Electronic Supplementary Material (ESI) for ChemComm.

Nitroreductase-sensitive fluorescent covalent organic framework for tumor hypoxia imaging in cells

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Supporting Information

General. All chemicals and solvents were purchased from Sigma-Aldrich and used without further purification. Deionized water was used from Adrona B30 water purification system. Routine nuclear magnetic resonance (NMR) spectra were recorded at 25 °C on a Bruker Avance spectrometer, with working frequencies of 400 MHz for ^{1}H, and 125 MHz for ^{13}C nuclei, respectively. All chemical shifts are reported in ppm relative to the signals corresponding to the residual solvent ($CDCl_3$: δ = 7.26 ppm and CD_3OD: δ = 3.31).

Materials Characterization. Fourier-transform (FT-IR) spectra were recorded on the Perkin Elmer Spectrum 100 with an attenuated total reflectance (ATR) attachment. NMR measurements were carried out on a 600 MHz Varian NMR system equipped with a 1.6 mm Varian T3 HXY MAS probe. Larmor frequencies for ^{1}H and ^{13}C nuclei were 599.50 MHz, and 150.72 MHz, respectively. Sample rotation frequency was 20 kHz. ^{1}H-^{13}C cross-polarization (CP) MAS NMR spectrum was recorded by first exciting protons and transferring polarization to carbon nuclei using the amplitude-ramped CP block with a duration of 4 ms. During the acquisition, high-power XiX heteronuclear decoupling was applied; repetition delay was 1 s and 53000 scans were collected. ^{1}H-^{13}C CP/MAS NMR spectrum was referenced to the corresponding signal of TMS. X-ray diffraction measurements were performed on Rigaku SmartLab II with Cu K_{α} (λ = 1.5405 Å) radiation source operating at 40 kV and 40 mA. The patterns were recorded with a divergent slit of 1/16° over the 2θ range of 1–50° with step size = 0.01°. Porosity analyses were performed on the Anton Paar Autosorb iQ combined physisorption and chemisorption instrument. For each measurement, 20 – 50 mg of sample was used. The samples were activated at 80 °C for 16 hours before being subject to N_2 gas adsorption in liquid N_2 bath (77 K) to collect full isotherms. Surface areas were calculated using the Brunauer – Emmett – Teller (BET) model, and pore size distributions were found using the non-local density functional theory (NLDFT). TGA experiments were performed on Mettler Toledo TGA/DSC2 with a heating rate of 10 °C min^{-1} over a temperature range of 75–1000 °C following an initial equilibration at 70°C. Elemental analysis was performed on Perkin Elmer Series II CHN 2400 analyser. Dynamic light scattering (DLS) experiments were performed on Brookhaven Instruments Corporation 90 Plus/BI-MAS using water as a solvent. Fluorescence properties were measured on Edinburg Instruments FLS920 Steady State and Fluorescence Lifetime Spectrometer. Scanning electron microscopy (SEM) images were recorded on JEOL JSM-7001 TTLS operating at 4.0 kV. Powder samples were drop-cast on Si wafer substrates, and electrodes were imaged by attaching them directly to the sample holder. Transmission electron microscopy (TEM) images were collected on JEOL JEM-2100 HR operating at 200 kV.

Tissue culture. HeLa cells were cultured at 37 °C and 5 % CO_2 in 25 mL tissue cultures flasks in Dulbecco's Modified Eagle's Medium (DMEM) supplemented with 10 % FBS, 100 µg mL^{-1} penicillin and 100 µg mL^{-1} streptomycin. Cells were detached with 0.25 % trypsin solution, resuspended in the medium and counted before being diluted to the final concentration depending on the experiment.

***In vitro* cell viability assays.** 96-well plates were seeded with cells (~10,000 cells per well in 100 µL of DMEM) and incubated at 37 °C for 24 hours. The medium was removed and replaced with fresh DMEM (control) or various concentrations of DNB, Tp, or **NI-COF** (all in 1 % DMSO) in triplicates, and incubated at 37 °C for 24 hours. Thereafter, cells were washed with PBS and incubated with the Presto-Blue^{TM} Cell Viability Reagent (ThermoFisher Scientific) diluted in DMEM as per manufacturer's instructions. The incubation at 37 °C lasted approximately 30 minutes. The contents of the 96-well plate were then transferred into a black flat-bottom 96-well plate, and the fluorescence signal was read using the Tecan Infinite F200 microplate reader ($\lambda_{ex}/\lambda_{em}$ 560 nm /595 nm). Untreated wells were used as a control.

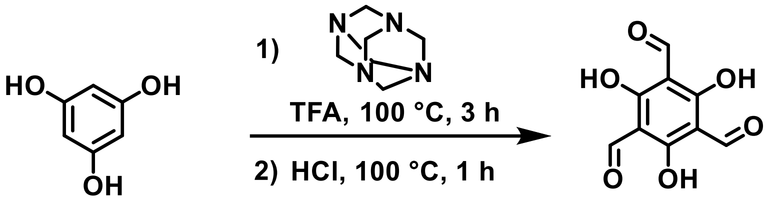
Cell internalization under hypoxic and normoxic conditions. HeLa cells were grown on square glass cover slips placed in petri dishes. 200,000 cells per petri dish were incubated at 37 °C for 48 h. The slides were then washed with PBS and incubated with fresh DMEM medium in either (i) the incubator as before, or (ii) under severe hypoxic conditions created in GENbag anaer (Biomerieux, France) in the incubator for four hours. An indicator strip was added into the GENbag to monitor the level of oxygen present. After the incubation period, the controls were left untreated whereas other samples were incubated with exfoliated **NI-COF** (4 µg mL^{-1}) at 37 °C for one hour. After the incubation, the cells were washed with PBS three times, fixed with 4 % formaldehyde solution for 15 minutes, and again washed with PBS three times. The cover slips were then mounted onto glass microscope slides with the aid of a mounting medium, and the edges of the coverslips were sealed.

Control experiments with **NO_2-COF** and **NH_2-COF** were performed using the same protocol as described above for **NI-COF**.

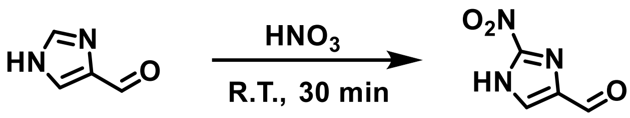
Another experiment was conducted under mild hypoxic conditions. The same protocol was carried out as described for sever hypoxic conditions above, except that GENbag anaer was replaced by GENbag microaer (Biomerieux, France). This created an environment with ~5 % O_2.

Fluorescence microscopy imaging was performed on Axio Observer Z.1 epifluorescence microscope (Zeiss, Germany). The microscope was equipped with the HXP 120C compact light source, the HAL100 halogen lamp and the AxioCam Mrm monochrome digital camera. Filter set 49 (Zeiss, Germany) with the emission wavelength at 445/50 nm. Images were acquired in the AxioVision 4 software and processed in the ImageJ software.

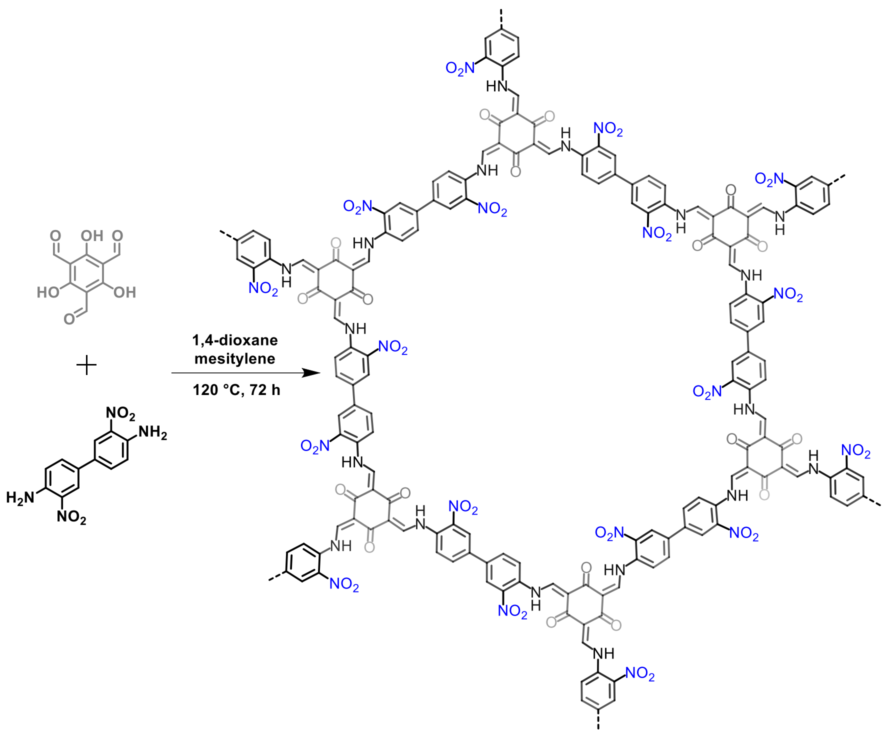
Synthesis of 1,3,5-triformylphloroglucinol (Tp). The compound was synthesized according to a published procedure with minor modifications.[1] Dry phloroglucinol (2.00 g, 16 mmol) and hexamethylenetetramine (5.00 g, 36 mmol) were added to a two-neck round bottom flask equipped with a condenser and a N_2-filled balloon. 30 mL of trifluoroacetic acid (TFA) was slowly added to the mixture, and the solution was heated at 100 °C for 3 h. Next, 50 mL of 3 M HCl was slowly added, and the heating was continued at 100 °C for 1 h. After cooling the mixture to room temperature, it was filtered through Celite, washed with water once, extracted with dichloromethane three times, and dried over $MgSO_4$. The combined dichloromethane phases were subsequently evaporated on rotary evaporator. The product appeared as a pale powder with a yield of 17.3 %, which is comparable to the literature. ^{1}H NMR (400 MHz, $CDCl_3$) δ 14.09 (s, 3H, OH), 10.15 (s, 3H, CHO) ppm. ^{13}C NMR (125 MHz, $CDCl_3$) δ 192.15 (s, CHO), 173.66 (s, C-OH), 102.92 (s, C-CHO) ppm.



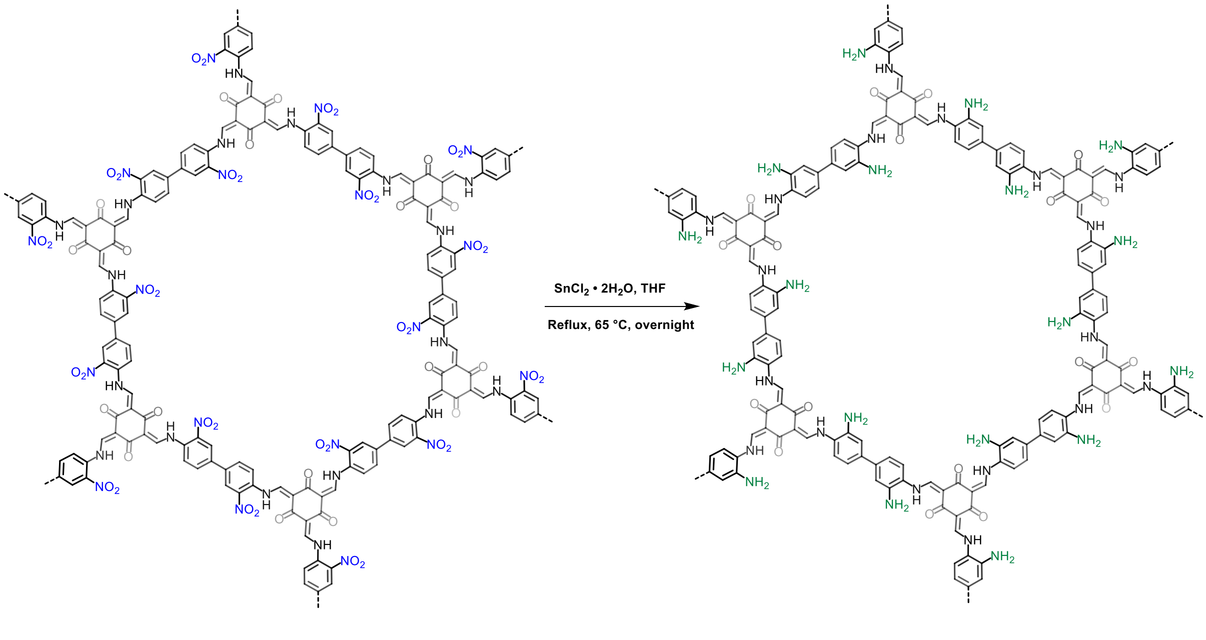
Synthesis of 4-nitro-1H-imidazole-2-carbaldehyde (Hyp) was based on the literature reports.[2,3] In brief, 4-imidazolecarboxaldehyde (143 mg, 1.5 mol) was stirred in 70 % nitric acid (3.0 mL) for 30 minutes at room temperature. Subsequently, rotary evaporation was used to remove the liquid and afford **Hyp**. ^{1}H NMR (400 MHz, CD_3OD) δ 8.84 – 8.90, 7.47 – 7.55, 5.63 – 5.72 ppm. ^{13}C NMR (125 MHz, CD_3OD) δ 136.2, 135.9, 135.3, 133.1, 117.7 – 118.9, 97.5, 91.8 ppm.



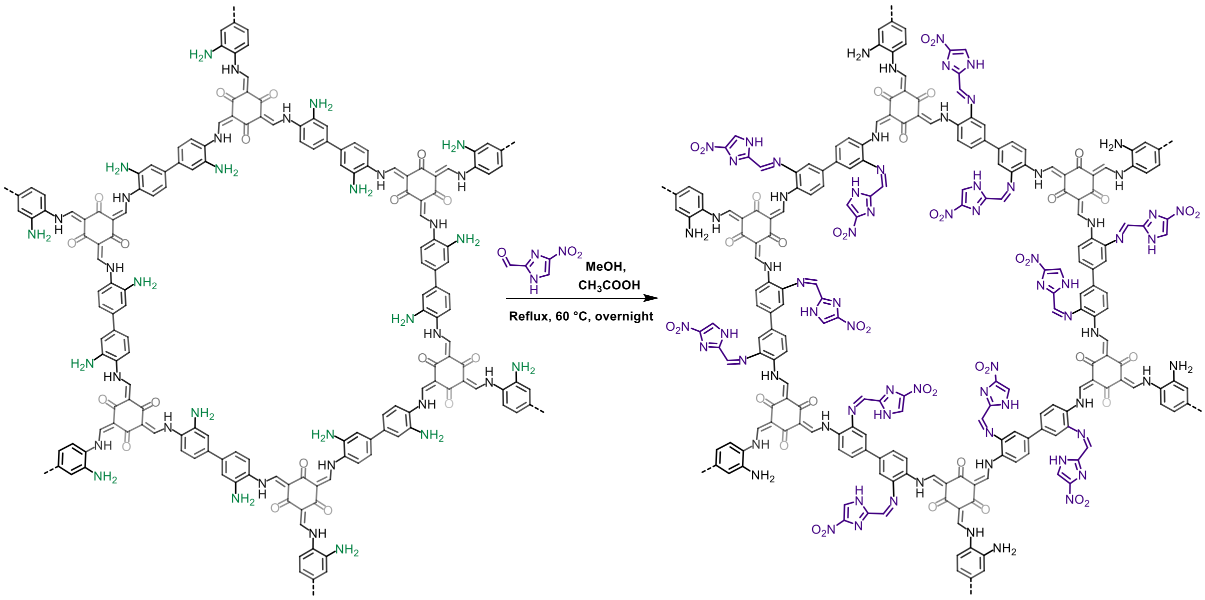
Synthesis of NO_2-COF. The material was synthesized by following a literature report.[4] In brief, Tp (63 mg, 0.300 mmol) and 3,3'-dinitrobenzidine (124 mg, 0.45 mmol) were placed in a Schlenk tube. A mixture of solvents (1.5 mL mesitylene, 1.5 mL 1,4-dioxane, and 0.5 mL 6 M acetic acid) was added. The tube was sonicated, sealed and treated with three freeze-pump-thaw cycles. Then, it was placed in an oven at 120 °C for 72 h. The precipitate was collected and washed with N,N'-dimethylformamide (DMF) and acetone. Finally, the material was exfoliated by five hours of exfoliation at 70 % power of the ultrasonic tip, and dried in a vacuum over (50 °C) overnight. Elemental analysis: 40.8 % C, 3.3 % H, 9.7 % N, <0.01 % S.



