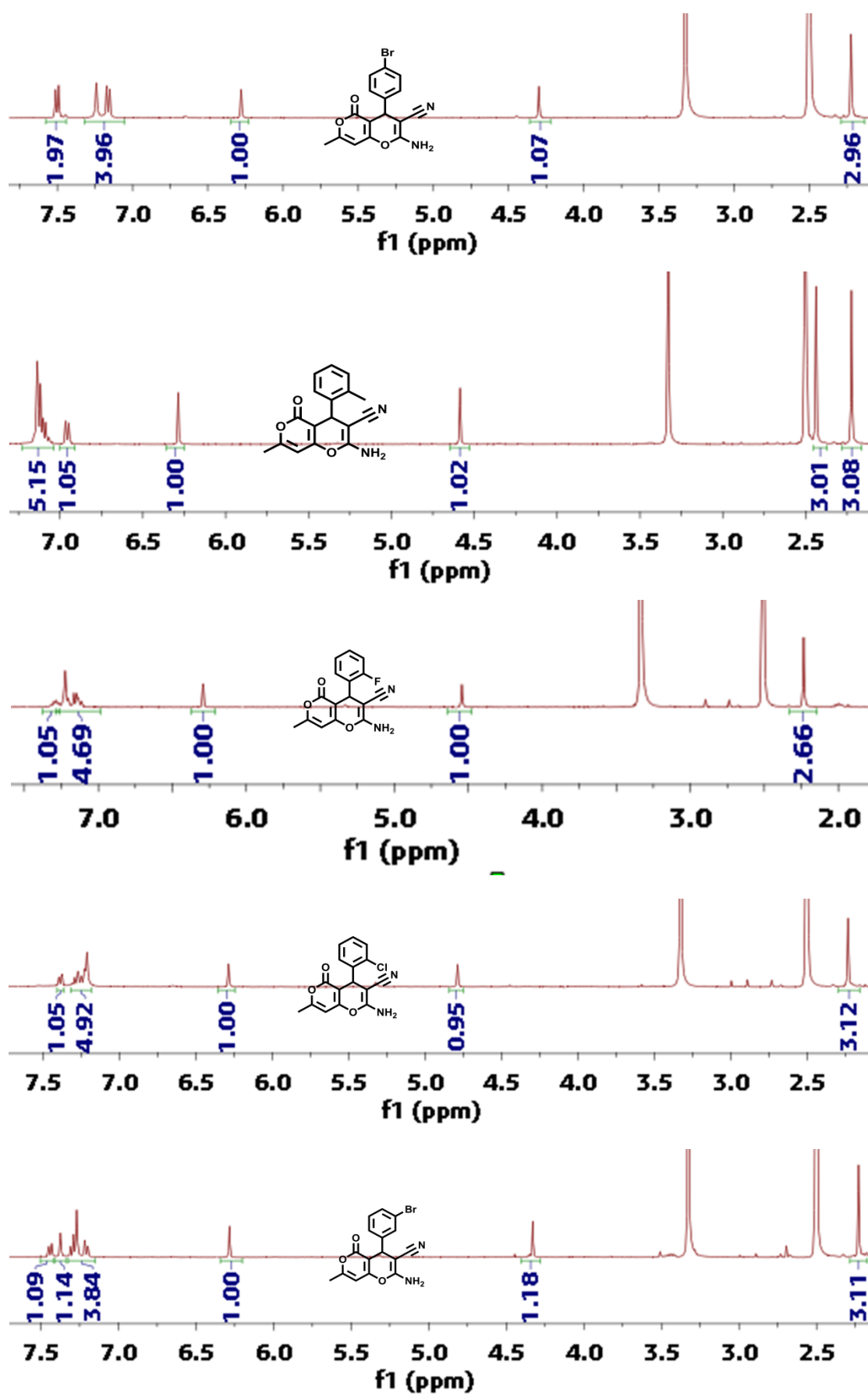
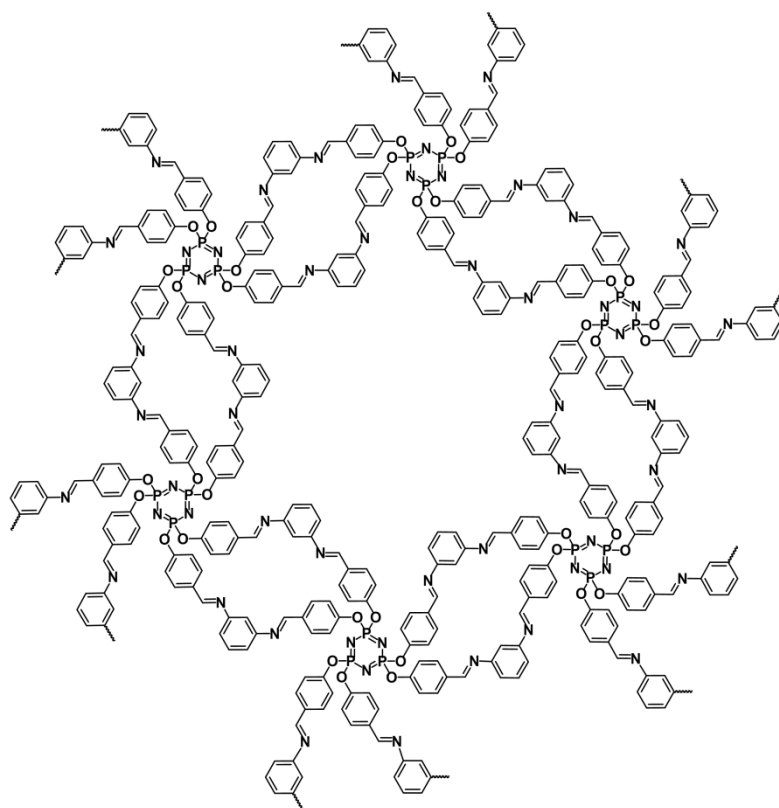
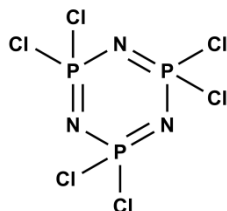