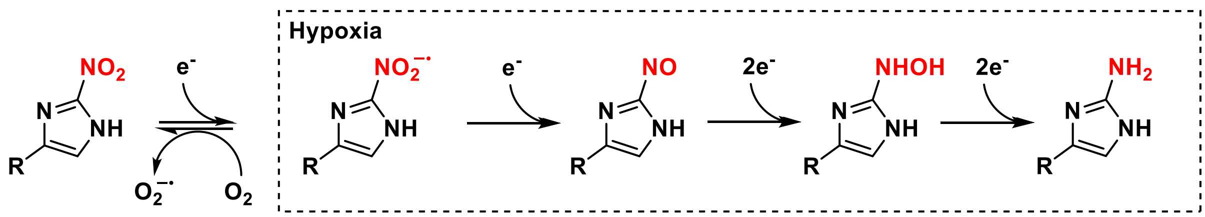
Synthesis of NH_2-COF.[5] NO_2-COF (30 mg) was placed in a two-neck flask equipped with a condenser and a N_2-filled balloon. In a separate flask, $SnCl_2 \cdot 2H_2O$ (750 mg, 3.3 mmol) was dissolved in anhydrous tetrahydrofuran (THF; 3 mL), and transferred to the two-neck flask *via* syringe. The mixture was heated under reflux at 65 °C overnight. Then, the powder was collected by centrifugation and resuspended in 5 mL of 1 M HCl. The mixture was stirred at room temperature for one hour. Then, it was washed 10 times with 1 M HCl, twice with water, and twice with THF, with each wash lasting for about one hour. Finally, thus-obtained brown-colored NH_2-COF was dried in a vacuum oven overnight (40 °C). Elemental analysis: 36.7 % C, 3.1 % H, 9.4 % N, <0.01 % S.



Synthesis of NI-COF. To conjugate the hypoxia targeting molecule to NH_2-COF, imine condensation was used. **NH_2-COF** (10 mg) and **Hyp** (3 mg) were placed in a round bottom flask, to which 3 mL of methanol and a catalytic amount of 6 M acetic acid were added. The mixture was heated under reflux at 60 °C overnight. After cooling to room temperature, the powder was collected by centrifugation and washed with methanol three times. Finally, the material was dried on air and in a vacuum oven (40 °C). Elemental analysis: 54.2 % C, 3.7 % H, 13.7 % N, <0.01 % S.



Stability testing of NI-COF. Around 10 mg of **NI-COF** was incubated in PBS for 24 hours, washed with water and ethanol to remove the PBS salts, and dried. Thus-obtained material was characterized by FT-IR, PXRD, and SEM to study possible changes in the chemical composition, crystallinity and morphology, respectively. Similarly, the stability of **NI-COF** was studied in 0.1 M acetate buffer at pH = 5.4. The material was incubated in the buffer for 24 hours, washed with water and ethanol, and dried. The same characterizations were performed as described for stability testing in PBS above.



R = NI-COF backbone

Figure S1. The mechanism of nitroreductase-sensitive **NI-COF** in hypoxic conditions.[6]

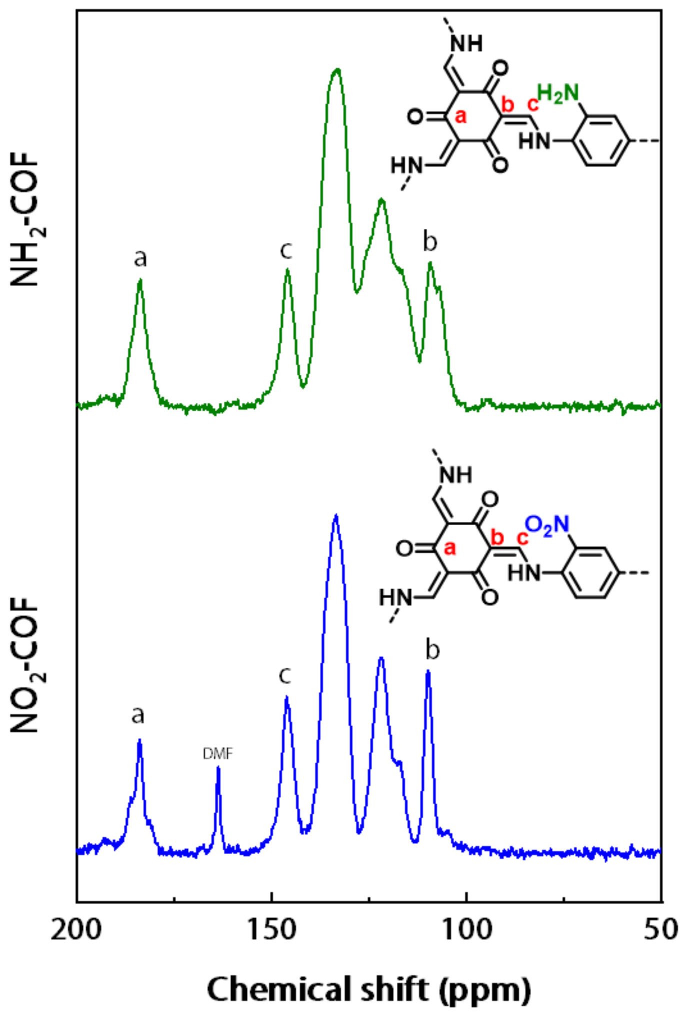


Figure S2. CP-MAS ^{13}C NMR spectra of **NO_2-COF** and **NH_2-COF**.

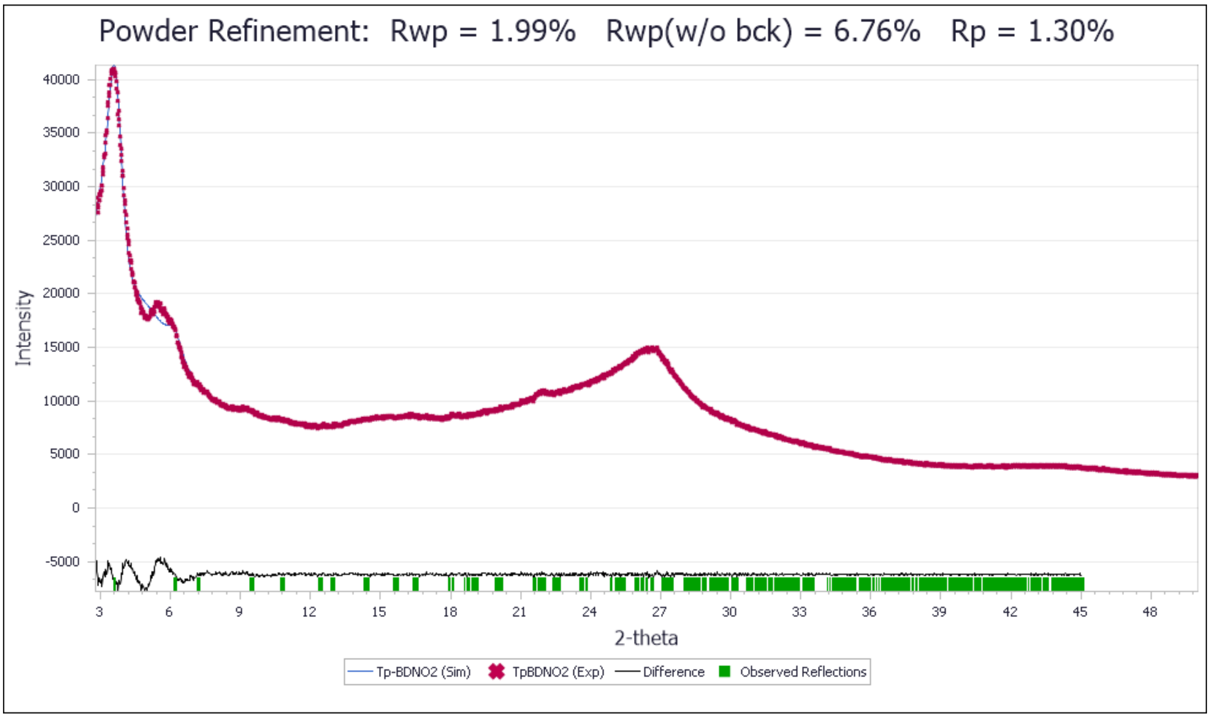


Figure S3. Pawley refinement of **NO_2-COF**. The experimental PXRD pattern collected after Pawley refinement was found to be in good agreement with the simulated one.

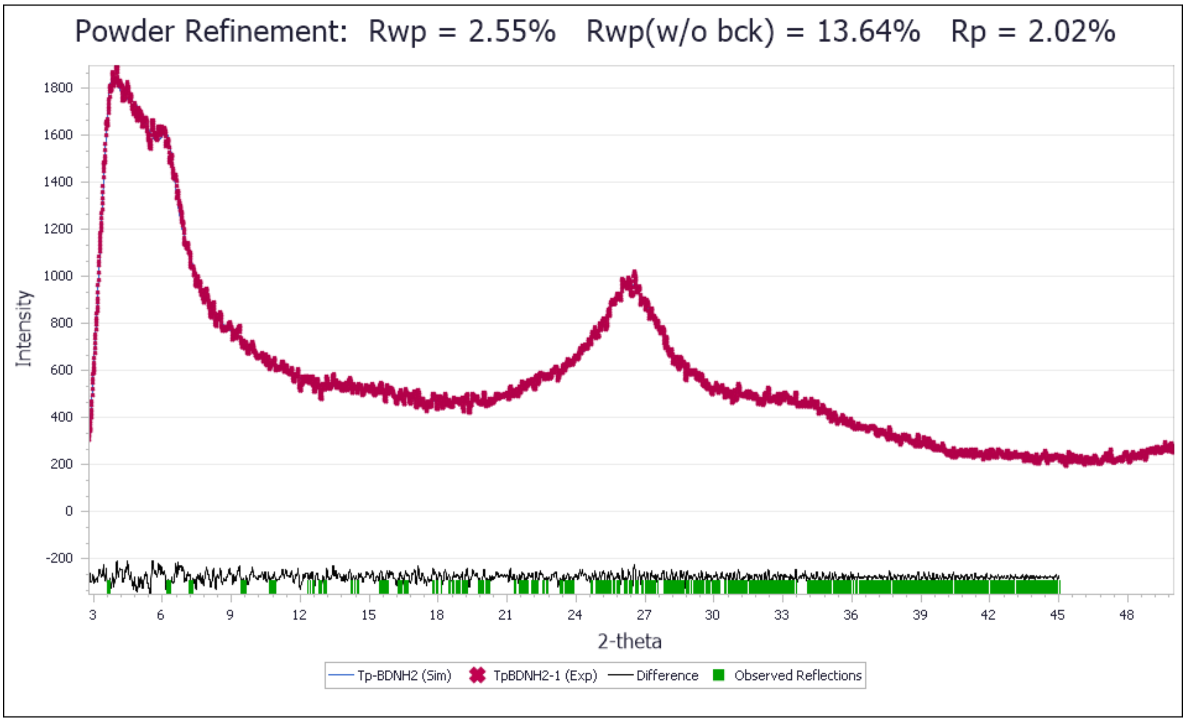


Figure S4. Pawley refinement of **NH_2-COF**. The experimental PXRD pattern collected after Pawley refinement was found to be in good agreement with the simulated one.

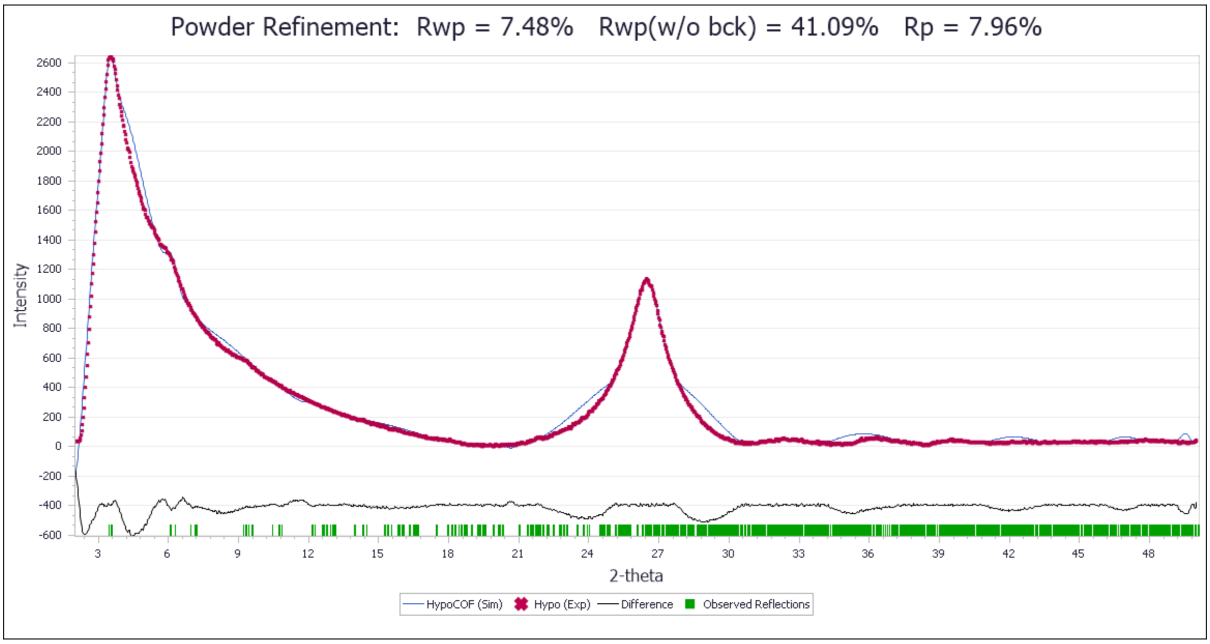


Figure S5. Pawley refinement of **NI-COF**. The experimental PXRD pattern collected after Pawley refinement was found to be in good agreement with the simulated one.

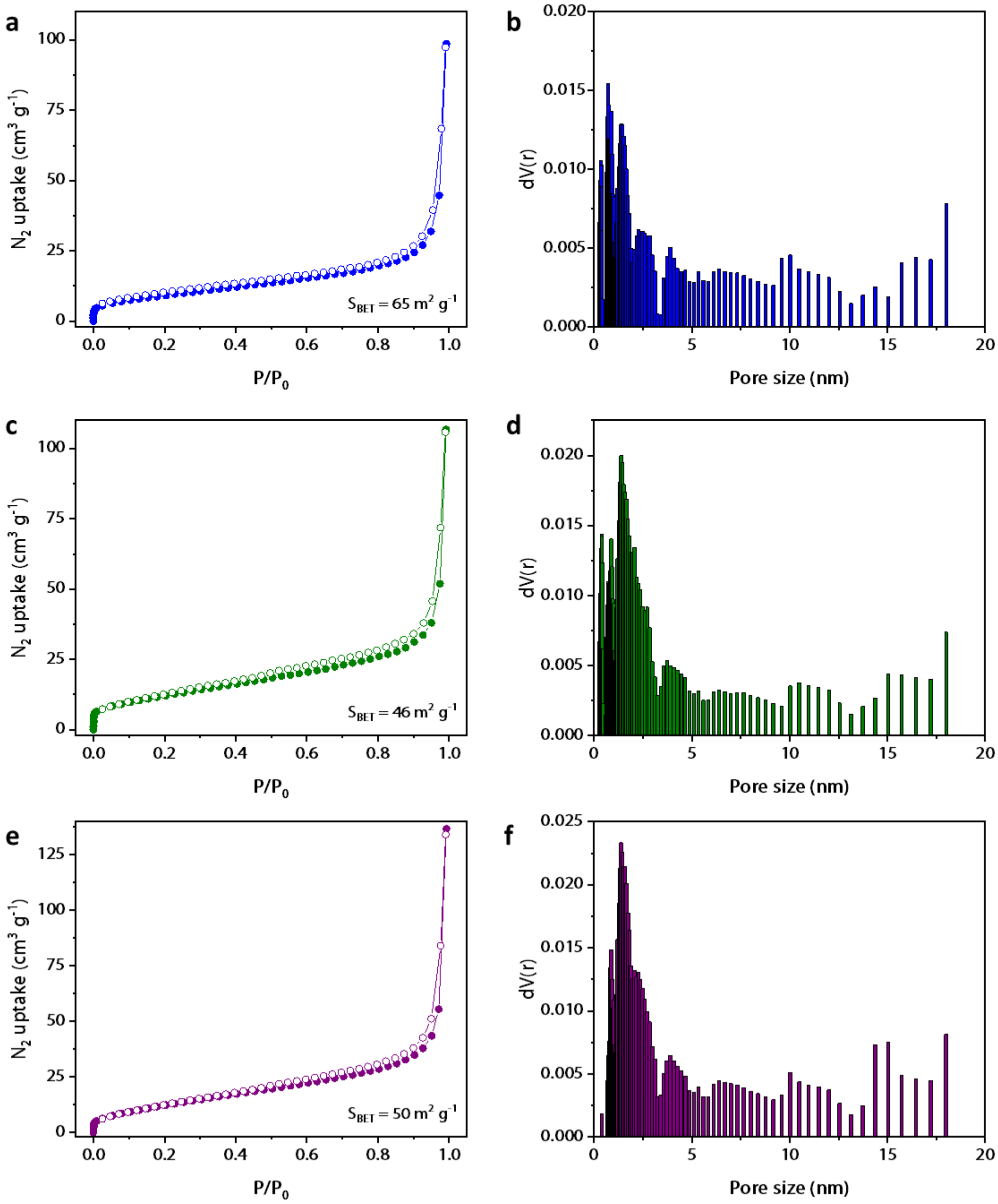


Figure S6. N_2 gas adsorption studies with all three COFs. a) N_2 adsorption isotherm for **NO_2-COF**; b) pore size distribution for **NO_2-COF**; c) N_2 adsorption isotherm for **NH_2-COF**; d) pore size distribution for **NH_2-COF**; e) N_2 adsorption isotherm for **NI-COF**; f) pore size distribution for **NI-COF**.

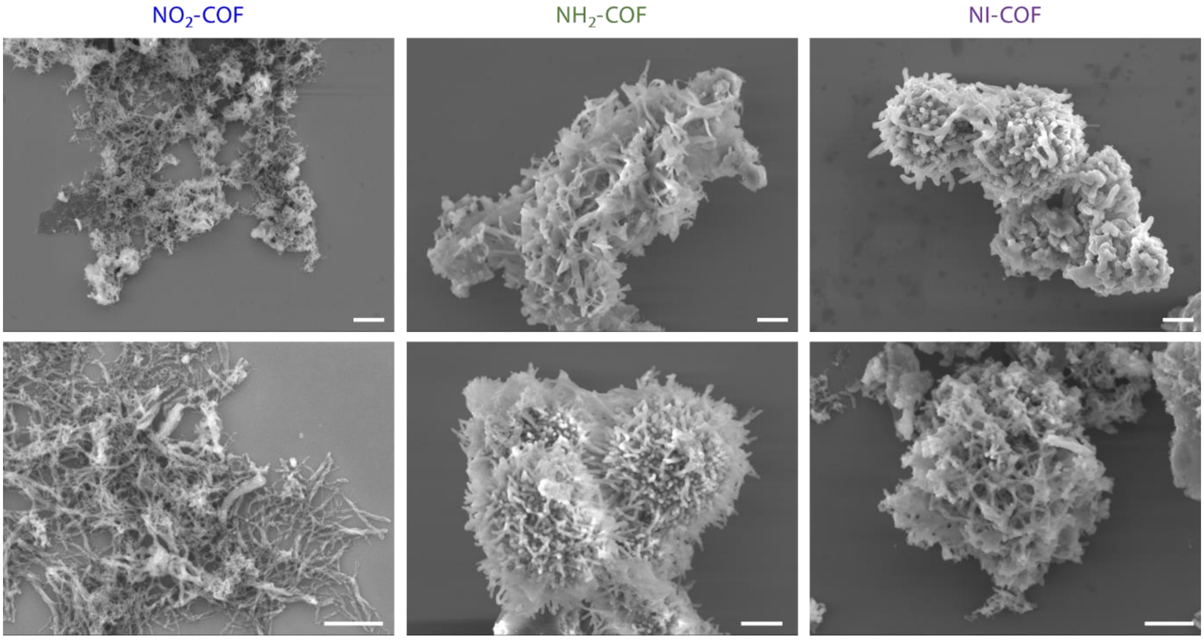


Figure S7. Morphology observed under SEM for **NO_2-COF**, **NH_2-COF**, and **NI-COF**. All scale bars represent 1 μm.

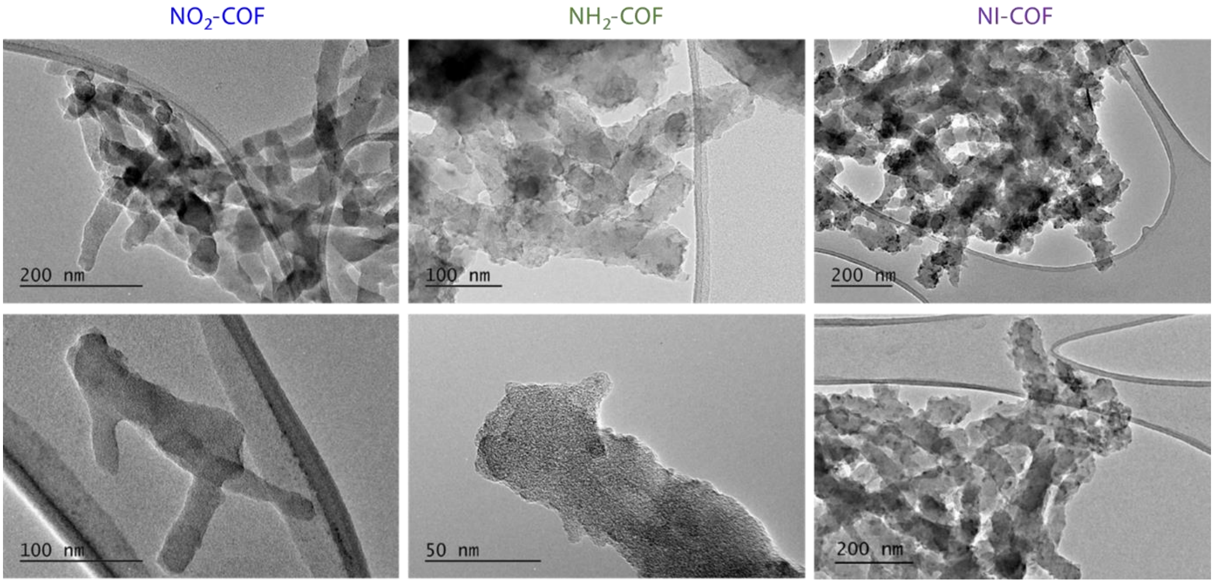


Figure S8. Morphology observed under TEM for **NO_2-COF**, **NH_2-COF**, and **NI-COF**.

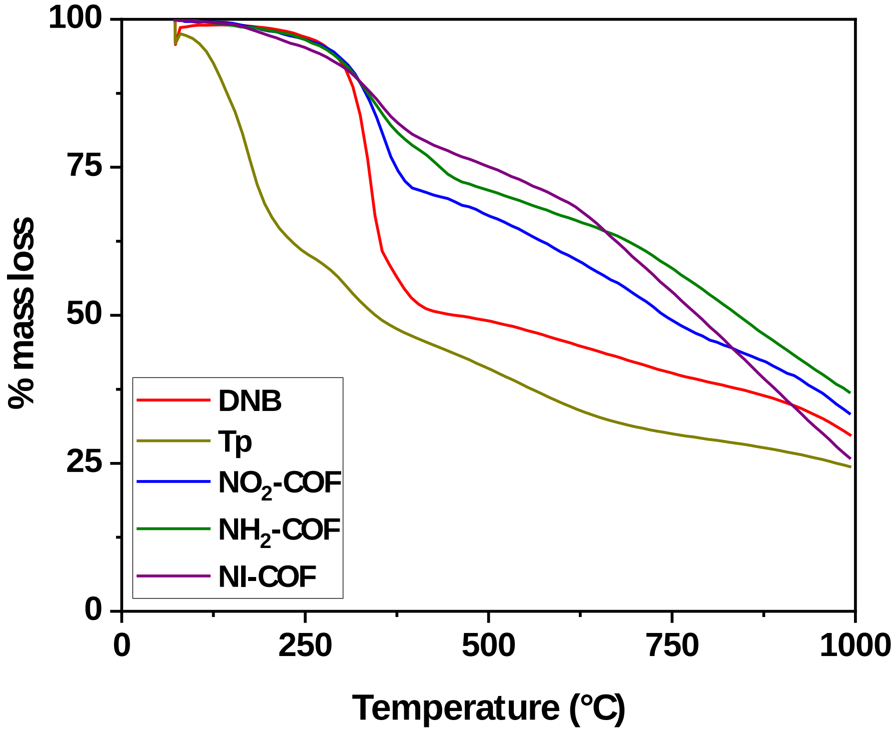


Figure S9. TGA profiles of both starting materials and the three COFs.

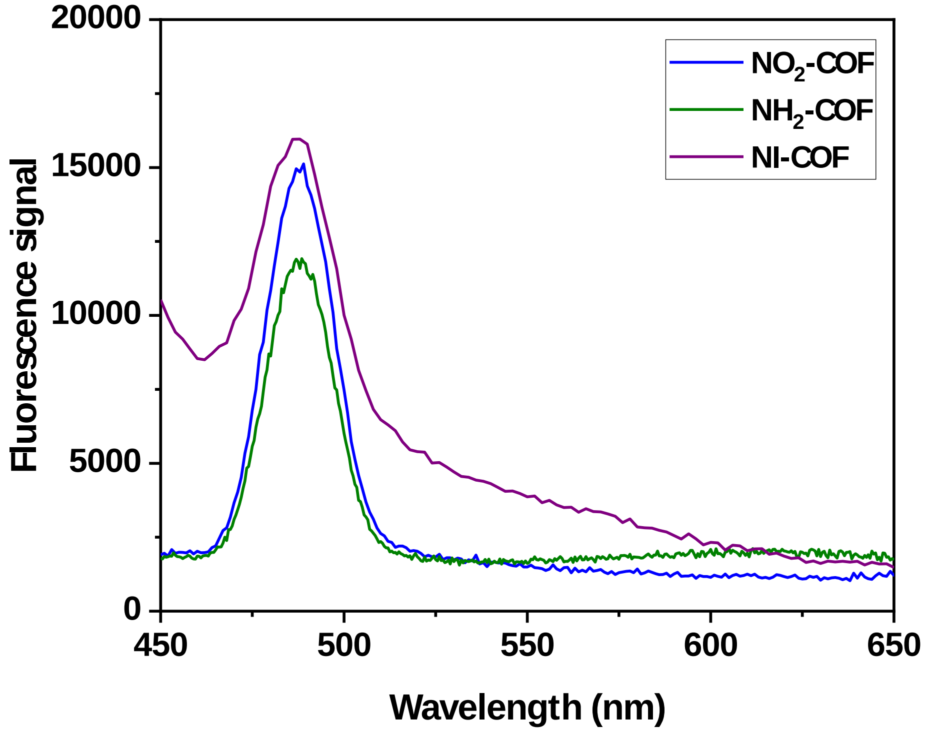


Figure S10. Emission spectra of **NI-COF**, **NH_2-COF**, and **NO_2-COF** in water upon excitation at 420 nm.

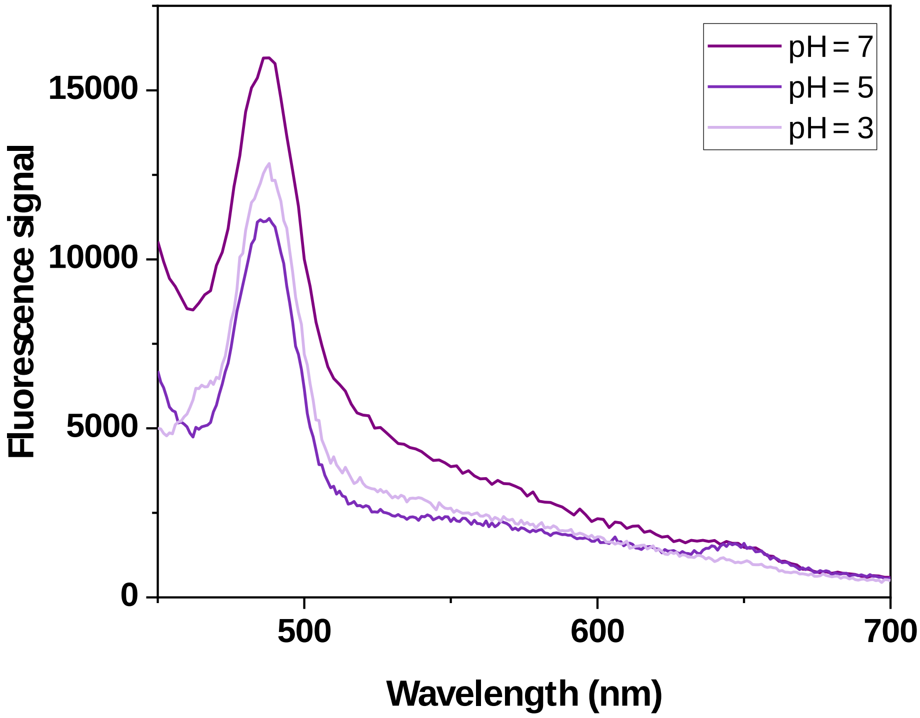


Figure S11. Emission spectra of **NI-COF** acquired at different pH levels (λ_{ex} = 420 nm).

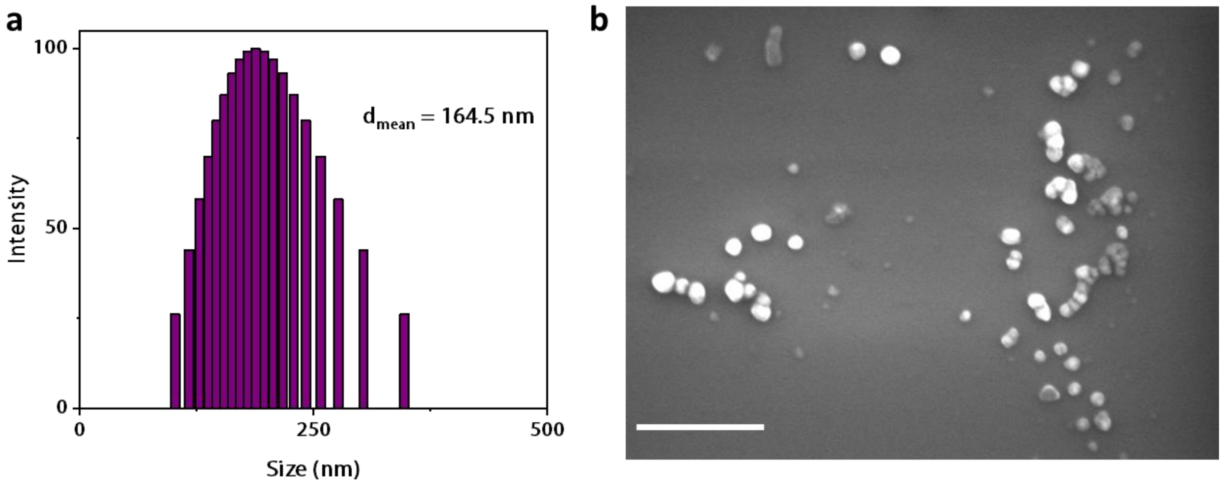


Figure S12. Particle size distribution of **NI-COF** in water measured by DLS (a), and imaged under SEM (b). Scale bar represents 1 µm.