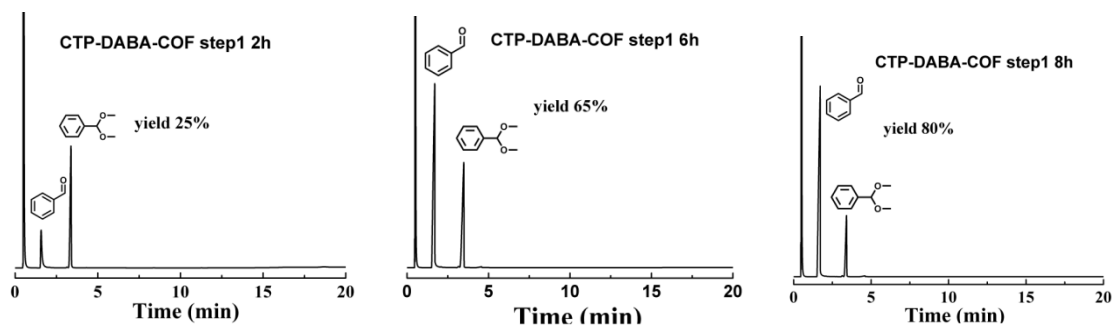
Fig. S17 <sup>1</sup>H NMR spectra of catalytic product various pyran heterocyclic complexes.