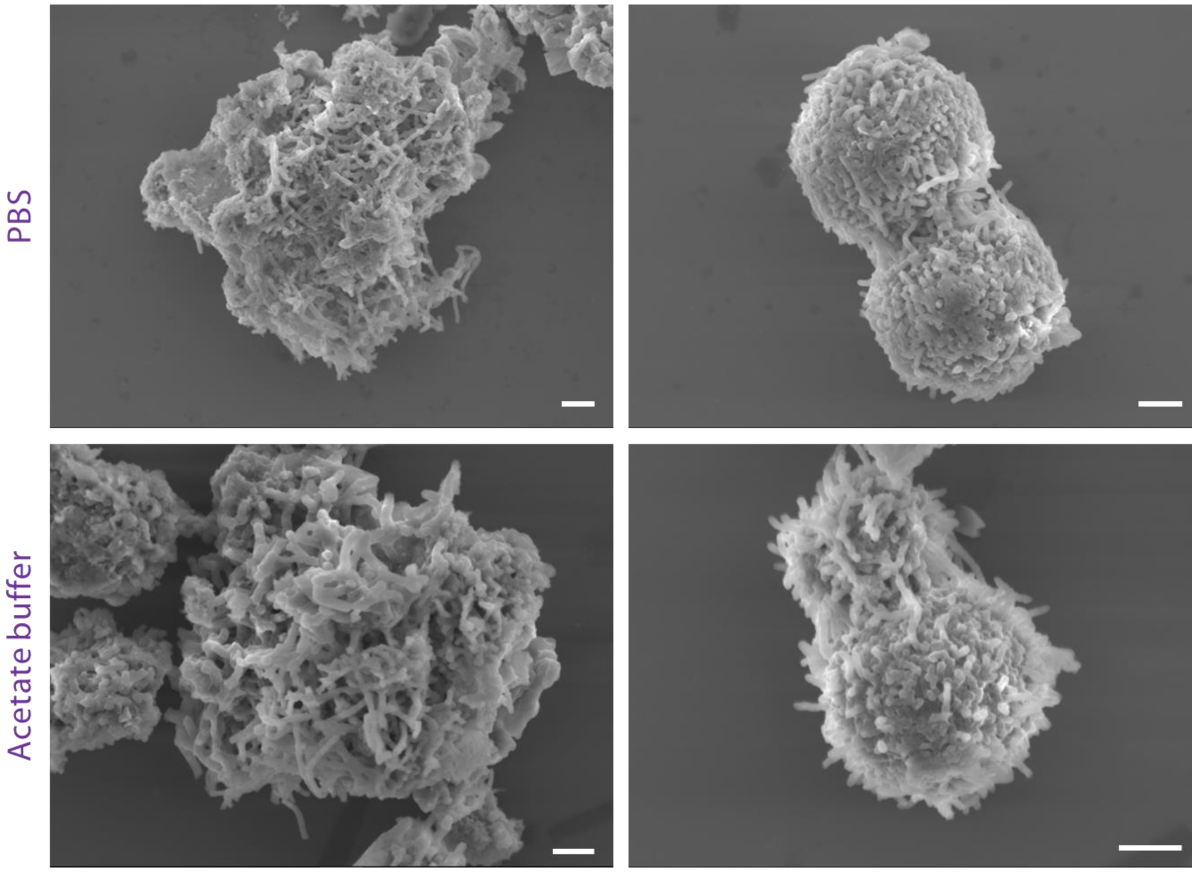


Figure S13. SEM micrographs of **NI-COF** following the stability tests in PBS and acetate buffers. All scale bars represent 1 µm.

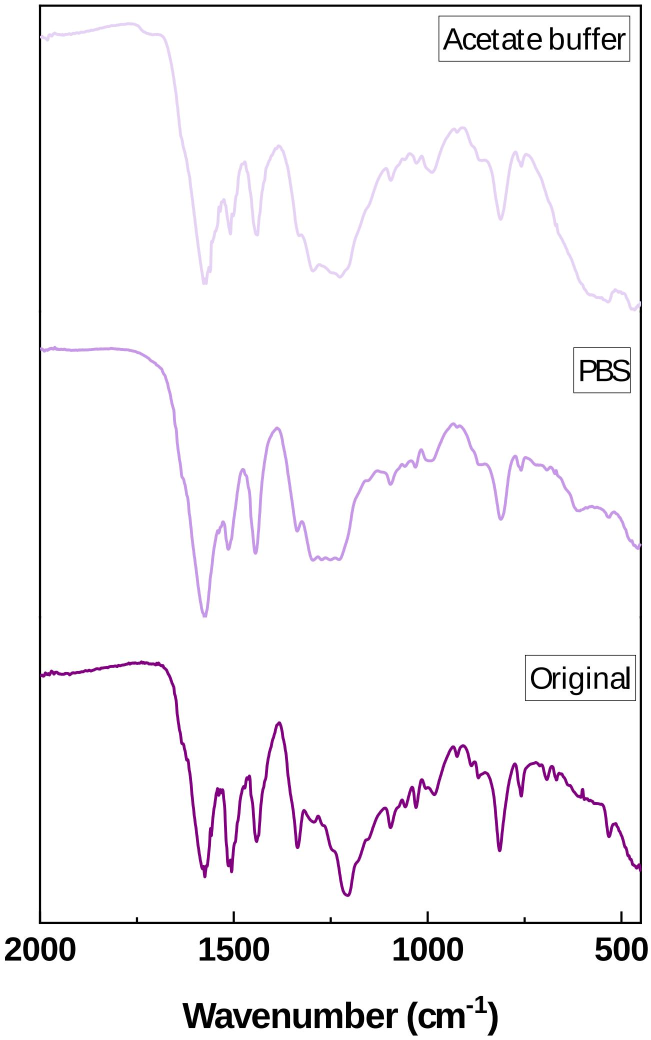


Figure S14. FT-IR spectrum of **NI-COF** following the stability tests in PBS and acetate buffers.

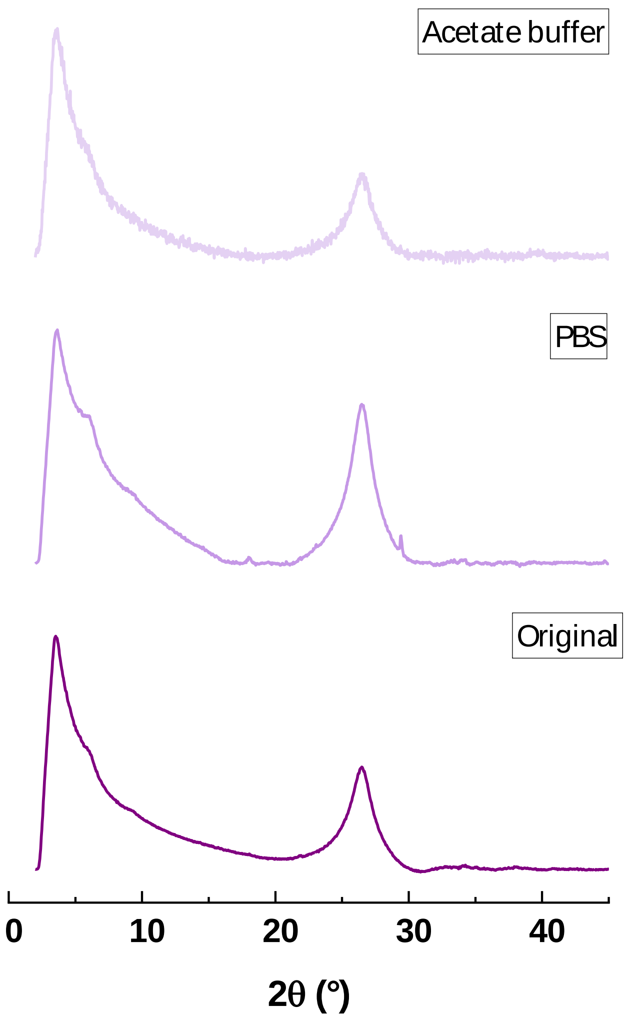


Figure S15. PXRD pattern of **NI-COF** following the stability tests in PBS and acetate buffers.

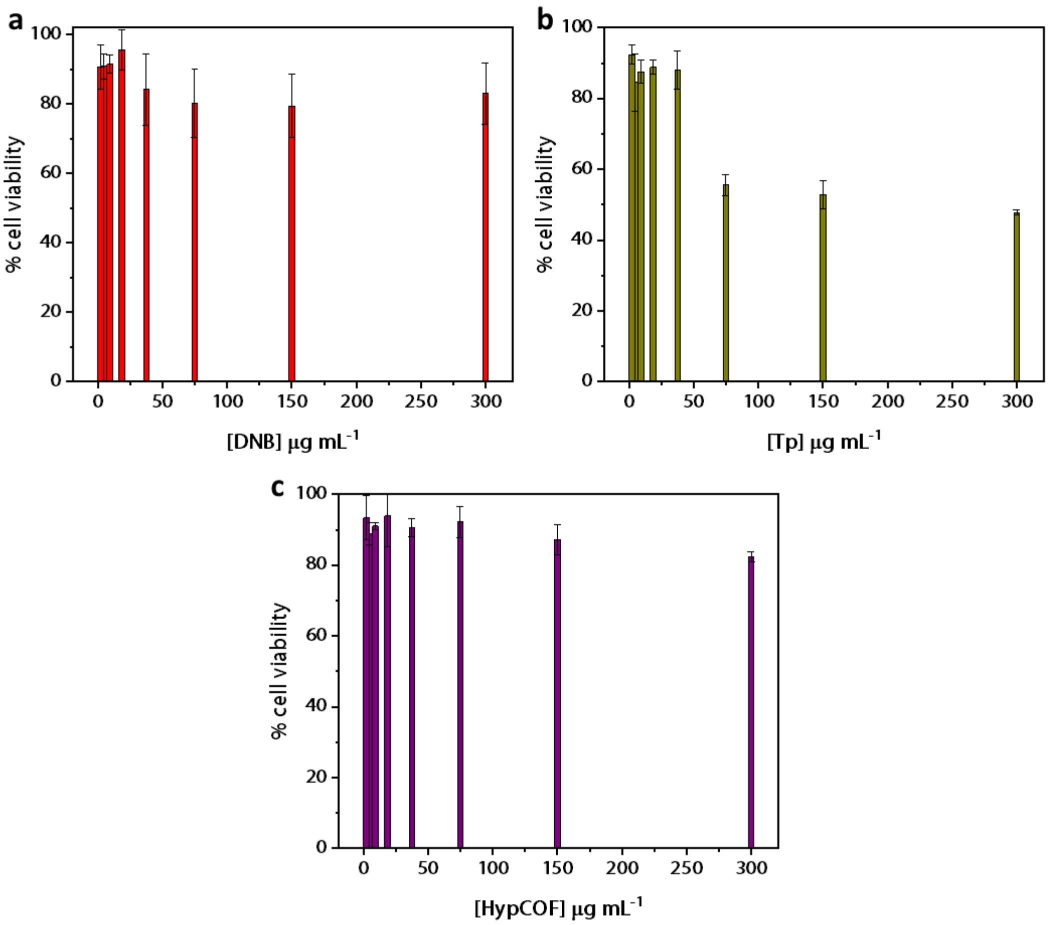


Figure S16. Cytotoxicity test results for a) 4,4'-dinitrobenzidine (DNB), b) 1,3,5-triformylphloroglucinol (Tp), and c) **NI-COF**. Results are expressed as means ± SD of three independent experiments.

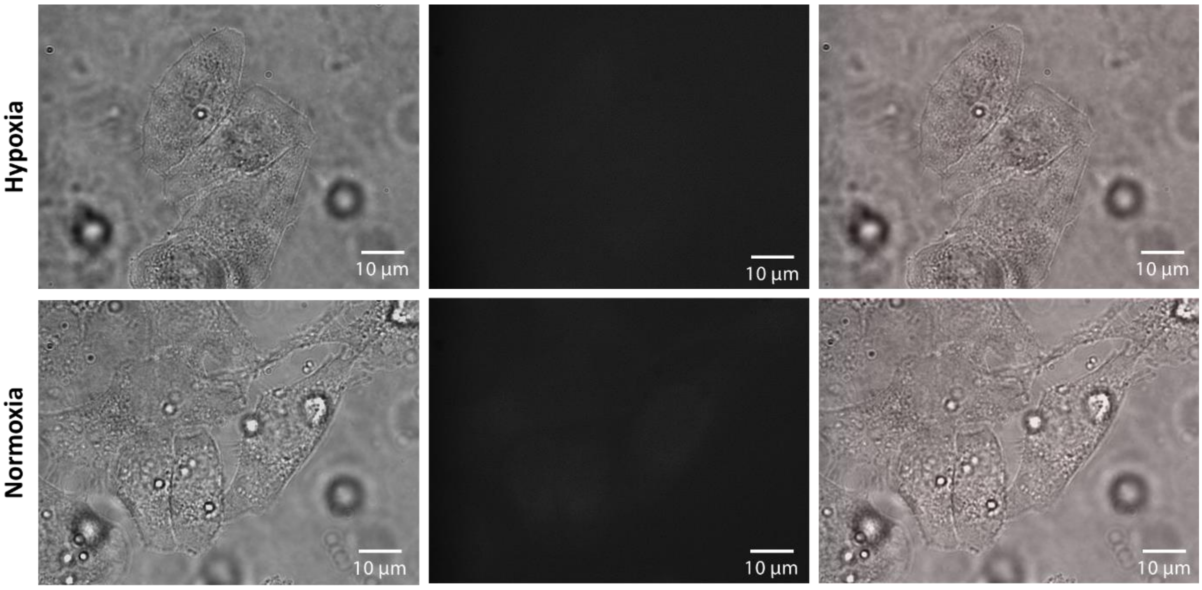


Figure S17. Fluorescence microscopy results for cells incubated under *severe* hypoxic (~0 % O_2; top) and normoxic (bottom) conditions. Images show brightfield, fluorescence and overlay of the two.

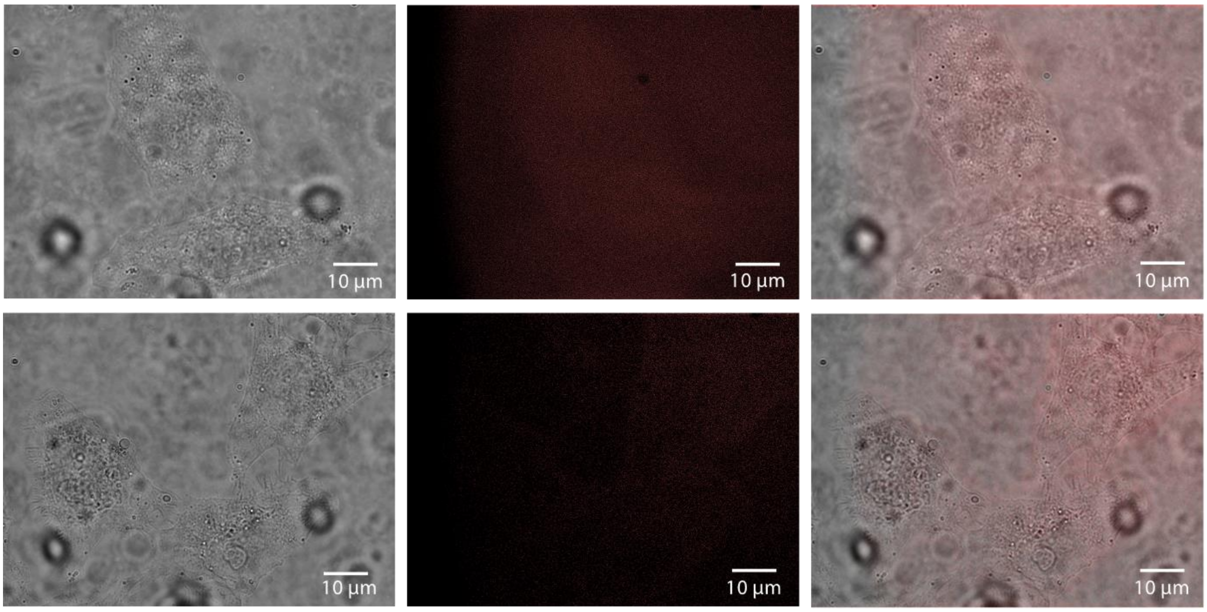


Figure S18. Fluorescence microscopy results for cells incubated under mild hypoxic (~5 % O_2; top) and normoxic (bottom) conditions. Images show brightfield, fluorescence and overlay of the two.

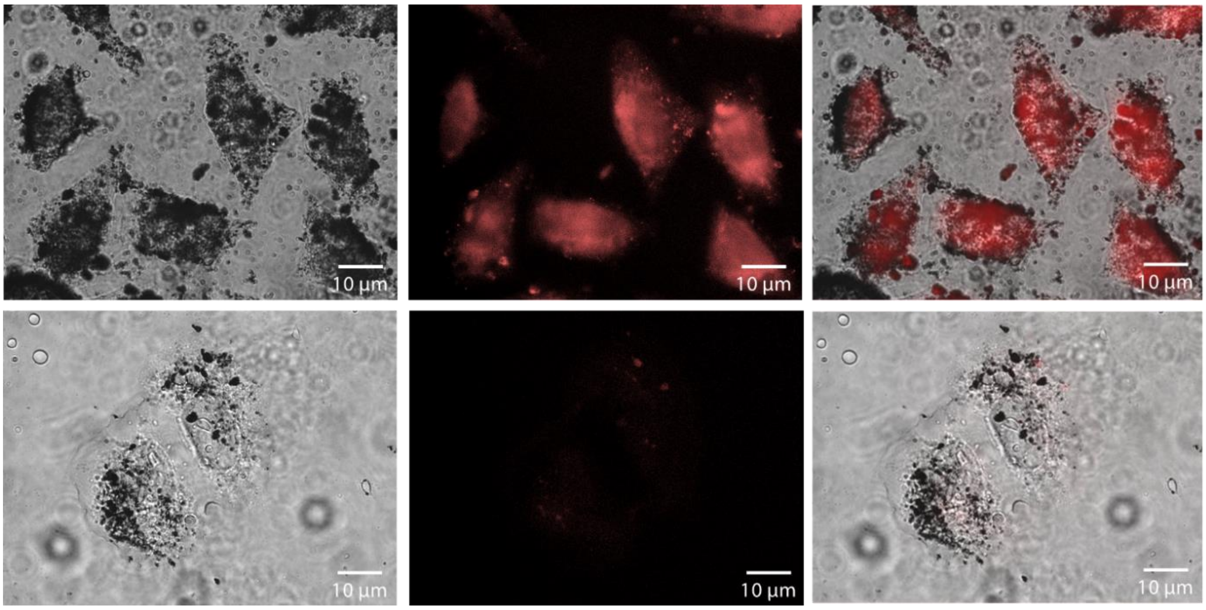


Figure S19. Fluorescence imaging results for *mild* hypoxia. The top row corresponds to HeLa cells incubated under hypoxia for 4 hours, the bottom row shows HeLa cells incubated under normoxia. [**NI-COF**] = 4 µg mL^{-1}, incubation time 60 minutes. Brightfield, fluorescence and overlay images are displayed.

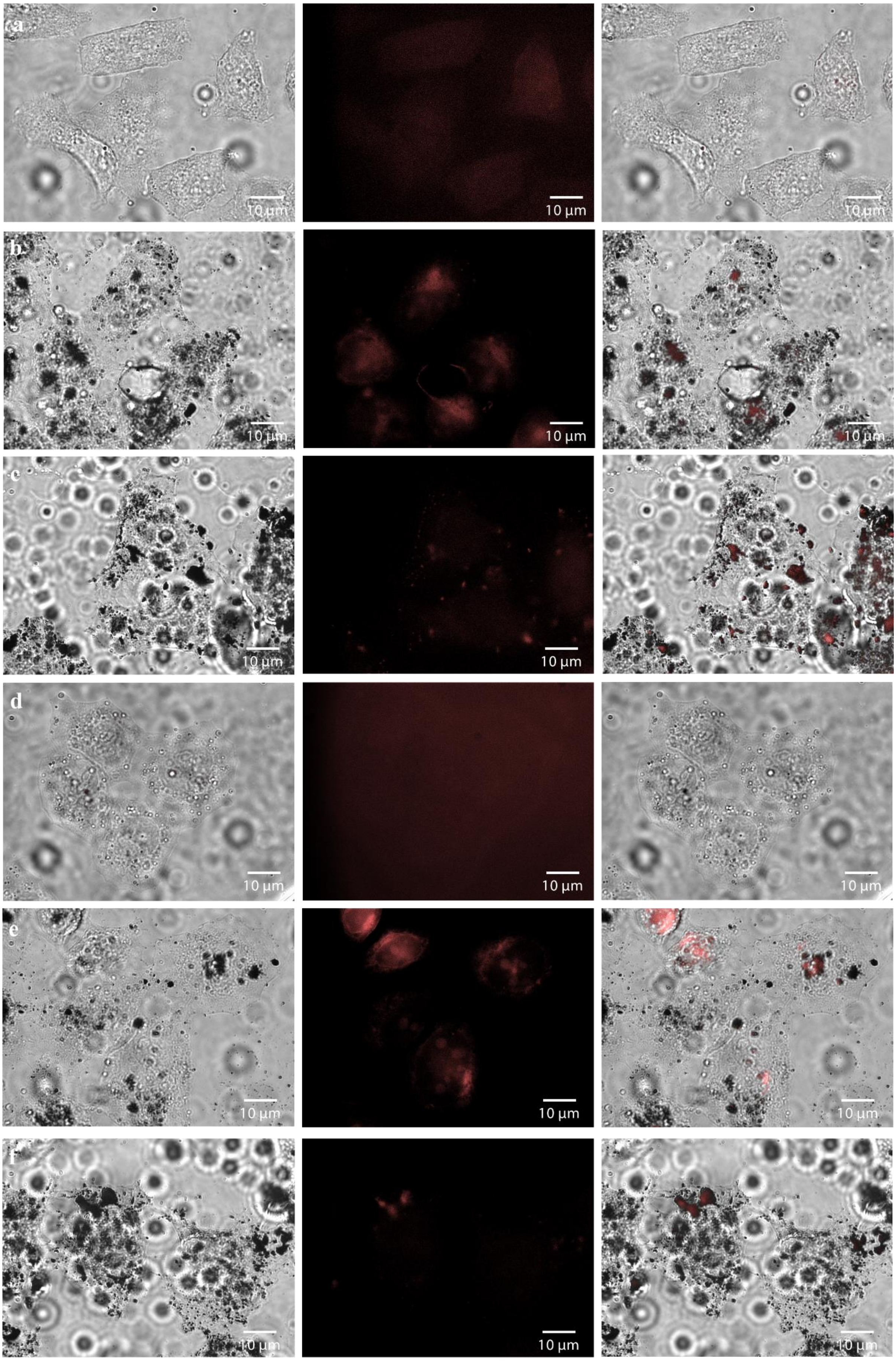

a
b
c
d
e
f
10 µm

Figure S20. Fluorescence imaging results for control experiments with **NO_2-COF** and **NH_2-COF**. HeLa cells incubated under a) normoxic conditions without any material, b) normoxic conditions with [**NO_2-COF**] = 4 μg mL^{-1}, c) normoxic conditions with [**NH_2-COF**] = 4 μg mL^{-1}, d) hypoxic conditions without any material, e) hypoxic conditions with [**NO_2-COF**] = 4 μg mL^{-1}, and f) hypoxic conditions with [**NH_2-COF**] = 4 μg mL^{-1}. In all cases, exposure to hypoxic/normoxic conditions for 4 hours, COF incubation time 60 minutes. Brightfield, fluorescence and overlay images are displayed.

Table S1. Fractional atomic coordinates of the unit cell of **NO_2-COF** in eclipsed AA conformation.

NO_2-COF in eclipsed AA conformation (Space group *P*1)											
a = 28.35, b = 28.64, c = 3.38; α = 89.70°, β = 90.0°, γ = 120.17°											
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C1	1.0238	-0.48194	-0.01182	**C41**	1.68419	-0.61336	-0.01182	**H81**	1.45427	-0.20628	-0.01182
C2	1.0578	-0.5025	-0.01182	**O42**	1.55464	-0.73578	-0.01182	**H82**	1.40835	-0.56984	-0.01182
C3	1.11242	-0.46842	-0.01182	**O43**	1.70482	-0.55872	-0.01182	**H83**	1.54656	-0.40693	-0.01182
C4	1.13305	-0.41378	-0.01182	**C44**	1.77306	-0.59998	-0.01182	**H84**	1.48406	-0.36911	-0.01182
C5	1.09905	-0.39323	-0.01182	**O45**	1.73181	-0.70925	-0.01182	**H85**	1.44785	-0.59369	-0.01182
C6	1.04443	-0.42731	-0.01182	**C46**	1.62288	-0.77704	-0.01182	**H86**	1.51035	-0.6315	-0.01182
N7	1.18735	-0.38008	-0.01182	**N47**	1.80706	-0.62054	-0.01182	**H87**	1.58605	-0.43078	-0.01182
C8	1.22135	-0.40063	-0.01182	**N48**	1.56826	-0.81112	-0.01182	**H88**	1.66072	-0.5445	-0.01182
C9	1.27622	-0.3667	-0.01182	**C49**	1.54737	-0.8658	-0.012	**H89**	1.54984	-0.65535	-0.01182
C10	1.31022	-0.38726	-0.01182	**C50**	1.49279	-0.9001	-0.01193	**H90**	1.79026	-0.55426	-0.01182
C11	1.36484	-0.35318	-0.01182	**C51**	1.47243	-0.9547	-0.01175	**H91**	1.65135	-0.7943	-0.01182
C12	1.38546	-0.29854	-0.01182	**C52**	1.50665	-0.97498	-0.01163	**H92**	1.79028	-0.66506	-0.01182
C13	1.35147	-0.27799	-0.01182	**C53**	1.56124	-0.94068	-0.0117	**H93**	1.54049	-0.79438	-0.01167
C14	1.29659	-0.31192	-0.01182	**C54**	1.58159	-0.88608	-0.01188	**H94**	1.42673	-0.98335	-0.01169
O15	1.2626	-0.29136	-0.01182	**C55**	1.44677	-0.13486	-0.01182	**H95**	1.58989	-0.95772	-0.01161
C16	1.37184	-0.2232	-0.01182	**C56**	1.86168	-0.58646	-0.01182	**H96**	1.62729	-0.85743	-0.01194
O17	1.44009	-0.26446	-0.01182	**C57**	1.50164	-0.10093	-0.01182	**H97**	1.56771	-0.01745	-0.01182
C18	1.39884	-0.37373	-0.01182	**C58**	1.52202	-0.04615	-0.01182	**H98**	1.40487	-0.04248	-0.01182
O19	1.28959	-0.44189	-0.01182	**C59**	1.48802	-0.02559	-0.01182	**H99**	1.36704	-0.14278	-0.01182
N20	1.37821	-0.42837	-0.01182	**C60**	1.4334	-0.05967	-0.01182	**H100**	1.97883	-0.59013	-0.01182
C21	1.41221	-0.44892	-0.01182	**C61**	1.41277	-0.11431	-0.01182	**H101**	1.95416	-0.45201	-0.01182
N22	1.42671	-0.18927	-0.01182	**C62**	1.89568	-0.60701	-0.01182	**H102**	1.85378	-0.51463	-0.01182
C23	1.39159	-0.50356	-0.01182	**C63**	1.9503	-0.57293	-0.01182	**O103**	1.31375	-0.59016	-0.02048
C24	1.42558	-0.52411	-0.01182	**C64**	1.97093	-0.5183	-0.01182	**O104**	1.30488	-0.51824	0.01321
C25	1.48021	-0.49003	-0.01182	**C65**	1.93693	-0.49774	-0.01182	**O105**	1.40788	-0.90949	-0.00838
C26	1.50083	-0.4354	-0.01182	**C66**	1.88231	-0.53182	-0.01182	**O106**	1.47763	-0.82675	-0.00598
C27	1.46683	-0.41484	-0.01182	**N67**	1.33713	-0.5382	-0.0061	**O107**	1.5133	-0.17606	-0.00252
C28	1.5142	-0.51059	-0.01182	**N68**	1.46052	-0.87786	-0.01407	**O108**	1.58573	-0.09589	0.01156
C29	1.49358	-0.56522	-0.01182	**N69**	1.53393	-0.12385	-0.00735	**O109**	1.6929	-0.47769	-0.02293
C30	1.52758	-0.58577	-0.01182	**N70**	1.65744	-0.46262	-0.01505	**O110**	1.6766	-0.41029	-0.00571
C31	1.5822	-0.55169	-0.01182	**N71**	1.12488	-0.33816	-0.01029	**O111**	1.17684	-0.30946	-0.01114
C32	1.60282	-0.49706	-0.01182	**N72**	1.87137	-0.66182	-0.01339	**O112**	1.09918	-0.31087	-0.00312
C33	1.56883	-0.4765	-0.01182	**H73**	1.04057	-0.54823	-0.01182	**O113**	1.90126	-0.68455	-0.00899
N34	1.6162	-0.57225	-0.01182	**H74**	1.14095	-0.48561	-0.01182	**O114**	1.81978	-0.69461	-0.02019
C35	1.59557	-0.62688	-0.01182	**H75**	1.0159	-0.41011	-0.01182	**C1**	2.0238	-0.48194	-0.01182
C36	1.62957	-0.64744	-0.01182	**H76**	1.20425	-0.33554	-0.01182	**C52**	1.50665	0.02502	-0.01163
C37	1.60926	-0.7017	-0.01182	**H77**	1.20412	-0.44636	-0.01182	**C59**	1.48802	-1.02559	-0.01182
C38	1.64351	-0.7224	-0.01182	**H78**	1.34314	-0.20621	-0.01182	**C64**	0.97093	-0.5183	-0.01182
C39	1.69781	-0.6887	-0.01182	**H79**	1.44456	-0.34523	-0.01182				
C40	1.71844	-0.63406	-0.01182	**H80**	1.33368	-0.45609	-0.01182				

Table S2. Fractional atomic coordinates of the unit cell of **NO_2-COF** in staggered AB conformation.