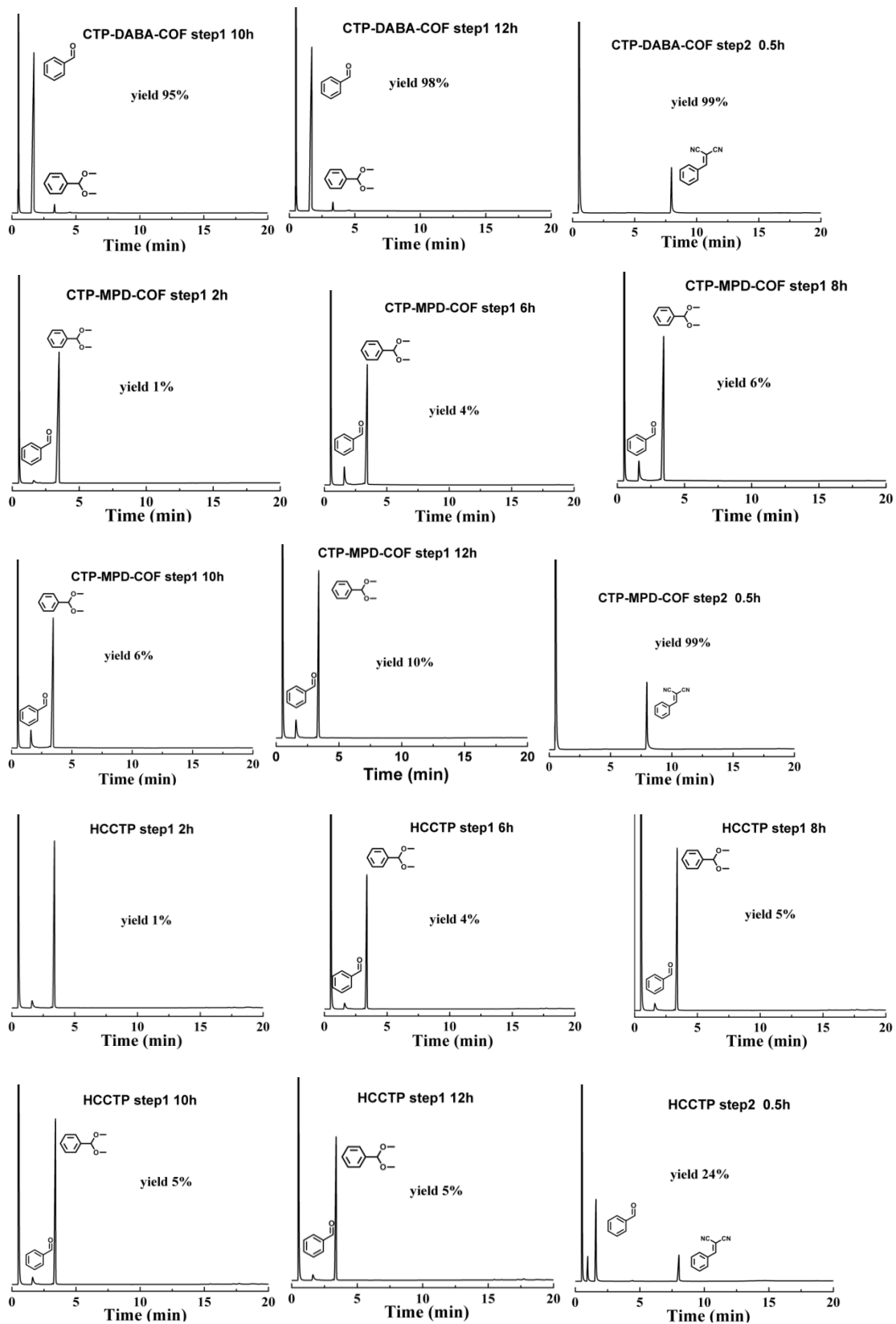


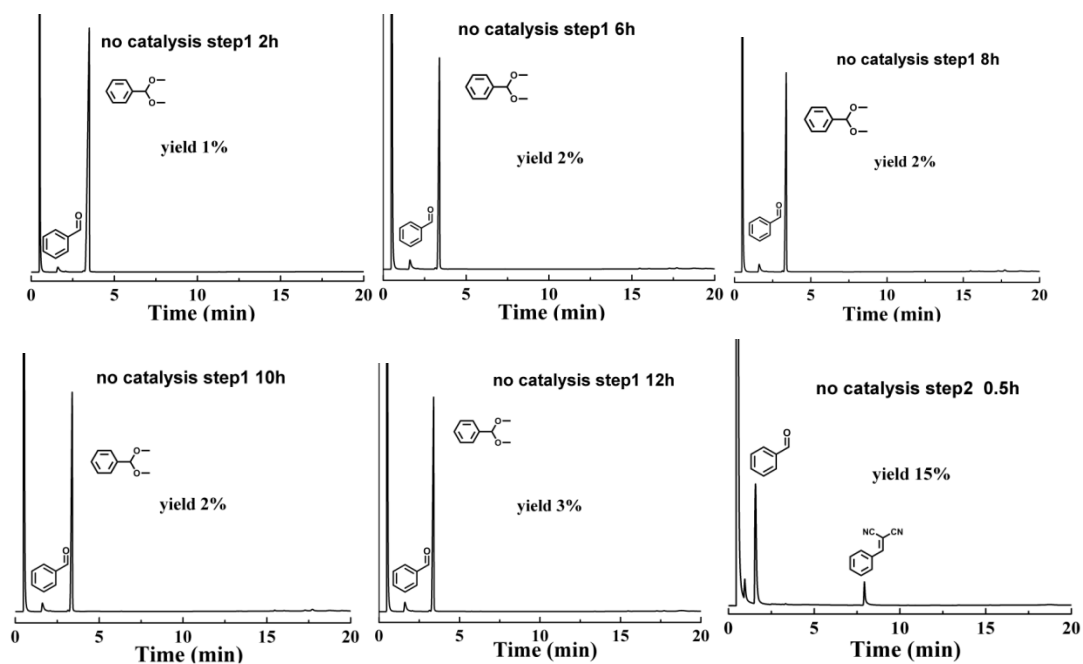
**Fig. S18** The structure of CTP -MPD-COF.