NO_2-COF in staggered AB conformation (Space group *P*1)											
a = 28.5, b = 28.5, c = 6.68; α = 90°, β = 90°, γ = 120°											
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
N1	0.05254	0.906	-0.78911	**H194**	0.33557	0.79056	-0.78003	**C113**	0.69356	0.39055	0.68738
C2	0.08662	0.88553	-0.78777	**H195**	0.2248	0.6796	-0.77776	**O114**	0.56424	0.26786	0.68742

C3	0.06608	0.83091	-0.78608	**H196**	0.46525	0.78107	-0.77749	**O115**	0.71401	0.44516	0.68738
C4	0.10015	0.81045	-0.78474	**H197**	0.32638	0.54062	-0.77086	**C116**	0.78256	0.40426	0.68736
C5	0.15476	0.84461	-0.7851	**H198**	0.4655	0.67038	-0.77336	**O117**	0.74166	0.29504	0.68737
C6	0.1753	0.89923	-0.78679	**H199**	0.2154	0.54032	-0.77272	**C118**	0.63279	0.22696	0.6874
C7	0.14123	0.91969	-0.78813	**H200**	0.10215	0.3521	-0.7676	**N119**	0.8167	0.38388	0.68735
C8	0.18884	0.82414	-0.78376	**H201**	0.26514	0.37721	-0.76579	**N120**	0.5782	0.19272	0.68742
C9	0.1683	0.76952	-0.78207	**H202**	0.30247	0.47724	-0.7689	**C121**	0.55748	0.13808	0.68733
C10	0.20237	0.74906	-0.78073	**H203**	0.07821	0.28852	-0.76563	**C122**	0.50293	0.10362	0.68738
C11	0.25698	0.78321	-0.78108	**H204**	0.04054	0.18824	-0.76253	**C123**	0.48275	0.04905	0.68748
C12	0.27752	0.83783	-0.78278	**H205**	0.2412	0.31362	-0.76382	**C124**	0.51713	0.02894	0.68753
C13	0.24344	0.8583	-0.78411	**H206**	0.12735	0.12487	-0.76377	**C125**	0.57168	0.0634	0.68748
N14	0.29105	0.76275	-0.77975	**H207**	0.65377	0.74525	-0.77298	**C126**	0.59186	0.11797	0.68738
C15	0.27052	0.70813	-0.77805	**H208**	0.6288	0.88316	-0.77855	**C127**	0.45374	0.86713	0.68743
C16	0.30459	0.68766	-0.77672	**H209**	0.52844	0.82041	-0.7779	**C128**	0.8713	0.41811	0.68734
C17	0.28406	0.63304	-0.77502	**H210**	0.71724	0.78496	-0.77339	**C129**	0.50858	0.90121	0.68742
C18	0.31838	0.61243	-0.77368	**H211**	0.81759	0.84771	-0.77404	**C130**	0.52878	0.95597	0.68741
C19	0.37299	0.64658	-0.77403	**H212**	0.69227	0.92288	-0.77896	**C131**	0.49463	0.97634	0.68742
C20	0.39352	0.7012	-0.77572	**H213**	0.88065	0.99776	-0.77858	**C132**	0.44003	0.94211	0.68744
C21	0.3592	0.72182	-0.77707	**H214**	0.88078	0.88706	-0.77445	**C133**	0.41959	0.8875	0.68744
O22	0.22945	0.59889	-0.77467	**H215**	1.0199	1.1276	-0.77648	**C134**	0.90545	0.39774	0.68733
O23	0.37974	0.77644	-0.77876	**H216**	1.1208	0.98848	-0.77529	**C135**	0.96004	0.43197	0.68732
C24	0.44813	0.73536	-0.77608	**O217**	-0.00649	0.74679	-0.78201	**C136**	0.98049	0.48658	0.68731
O25	0.40706	0.62612	-0.77269	**O218**	-0.02126	0.81423	-0.78163	**C137**	0.94634	0.50695	0.68732
C26	0.29784	0.55781	-0.77198	**O219**	0.36145	0.85093	-0.78035	**C138**	0.89175	0.47272	0.68733
N27	0.48221	0.7149	-0.77474	**O220**	0.35361	0.92251	-0.77891	**N139**	0.3455	0.46416	0.69032
N28	0.24323	0.52365	-0.77163	**O221**	0.08411	0.42343	-0.76666	**N140**	0.47051	0.12568	0.68632
C29	0.2227	0.46903	-0.76994	**O222**	0.15121	0.50545	-0.76895	**N141**	0.54102	0.87847	0.68964
C30	0.16841	0.43526	-0.76959	**O223**	0.18851	0.15976	-0.76981	**N142**	0.66615	0.54087	0.68578
C31	0.14787	0.38064	-0.7679	**O224**	0.2594	0.23935	-0.75772	**N143**	0.13202	0.66295	0.68828
C32	0.18195	0.36017	-0.76656	**O225**	0.58194	0.65528	-0.76812	**N144**	0.88131	0.34294	0.68655
C33	0.23655	0.39433	-0.76691	**O226**	0.50007	0.64187	-0.76671	**H145**	0.04838	0.45296	0.68754
C34	0.25677	0.44857	-0.7686	**O227**	0.84561	1.02725	-0.77835	**H146**	0.14871	0.51585	0.68752
C35	0.16141	0.30555	-0.76487	**O228**	0.76321	1.01154	-0.78302	**H147**	0.02311	0.59069	0.68755
C36	0.1068	0.2714	-0.76451	**N1**	1.05254	0.906	-0.78911	**H148**	0.21153	0.66588	0.6875
C37	0.08627	0.21678	-0.76282	**N41**	1.0998	1.14169	-0.75979	**H149**	0.21185	0.55528	0.6875
C38	0.12034	0.19631	-0.76148	**C63**	0.04819	0.11032	-0.77996	**H150**	0.35019	0.79551	0.68746
C39	0.17495	0.23047	-0.76184	**C65**	0.07527	0.96015	-0.7739	**H151**	0.45237	0.65717	0.68744
C40	0.19548	0.28509	-0.76353	**C73**	0.03132	0.51904	0.68755	**H152**	0.34172	0.54609	0.68747
N41	0.0998	0.14169	-0.75979	**C74**	0.06546	0.49867	0.68754	**H153**	0.46154	0.79588	0.68743
C42	0.5365	0.74867	-0.77509	**C75**	0.12006	0.5329	0.68752	**H154**	0.41699	0.43287	0.68745
C43	0.57057	0.72821	-0.77375	**C76**	0.14051	0.5875	0.68752	**H155**	0.55483	0.59601	0.68741
C44	0.62518	0.76237	-0.7741	**C77**	0.10636	0.60788	0.68753	**H156**	0.49205	0.6335	0.68743
C45	0.64571	0.81699	-0.77579	**C78**	0.05176	0.57365	0.68754	**H157**	0.45666	0.40923	0.68744
C46	0.61164	0.83745	-0.77713	**N79**	0.19478	0.62136	0.6875	**H158**	0.51944	0.37175	0.68743
C47	0.55703	0.80329	-0.77678	**C80**	0.22893	0.60098	0.6875	**H159**	0.59449	0.57237	0.68741
C48	0.70032	0.85114	-0.77615	**C81**	0.28378	0.63507	0.68748	**H160**	0.66977	0.45918	0.68739
C49	0.7344	0.83068	-0.77481	**C82**	0.31793	0.61469	0.68747	**H161**	0.55911	0.3481	0.68742
C50	0.789	0.86483	-0.77516	**C83**	0.37252	0.64892	0.68746	**H162**	0.7996	0.44996	0.68736
C51	0.80954	0.91945	-0.77686	**C84**	0.39297	0.70353	0.68745	**H163**	0.66139	0.20984	0.6874
C52	0.77547	0.93992	-0.7782	**C85**	0.35882	0.72391	0.68746	**H164**	0.80007	0.33938	0.68736
C53	0.72086	0.90576	-0.77784	**C86**	0.30397	0.68982	0.68748	**H165**	0.5503	0.20932	0.6875
N54	0.86383	0.95323	-0.7772	**O87**	0.26982	0.7102	0.68748	**H166**	0.43708	0.02027	0.68752
C55	0.8979	0.93277	-0.77587	**C88**	0.37901	0.77866	0.68745	**H167**	0.60046	0.04651	0.68752
C56	0.95251	0.96692	-0.77622	**O89**	0.44756	0.73776	0.68744	**H168**	0.63753	0.14675	0.68734
C57	0.98659	0.94646	-0.77488	**C90**	0.40667	0.62855	0.68745	**H169**	0.57444	0.98479	0.6874
C58	1.04119	0.98061	-0.77524	**O91**	0.29748	0.56008	0.68748	**H170**	0.41138	0.95915	0.68744
C59	1.06173	1.03523	-0.77693	**N92**	0.38622	0.57394	0.68746	**H171**	0.37388	0.85891	0.68745
C60	1.02766	1.0557	-0.77827	**C93**	0.42037	0.55356	0.68745	**H172**	0.9887	0.41493	0.68731
C61	0.97305	1.02154	-0.77791	**N94**	0.43386	0.81274	0.68744	**H173**	0.96342	0.55266	0.68731
O62	0.93898	1.04201	-0.77925	**C95**	0.39993	0.49895	0.68746	**H174**	0.86309	0.48977	0.68734
C63	1.04819	1.11032	-0.77996	**C96**	0.43407	0.47858	0.68745	**O175**	0.32979	0.41587	0.6873
O64	1.11634	1.06939	-0.77728	**C97**	0.48867	0.51281	0.68743	**O176**	0.31731	0.48499	0.68839
C65	1.07527	0.96015	-0.7739	**C98**	0.50912	0.56742	0.68743	**O177**	0.4221	0.09464	0.68642
O66	0.96605	0.89184	-0.77319	**C99**	0.47497	0.58779	0.68743	**O178**	0.49285	0.1746	0.69307
N67	0.00824	0.79473	-0.78571	**C100**	0.52282	0.49243	0.68742	**O179**	0.51774	0.82926	0.68374
N68	0.33504	0.87364	-0.78314	**C101**	0.50237	0.43783	0.68743	**O180**	0.58968	0.90853	0.68977
N69	0.13201	0.45655	-0.771	**C102**	0.53652	0.41745	0.68742	**O181**	0.69417	0.51923	0.68879
N70	0.21102	0.2088	-0.76042	**C103**	0.59112	0.45168	0.68741	**O182**	0.68273	0.58941	0.6888
N71	0.54913	0.67073	-0.77196	**C104**	0.61156	0.50629	0.6874	**O183**	0.18083	0.6921	0.68874
N72	0.79691	0.99739	-0.77998	**C105**	0.57741	0.52667	0.68741	**O184**	0.09881	0.67788	0.68803
H187	0.00824	0.87846	-0.77988	**N106**	0.62526	0.43131	0.6874	**O185**	0.91353	0.32663	0.69109

H188	0.083	0.76474	-0.78333	**C107**	0.60482	0.3767	0.68741	**O186**	0.83223	0.31464	0.68234
H189	0.22102	0.92776	-0.78708	**C108**	0.63897	0.35632	0.6874	**C73**	1.03132	0.51904	0.68755
H190	0.15838	0.9654	-0.78955	**C109**	0.61884	0.30209	0.68741	**C124**	0.51713	1.02894	0.68753
H191	0.12258	0.74099	-0.78177	**C110**	0.65324	0.28156	0.6874	**C131**	0.49463	-0.02366	0.68742
H192	0.18522	0.70334	-0.77931	**C111**	0.70752	0.31542	0.68738	**C136**	-0.01951	0.48658	0.68731
H193	0.2606	0.90401	-0.78553	**C112**	0.72796	0.37003	0.68738				

Table S3. Fractional atomic coordinates of unit cell of **NH_2-COF** in eclipsed AA conformation.

NH_2-COF in eclipsed AA conformation (Space group *P*1)											
a = 28.40, b = 28.98, c = 3.39; α = 89.91°, β = 89.99°, γ = 119.96°											
Atom	**x**	**y**	**z**	**Atom**	**x**	**y**	**z**	**Atom**	**x**	**y**	**z**
C1	1.0238	-0.48194	-0.01182	**C41**	1.68419	-0.61336	-0.01182	**H81**	1.45427	-0.20628	-0.01182
C2	1.0578	-0.5025	-0.01182	**O42**	1.55464	-0.73578	-0.01182	**H82**	1.40835	-0.56984	-0.01182
C3	1.11242	-0.46842	-0.01182	**O43**	1.70482	-0.55872	-0.01182	**H83**	1.54656	-0.40693	-0.01182
C4	1.13305	-0.41378	-0.01182	**C44**	1.77306	-0.59998	-0.01182	**H84**	1.48406	-0.36911	-0.01182
C5	1.09905	-0.39323	-0.01182	**O45**	1.73181	-0.70925	-0.01182	**H85**	1.44785	-0.59369	-0.01182
C6	1.04443	-0.42731	-0.01182	**C46**	1.62288	-0.77704	-0.01182	**H86**	1.51035	-0.6315	-0.01182
N7	1.18735	-0.38008	-0.01182	**N47**	1.80706	-0.62054	-0.01182	**H87**	1.58605	-0.43078	-0.01182
C8	1.22135	-0.40063	-0.01182	**N48**	1.56826	-0.81112	-0.01182	**H88**	1.66072	-0.5445	-0.01182
C9	1.27622	-0.3667	-0.01182	**C49**	1.54737	-0.8658	-0.012	**H89**	1.54984	-0.65535	-0.01182
C10	1.31022	-0.38726	-0.01182	**C50**	1.49279	-0.9001	-0.01193	**H90**	1.79026	-0.55426	-0.01182
C11	1.36484	-0.35318	-0.01182	**C51**	1.47243	-0.9547	-0.01175	**H91**	1.65135	-0.7943	-0.01182
C12	1.38546	-0.29854	-0.01182	**C52**	1.50665	-0.97498	-0.01163	**H92**	1.79028	-0.66506	-0.01182
C13	1.35147	-0.27799	-0.01182	**C53**	1.56124	-0.94068	-0.0117	**H93**	1.54049	-0.79438	-0.01167
C14	1.29659	-0.31192	-0.01182	**C54**	1.58159	-0.88608	-0.01188	**H94**	1.42673	-0.98335	-0.01169
O15	1.2626	-0.29136	-0.01182	**C55**	1.44677	-0.13486	-0.01182	**H95**	1.58989	-0.95772	-0.01161
C16	1.37184	-0.2232	-0.01182	**C56**	1.86168	-0.58646	-0.01182	**H96**	1.62729	-0.85743	-0.01194
O17	1.44009	-0.26446	-0.01182	**C57**	1.50164	-0.10093	-0.01182	**H97**	1.56771	-0.01745	-0.01182
C18	1.39884	-0.37373	-0.01182	**C58**	1.52202	-0.04615	-0.01182	**H98**	1.40487	-0.04248	-0.01182
O19	1.28959	-0.44189	-0.01182	**C59**	1.48802	-0.02559	-0.01182	**H99**	1.36704	-0.14278	-0.01182
N20	1.37821	-0.42837	-0.01182	**C60**	1.4334	-0.05967	-0.01182	**H100**	1.97883	-0.59013	-0.01182
C21	1.41221	-0.44892	-0.01182	**C61**	1.41277	-0.11431	-0.01182	**H101**	1.95416	-0.45201	-0.01182
N22	1.42671	-0.18927	-0.01182	**C62**	1.89568	-0.60701	-0.01182	**H102**	1.85378	-0.51463	-0.01182
C23	1.39159	-0.50356	-0.01182	**C63**	1.9503	-0.57293	-0.01182	**H103**	1.3199	-0.58258	-0.02332
C24	1.42558	-0.52411	-0.01182	**C64**	1.97093	-0.5183	-0.01182	**H104**	1.30345	-0.5294	0.01409
C25	1.48021	-0.49003	-0.01182	**C65**	1.93693	-0.49774	-0.01182	**H105**	1.41596	-0.90189	-0.00544
C26	1.50083	-0.4354	-0.01182	**C66**	1.88231	-0.53182	-0.01182	**H106**	1.47526	-0.8339	-0.00596
C27	1.46683	-0.41484	-0.01182	**N67**	1.33713	-0.5382	-0.0061	**H107**	1.5201	-0.16409	-0.00258
C28	1.5142	-0.51059	-0.01182	**N68**	1.46052	-0.87786	-0.01407	**H108**	1.57396	-0.10221	0.0064
C29	1.49358	-0.56522	-0.01182	**N69**	1.53393	-0.12385	-0.00735	**H109**	1.6919	-0.47031	-0.01555
C30	1.52758	-0.58577	-0.01182	**N70**	1.65744	-0.46262	-0.01505	**H110**	1.67985	-0.41891	-0.00171
C31	1.5822	-0.55169	-0.01182	**N71**	1.12488	-0.33816	-0.01029	**H111**	1.16912	-0.31081	-0.01114
C32	1.60282	-0.49706	-0.01182	**N72**	1.87137	-0.66182	-0.01339	**H112**	1.10605	-0.31161	-0.00349
C33	1.56883	-0.4765	-0.01182	**H73**	1.04057	-0.54823	-0.01182	**H113**	1.89314	-0.68475	-0.00439
N34	1.6162	-0.57225	-0.01182	**H74**	1.14095	-0.48561	-0.01182	**H114**	1.82872	-0.69461	-0.01659
C35	1.59557	-0.62688	-0.01182	**H75**	1.0159	-0.41011	-0.01182	**C1**	2.0238	-0.48194	-0.01182
C36	1.62957	-0.64744	-0.01182	**H76**	1.20425	-0.33554	-0.01182	**C52**	1.50665	0.02502	-0.01163
C37	1.60926	-0.7017	-0.01182	**H77**	1.20412	-0.44636	-0.01182	**C59**	1.48802	-1.02559	-0.01182
C38	1.64351	-0.7224	-0.01182	**H78**	1.34314	-0.20621	-0.01182	**C64**	0.97093	-0.5183	-0.01182
C39	1.69781	-0.6887	-0.01182	**H79**	1.44456	-0.34523	-0.01182				
C40	1.71844	-0.63406	-0.01182	**H80**	1.33368	-0.45609	-0.01182				

Table S4. Fractional atomic coordinates of the unit cell of **NH_2-COF** in staggered AB conformation.

NH_2-COF in staggered AB conformation (Space group *P*1)											
a = 28.5, b = 28.5, c = 6.68; α = 90°, β = 90°, γ = 120°											
Atom	**x**	**y**	**z**	**Atom**	**x**	**y**	**z**	**Atom**	**x**	**y**	**z**
N1	0.05254	0.906	-0.78911	**H194**	0.33557	0.79056	-0.78003	**C113**	0.69356	0.39055	0.68738
C2	0.08662	0.88553	-0.78777	**H195**	0.2248	0.6796	-0.77776	**O114**	0.56424	0.26786	0.68742
C3	0.06608	0.83091	-0.78608	**H196**	0.46525	0.78107	-0.77749	**O115**	0.71401	0.44516	0.68738
C4	0.10015	0.81045	-0.78474	**H197**	0.32638	0.54062	-0.77086	**C116**	0.78256	0.40426	0.68736
C5	0.15476	0.84461	-0.7851	**H198**	0.4655	0.67038	-0.77336	**O117**	0.74166	0.29504	0.68737
C6	0.1753	0.89923	-0.78679	**H199**	0.2154	0.54032	-0.77272	**C118**	0.63279	0.22696	0.6874
C7	0.14123	0.91969	-0.78813	**H200**	0.10215	0.3521	-0.7676	**N119**	0.8167	0.38388	0.68735
C8	0.18884	0.82414	-0.78376	**H201**	0.26514	0.37721	-0.76579	**N120**	0.5782	0.19272	0.68742

C9	0.1683	0.76952	-0.78207	**H202**	0.30247	0.47724	-0.7689	**C121**	0.55748	0.13808	0.68733
C10	0.20237	0.74906	-0.78073	**H203**	0.07821	0.28852	-0.76563	**C122**	0.50293	0.10362	0.68738
C11	0.25698	0.78321	-0.78108	**H204**	0.04054	0.18824	-0.76253	**C123**	0.48275	0.04905	0.68748
C12	0.27752	0.83783	-0.78278	**H205**	0.2412	0.31362	-0.76382	**C124**	0.51713	0.02894	0.68753
C13	0.24344	0.8583	-0.78411	**H206**	0.12735	0.12487	-0.76377	**C125**	0.57168	0.0634	0.68748
N14	0.29105	0.76275	-0.77975	**H207**	0.65377	0.74525	-0.77298	**C126**	0.59186	0.11797	0.68738
C15	0.27052	0.70813	-0.77805	**H208**	0.6288	0.88316	-0.77855	**C127**	0.45374	0.86713	0.68743
C16	0.30459	0.68766	-0.77672	**H209**	0.52844	0.82041	-0.7779	**C128**	0.8713	0.41811	0.68734
C17	0.28406	0.63304	-0.77502	**H210**	0.71724	0.78496	-0.77339	**C129**	0.50858	0.90121	0.68742
C18	0.31838	0.61243	-0.77368	**H211**	0.81759	0.84771	-0.77404	**C130**	0.52878	0.95597	0.68741
C19	0.37299	0.64658	-0.77403	**H212**	0.69227	0.92288	-0.77896	**C131**	0.49463	0.97634	0.68742
C20	0.39352	0.7012	-0.77572	**H213**	0.88065	0.99776	-0.77858	**C132**	0.44003	0.94211	0.68744
C21	0.3592	0.72182	-0.77707	**H214**	0.88078	0.88706	-0.77445	**C133**	0.41959	0.8875	0.68744
O22	0.22945	0.59889	-0.77467	**H215**	1.0199	1.1276	-0.77648	**C134**	0.90545	0.39774	0.68733
O23	0.37974	0.77644	-0.77876	**H216**	1.1208	0.98848	-0.77529	**C135**	0.96004	0.43197	0.68732
C24	0.44813	0.73536	-0.77608	**H217**	-0.00976	0.75969	-0.78204	**C136**	0.98049	0.48658	0.68731
O25	0.40706	0.62612	-0.77269	**H218**	-0.01824	0.80196	-0.7816	**C137**	0.94634	0.50695	0.68732
C26	0.29784	0.55781	-0.77198	**H219**	0.36197	0.86036	-0.77989	**C138**	0.89175	0.47272	0.68733
N27	0.48221	0.7149	-0.77474	**H220**	0.35399	0.91475	-0.77923	**N139**	0.3455	0.46416	0.69032
N28	0.24323	0.52365	-0.77163	**H221**	0.09144	0.43365	-0.76562	**N140**	0.47051	0.12568	0.68632
C29	0.2227	0.46903	-0.76994	**H222**	0.14419	0.49612	-0.76992	**N141**	0.54102	0.87847	0.68964
C30	0.16841	0.43526	-0.76959	**H223**	0.19924	0.17014	-0.7685	**N142**	0.66615	0.54087	0.68578
C31	0.14787	0.38064	-0.7679	**H224**	0.25073	0.23119	-0.75875	**N143**	0.13202	0.66295	0.68828
C32	0.18195	0.36017	-0.76656	**H225**	0.57109	0.65156	-0.76902	**N144**	0.88131	0.34294	0.68655
C33	0.23655	0.39433	-0.76691	**H226**	0.50861	0.64399	-0.76602	**H145**	0.04838	0.45296	0.68754
C34	0.25677	0.44857	-0.7686	**H227**	0.83681	1.02443	-0.7784	**H146**	0.14871	0.51585	0.68752
C35	0.16141	0.30555	-0.76487	**H228**	0.77488	1.01568	-0.78295	**H147**	0.02311	0.59069	0.68755
C36	0.1068	0.2714	-0.76451	**N1**	1.05254	0.906	-0.78911	**H148**	0.21153	0.66588	0.6875
C37	0.08627	0.21678	-0.76282	**N41**	1.0998	1.14169	-0.75979	**H149**	0.21185	0.55528	0.6875
C38	0.12034	0.19631	-0.76148	**C63**	0.04819	0.11032	-0.77996	**H150**	0.35019	0.79551	0.68746
C39	0.17495	0.23047	-0.76184	**C65**	0.07527	0.96015	-0.7739	**H151**	0.45237	0.65717	0.68744
C40	0.19548	0.28509	-0.76353	**C73**	0.03132	0.51904	0.68755	**H152**	0.34172	0.54609	0.68747
N41	0.0998	0.14169	-0.75979	**C74**	0.06546	0.49867	0.68754	**H153**	0.46154	0.79588	0.68743
C42	0.5365	0.74867	-0.77509	**C75**	0.12006	0.5329	0.68752	**H154**	0.41699	0.43287	0.68745
C43	0.57057	0.72821	-0.77375	**C76**	0.14051	0.5875	0.68752	**H155**	0.55483	0.59601	0.68741
C44	0.62518	0.76237	-0.7741	**C77**	0.10636	0.60788	0.68753	**H156**	0.49205	0.6335	0.68743
C45	0.64571	0.81699	-0.77579	**C78**	0.05176	0.57365	0.68754	**H157**	0.45666	0.40923	0.68744
C46	0.61164	0.83745	-0.77713	**N79**	0.19478	0.62136	0.6875	**H158**	0.51944	0.37175	0.68743
C47	0.55703	0.80329	-0.77678	**C80**	0.22893	0.60098	0.6875	**H159**	0.59449	0.57237	0.68741
C48	0.70032	0.85114	-0.77615	**C81**	0.28378	0.63507	0.68748	**H160**	0.66977	0.45918	0.68739
C49	0.7344	0.83068	-0.77481	**C82**	0.31793	0.61469	0.68747	**H161**	0.55911	0.3481	0.68742
C50	0.789	0.86483	-0.77516	**C83**	0.37252	0.64892	0.68746	**H162**	0.7996	0.44996	0.68736
C51	0.80954	0.91945	-0.77686	**C84**	0.39297	0.70353	0.68745	**H163**	0.66139	0.20984	0.6874
C52	0.77547	0.93992	-0.7782	**C85**	0.35882	0.72391	0.68746	**H164**	0.80007	0.33938	0.68736
C53	0.72086	0.90576	-0.77784	**C86**	0.30397	0.68982	0.68748	**H165**	0.5503	0.20932	0.6875
N54	0.86383	0.95323	-0.7772	**O87**	0.26982	0.7102	0.68748	**H166**	0.43708	0.02027	0.68752
C55	0.8979	0.93277	-0.77587	**C88**	0.37901	0.77866	0.68745	**H167**	0.60046	0.04651	0.68752
C56	0.95251	0.96692	-0.77622	**O89**	0.44756	0.73776	0.68744	**H168**	0.63753	0.14675	0.68734
C57	0.98659	0.94646	-0.77488	**C90**	0.40667	0.62855	0.68745	**H169**	0.57444	0.98479	0.6874
C58	1.04119	0.98061	-0.77524	**O91**	0.29748	0.56008	0.68748	**H170**	0.41138	0.95915	0.68744
C59	1.06173	1.03523	-0.77693	**N92**	0.38622	0.57394	0.68746	**H171**	0.37388	0.85891	0.68745
C60	1.02766	1.0557	-0.77827	**C93**	0.42037	0.55356	0.68745	**H172**	0.9887	0.41493	0.68731
C61	0.97305	1.02154	-0.77791	**N94**	0.43386	0.81274	0.68744	**H173**	0.96342	0.55266	0.68731
O62	0.93898	1.04201	-0.77925	**C95**	0.39993	0.49895	0.68746	**H174**	0.86309	0.48977	0.68734
C63	1.04819	1.11032	-0.77996	**C96**	0.43407	0.47858	0.68745	**H175**	0.32771	0.42331	0.68747
O64	1.11634	1.06939	-0.77728	**C97**	0.48867	0.51281	0.68743	**H176**	0.31794	0.47611	0.68804
C65	1.07527	0.96015	-0.7739	**C98**	0.50912	0.56742	0.68743	**H177**	0.42939	0.10387	0.68724
O66	0.96605	0.89184	-0.77319	**C99**	0.47497	0.58779	0.68743	**H178**	0.48416	0.16593	0.69205
N67	0.00824	0.79473	-0.78571	**C100**	0.52282	0.49243	0.68742	**H179**	0.52761	0.83897	0.68474
N68	0.33504	0.87364	-0.78314	**C101**	0.50237	0.43783	0.68743	**H180**	0.58069	0.89949	0.68885
N69	0.13201	0.45655	-0.771	**C102**	0.53652	0.41745	0.68742	**H181**	0.69382	0.52849	0.68856
N70	0.21102	0.2088	-0.76042	**C103**	0.59112	0.45168	0.68741	**H182**	0.68395	0.58132	0.68913
N71	0.54913	0.67073	-0.77196	**C104**	0.61156	0.50629	0.6874	**H183**	0.17253	0.68836	0.68791
N72	0.79691	0.99739	-0.77998	**C105**	0.57741	0.52667	0.68741	**H184**	0.11167	0.68332	0.68928
H187	0.00824	0.87846	-0.77988	**N106**	0.62526	0.43131	0.6874	**H185**	0.90126	0.32196	0.68948
H188	0.083	0.76474	-0.78333	**C107**	0.60482	0.3767	0.68741	**H186**	0.84108	0.31816	0.68337
H189	0.22102	0.92776	-0.78708	**C108**	0.63897	0.35632	0.6874	**C73**	1.03132	0.51904	0.68755
H190	0.15838	0.9654	-0.78955	**C109**	0.61884	0.30209	0.68741	**C124**	0.51713	1.02894	0.68753
H191	0.12258	0.74099	-0.78177	**C110**	0.65324	0.28156	0.6874	**C131**	0.49463	-0.02366	0.68742
H192	0.18522	0.70334	-0.77931	**C111**	0.70752	0.31542	0.68738	**C136**	-0.01951	0.48658	0.68731
H193	0.2606	0.90401	-0.78553	**C112**	0.72796	0.37003	0.68738				

Table S5. Fractional atomic coordinates of the unit cell of **NI-COF** in eclipsed AA conformation.