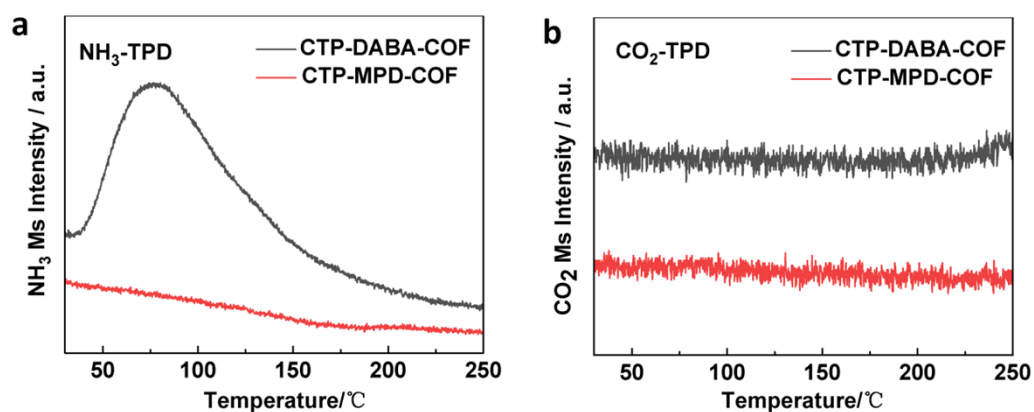
**Fig. S19** The structure of HCCTP.



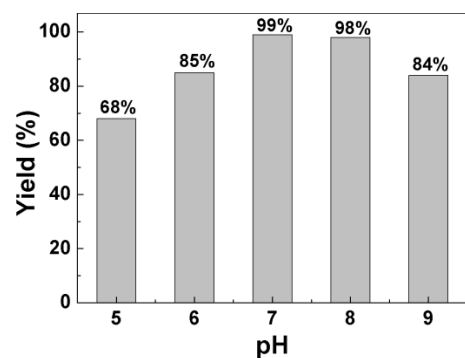




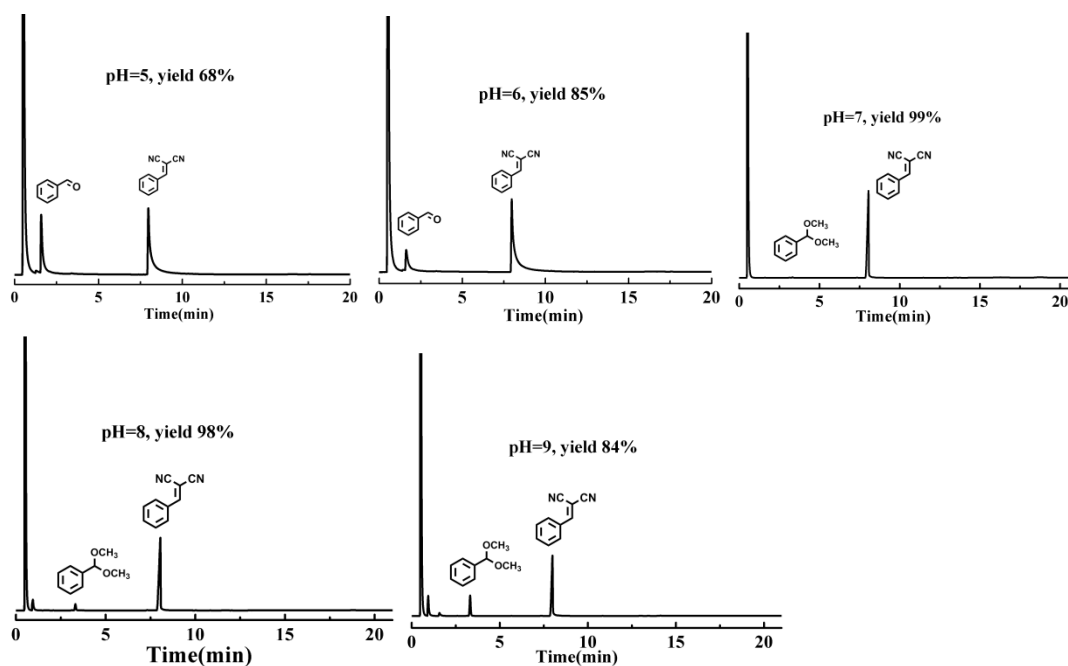
**Fig. S20** The GC of the deacetalization (Step 1) and the Knoevenagel condensation (Step2) by CTP-DABA-COF, CTP-DABA-COF, HCCTP and no catalysis.



**Fig. S21** a)  $\text{NH}_3$ -TPD and b)  $\text{CO}_2$ -TPD by CTP-DABA-COF and CTP-MPD-COF.



**Fig. S22** The comparative experiment of deacetalization-Knoevenagel reaction at different pH.



**Fig. S23** The GC of the deacetalization-Knoevenagel reaction at different pH.

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