NI-COF in eclipsed AA conformation (Space group *P*1)											
a = 28.0, b = 29.1, c = 3.37; α = 91.8°, β = 90.4°, γ = 119.4°											
Atoms	**X**	**Y**	**Z**	**Atoms**	**X**	**Y**	**Z**	**Atoms**	**X**	**Y**	**Z**
C1	1.02325	-0.48342	0	**C61**	1.41151	-0.11495	0	**H121**	1.44431	-0.34527	0
C2	1.0574	-0.5038	0	**C62**	1.89742	-0.60467	0	**H122**	1.33366	-0.45635	0
C3	1.112	-0.46956	0	**C63**	1.95201	-0.57044	0	**H123**	1.45302	-0.2071	0
C4	1.13212	-0.41533	0	**C64**	1.97214	-0.51621	0	**H124**	1.40895	-0.56957	0
C5	1.09797	-0.39496	0	**C65**	1.93799	-0.49584	0	**H125**	1.54677	-0.40642	0
C6	1.0437	-0.42882	0	**C66**	1.88371	-0.52969	0	**H126**	1.48399	-0.36894	0
N7	1.18672	-0.3811	0	**N67**	1.11842	-0.34035	0	**H127**	1.44862	-0.59321	0
C8	1.22087	-0.40147	0	**N68**	1.33728	-0.53772	0	**H128**	1.5114	-0.63069	0
C9	1.27571	-0.36739	0	**N69**	1.65811	-0.46191	0	**H129**	1.58644	-0.43006	0
C10	1.30987	-0.38776	0	**N70**	1.46073	-0.87802	0	**H130**	1.66172	-0.54325	0
C11	1.36446	-0.35353	0	**N71**	1.87697	-0.65928	0	**H131**	1.55107	-0.65433	0
C12	1.3849	-0.29892	0	**N72**	1.53466	-0.12161	0	**H132**	1.79156	-0.55246	0
C13	1.35075	-0.27855	0	**C73**	1.08427	-0.31998	0	**H133**	1.65349	-0.79242	0
C14	1.29591	-0.31263	0	**C74**	1.10471	-0.26537	0	**H134**	1.79204	-0.66304	0
O15	1.26176	-0.29226	0	**N75**	1.15795	-0.22693	0	**H135**	1.54227	-0.79311	0
C16	1.37095	-0.22379	0	**C76**	1.16152	-0.17754	0	**H136**	1.42898	-0.98175	0
O17	1.4395	-0.26469	0	**C77**	1.11052	-0.18561	0	**H137**	1.59209	-0.95633	0
C18	1.39861	-0.3739	0	**N78**	1.07526	-0.23988	0	**H138**	1.62958	-0.85608	0
O19	1.28942	-0.44237	0	**N79**	1.09694	-0.14581	0	**H139**	1.56637	-0.01766	0
N20	1.37817	-0.42851	0	**C80**	1.31715	-0.59195	0	**H140**	1.4033	-0.0433	0
C21	1.41232	-0.44888	0	**C81**	1.26256	-0.62619	0	**H141**	1.36581	-0.14355	0
N22	1.42547	-0.19008	0	**C82**	1.67855	-0.4073	0	**H142**	1.98067	-0.58748	0
C23	1.39187	-0.50349	0	**C83**	1.73283	-0.37344	0	**H143**	1.95506	-0.45013	0
C24	1.42602	-0.52386	0	**C84**	1.40613	-0.91225	0	**H144**	1.85519	-0.51249	0
C25	1.48062	-0.48963	0	**C85**	1.37198	-0.89188	0	**H145**	1.03856	-0.3486	0
C26	1.50106	-0.43502	0	**C86**	1.91112	-0.67965	0	**H146**	1.1894	-0.23904	0
C27	1.46691	-0.41465	0	**C87**	1.89068	-0.73426	0	**H147**	1.20293	-0.13913	0
C28	1.51477	-0.51	0	**N88**	1.22389	-0.61161	0	**O148**	1.04749	-0.15608	-0.06759
C29	1.49433	-0.56461	0	**C89**	1.17432	-0.65733	0	**O149**	1.13159	-0.09592	0.06789
C30	1.52848	-0.58498	0	**C90**	1.18233	-0.70061	0	**H150**	1.34588	-0.60891	0
C31	1.58307	-0.55075	0	**N91**	1.23663	-0.68148	0	**H151**	1.64996	-0.39019	0
C32	1.60352	-0.49614	0	**N92**	1.77175	-0.38817	0	**H152**	1.38909	-0.95795	0
C33	1.56936	-0.47577	0	**C93**	1.82107	-0.3423	0	**H153**	1.95683	-0.65103	0
N34	1.61722	-0.57112	0	**C94**	1.81306	-0.29902	0	**H154**	1.13603	-0.65411	0
C35	1.59678	-0.62573	0	**N95**	1.75876	-0.31815	0	**H155**	1.7598	-0.43169	0
C36	1.63093	-0.6461	0	**N96**	1.38687	-0.83848	0	**H156**	1.85955	-0.34519	0
C37	1.61049	-0.70071	0	**C97**	1.34112	-0.83497	0	**H157**	1.43044	-0.80706	0
C38	1.64489	-0.72124	0	**C98**	1.29788	-0.88617	0	**H158**	1.34407	-0.79358	0
C39	1.69948	-0.687	0	**N99**	1.31692	-0.9213	0	**H159**	1.80599	-0.76059	0
C40	1.71993	-0.63239	0	**N100**	1.83744	-0.7727	0	**H160**	1.79246	-0.86051	0
C41	1.68552	-0.61187	0	**C101**	1.83387	-0.82209	0	**H161**	1.6063	-0.04168	0
O42	1.55621	-0.73457	0	**C102**	1.88512	-0.81417	0	**H162**	1.56495	-0.19257	0
O43	1.70597	-0.55726	0	**N103**	1.92013	-0.75976	0	**H163**	1.65131	-0.20606	0
C44	1.77452	-0.59816	0	**C104**	1.58926	-0.08738	0	**O164**	1.76668	-0.13547	0.01105
O45	1.73363	-0.70738	0	**C105**	1.62341	-0.10775	0	**O165**	1.7879	-0.05028	0.00772
C46	1.62476	-0.77547	0	**N106**	1.60852	-0.16115	0	**O166**	1.15234	-0.7939	-0.00161
N47	1.80867	-0.61853	0	**C107**	1.65427	-0.16466	0	**O167**	1.09242	-0.76699	-0.00471
N48	1.57017	-0.8097	0	**C108**	1.69751	-0.11347	0	**O168**	1.90218	-0.23444	-0.00799
C49	1.54972	-0.86431	0	**N109**	1.67847	-0.07833	0	**O169**	1.84433	-0.2049	-0.00679
C50	1.49513	-0.89854	0	**N110**	1.75057	-0.09983	0	**O170**	1.20626	-0.9501	0.01132
C51	1.47469	-0.95315	0	**N111**	1.14292	-0.75353	0	**O171**	1.22922	-0.86398	-0.01106
C52	1.50884	-0.97352	0	**N112**	1.85247	-0.24611	0	**O172**	1.863	-0.90549	0.00896
C53	1.56343	-0.93929	0	**N113**	1.24482	-0.8998	0	**O173**	1.94847	-0.84153	0.00978
C54	1.58387	-0.88468	0	**N114**	1.89845	-0.85382	0	**H174**	1.2358	-0.5681	0
C55	1.44567	-0.13532	0	**H115**	1.04033	-0.5495	0	**C1**	2.02325	-0.48342	0
C56	1.86327	-0.5843	0	**H116**	1.14065	-0.48661	0	**C52**	1.50884	0.02648	0
C57	1.50051	-0.10124	0	**H117**	1.01517	-0.41161	0	**C59**	1.48655	-1.02611	0
C58	1.5207	-0.04648	0	**H118**	1.20331	-0.3366	0	**C64**	0.97214	-0.51621	0
C59	1.48655	-0.02611	0	**H119**	1.20379	-0.44718	0				
C60	1.43196	-0.06034	0	**H120**	1.34212	-0.20695	0				

Table S6. Fractional atomic coordinates of the unit cell of **NI-COF** in staggered AB conformation.

NI-COF in staggered AB conformation (Space group *P*1)											
a = 28.5, b = 28.5, c = 6.76; α = 90°, β = 90°, γ = 120°											
Atoms	**X**	**Y**	**Z**	**Atoms**	**X**	**Y**	**Z**	**Atoms**	**X**	**Y**	**Z**
C1	1.07817	-0.11487	0.68363	**H294**	1.85882	0.09561	0.68362	**C175**	0.41162	0.88523	0.22189
C2	1.05773	-0.1694	0.68363	**H295**	1.87245	0.19552	0.68362	**C176**	0.89752	0.39551	0.22189
C3	1.0919	-0.18984	0.68363	**O296**	1.71871	0.17435	0.68574	**C177**	0.95212	0.42974	0.22189
C4	1.14652	-0.15573	0.68363	**O297**	1.80325	0.23583	0.68446	**C178**	0.97224	0.48397	0.22189
C5	1.16696	-0.1012	0.68363	**H298**	2.11319	-0.01101	0.68362	**C179**	0.93809	0.50435	0.22189
C6	1.13279	-0.08076	0.68363	**H299**	2.00253	-0.12197	0.68361	**C180**	0.88382	0.47049	0.22189
C7	1.18069	-0.17616	0.68363	**H300**	1.0748	-0.23554	0.68363	**N181**	0.11852	0.65983	0.22189
C8	1.16025	-0.2307	0.68363	**H301**	1.21268	-0.07262	0.68363	**N182**	0.33739	0.46246	0.22189
C9	1.19442	-0.25113	0.68363	**H302**	1.14989	-0.03506	0.68363	**N183**	0.65822	0.53827	0.22189
C10	1.24866	-0.21708	0.68363	**H303**	1.11453	-0.25927	0.68363	**N184**	0.46083	0.12216	0.22189
C11	1.26911	-0.16255	0.68363	**H304**	1.17732	-0.29684	0.68363	**N185**	0.87708	0.3409	0.22189
C12	1.23531	-0.14206	0.68363	**H305**	1.25257	-0.09633	0.68363	**N186**	0.53477	0.87857	0.22189
N13	1.28284	-0.23752	0.68363	**H306**	1.32734	-0.20966	0.68363	**C187**	0.08437	0.6802	0.22189
C14	1.26239	-0.29205	0.68363	**H307**	1.21668	-0.32063	0.68363	**C188**	0.10482	0.73481	0.22189
C15	1.29657	-0.31248	0.68363	**H308**	1.45715	-0.21899	0.68363	**N189**	0.15805	0.77325	0.22189
C16	1.27597	-0.36742	0.68363	**H309**	1.31828	-0.45952	0.68363	**C190**	0.16163	0.82264	0.22189
C17	1.31015	-0.38785	0.68363	**H310**	1.20729	-0.45977	0.68363	**C191**	0.11063	0.81457	0.22189
C18	1.36477	-0.35375	0.68363	**H311**	1.4575	-0.32964	0.68363	**N192**	0.07537	0.76031	0.22189
C19	1.38536	-0.29881	0.68363	**H312**	1.09386	-0.64824	0.68363	**N193**	0.09704	0.85437	0.22189
C20	1.35119	-0.27838	0.68363	**H313**	1.25692	-0.62316	0.68363	**C194**	0.31726	0.40823	0.22189
O21	1.37163	-0.22384	0.68363	**H314**	1.29453	-0.52288	0.68363	**C195**	0.26267	0.37399	0.22189
C22	1.43998	-0.26471	0.68363	**H315**	1.07014	-0.71156	0.68363	**C196**	0.67866	0.59288	0.22189
O23	1.39894	-0.37418	0.68363	**H316**	1.03253	-0.81185	0.68363	**C197**	0.73294	0.62674	0.22189
C24	1.2897	-0.44238	0.68363	**H317**	1.2332	-0.68648	0.68363	**C198**	0.40624	0.08793	0.22189
O25	1.22135	-0.40152	0.68363	**H318**	1.64573	-0.25459	0.68362	**C199**	0.37209	0.1083	0.22189
N26	1.23508	-0.47649	0.68363	**H319**	1.62056	-0.11674	0.68362	**C200**	0.91123	0.32053	0.22189
C27	1.21464	-0.53102	0.68363	**H320**	1.52029	-0.17938	0.68363	**C201**	0.89079	0.26592	0.22189
N28	1.47415	-0.28514	0.68363	**H321**	1.70932	-0.21492	0.68362	**N202**	0.224	0.38857	0.22189
C29	1.16002	-0.56513	0.68363	**H322**	1.80959	-0.15228	0.68362	**C203**	0.17443	0.34285	0.22189
C30	1.13958	-0.61966	0.68363	**H323**	1.68415	-0.07707	0.68362	**C204**	0.18244	0.29957	0.22189
C31	1.17375	-0.64009	0.68363	**H324**	1.87282	-0.00195	0.68362	**N205**	0.23673	0.3187	0.22189
C32	1.22837	-0.60599	0.68363	**H325**	1.87264	-0.11269	0.68362	**N206**	0.77186	0.61201	0.22189
C33	1.24881	-0.55146	0.68363	**H326**	1.31559	-0.05677	0.68363	**C207**	0.82118	0.65788	0.22189
C34	1.15331	-0.69463	0.68363	**H327**	1.42501	-0.09826	0.68363	**C208**	0.81317	0.70116	0.22189
C35	1.09869	-0.72873	0.68363	**H328**	1.52521	-0.01216	0.68363	**N209**	0.75887	0.68203	0.22189
C36	1.07825	-0.78327	0.68363	**H329**	1.05459	-0.62444	0.68363	**N210**	0.38697	0.1617	0.22189
C37	1.11242	-0.8037	0.68363	**H330**	1.273	-0.71021	0.68363	**C211**	0.34123	0.16521	0.22189
C38	1.16704	-0.7696	0.68363	**H331**	1.00929	-0.45976	0.68363	**C212**	0.29799	0.11401	0.22189
C39	1.18748	-0.71506	0.68363	**H332**	1.23121	-0.86138	0.68363	**N213**	0.31702	0.07888	0.22189
C40	1.52839	-0.25109	0.68363	**H333**	1.3177	-0.875	0.68362	**N214**	0.83755	0.22748	0.22189
C41	1.56257	-0.27152	0.68362	**H334**	1.62186	-0.31828	0.68362	**C215**	0.83398	0.17809	0.22189
C42	1.61719	-0.23742	0.68362	**H335**	1.47091	-0.42767	0.68362	**C216**	0.88523	0.18601	0.22189
C43	1.63763	-0.18288	0.68362	**H336**	1.45728	-0.52758	0.68362	**N217**	0.92023	0.24042	0.22189
C44	1.60346	-0.16245	0.68362	**O337**	1.52645	-0.56729	0.68227	**C218**	0.58936	0.9128	0.22189
C45	1.54884	-0.19656	0.68363	**O338**	1.61148	-0.50646	0.6835	**C219**	0.62351	0.89243	0.22189
C46	1.69225	-0.14878	0.68362	**O339**	1.42893	-0.80425	0.68523	**N220**	0.60863	0.83903	0.22189
C47	1.72642	-0.16921	0.68362	**O340**	1.44843	-0.72033	0.68505	**C221**	0.65437	0.83552	0.22189
C48	1.78104	-0.13511	0.68362	**H341**	1.01124	-0.27518	0.68363	**C222**	0.69762	0.88672	0.22189
C49	1.80149	-0.08057	0.68362	**H342**	0.9017	-0.23373	0.68363	**N223**	0.67858	0.92185	0.22189
C50	1.76731	-0.06014	0.68362	**H343**	0.80186	-0.31999	0.68363	**N224**	0.75067	0.90035	0.22189
C51	1.71269	-0.09424	0.68362	**O344**	0.82267	-0.45305	0.70275	**N225**	0.14303	0.24665	0.22189
N52	1.8561	-0.04647	0.68362	**O345**	0.76267	-0.42856	0.66434	**N226**	0.85257	0.75408	0.22189
C53	1.8899	-0.06696	0.68362	**H346**	0.9633	-0.55253	0.68363	**N227**	0.24493	0.10038	0.22189
C54	1.94452	-0.03285	0.68362	**O347**	0.87342	-0.61218	0.6804	**N228**	0.89856	0.14636	0.22189
C55	1.97869	-0.05328	0.68362	**O348**	0.90532	-0.52577	0.68194	**H229**	0.04043	0.45068	0.22189
C56	2.03331	-0.01918	0.68362	**C1**	2.07817	-0.11487	0.68363	**H230**	0.14076	0.51358	0.22189
C57	2.05376	0.03535	0.68362	**C37**	2.11242	0.1963	0.68363	**H231**	0.01528	0.58857	0.22189
C58	2.01958	0.05579	0.68362	**N65**	1.09464	-0.85557	0.68362	**H232**	0.20342	0.66358	0.22189
C59	1.96496	0.02168	0.68362	**N66**	1.04704	-0.09415	0.68362	**H233**	0.2039	0.55301	0.22189
O60	1.93079	0.04211	0.68362	**C115**	0.02336	0.51676	0.22189	**H234**	0.34223	0.79323	0.22189
C61	2.04003	0.11032	0.68362	**C116**	0.05751	0.49638	0.22189	**H235**	0.44442	0.65491	0.22189
O62	2.10837	0.06946	0.68362	**C117**	0.1121	0.53062	0.22189	**H236**	0.33377	0.54383	0.22189
C63	2.06749	-0.03961	0.68362	**C118**	0.13223	0.58485	0.22189	**H237**	0.45312	0.79309	0.22189
O64	1.95825	-0.10782	0.68362	**C119**	0.09808	0.60522	0.22189	**H238**	0.40905	0.43061	0.22189
N65	2.09464	0.14443	0.68362	**C120**	0.0438	0.57137	0.22189	**H239**	0.54688	0.59376	0.22189

N66	2.04704	-0.09415	0.68362	**N121**	0.18682	0.61908	0.22189	**H240**	0.4841	0.63124	0.22189
N67	1.00311	-0.20351	0.68363	**C122**	0.22098	0.59871	0.22189	**H241**	0.44872	0.40697	0.22189
N68	1.32373	-0.12844	0.68363	**C123**	0.27582	0.63279	0.22189	**H242**	0.51151	0.36949	0.22189
N69	1.12585	-0.5447	0.68363	**C124**	0.30997	0.61242	0.22189	**H243**	0.58655	0.57012	0.22189
N70	1.20121	-0.79003	0.68363	**C125**	0.36457	0.64665	0.22189	**H244**	0.66183	0.45693	0.22189
N71	1.54197	-0.32646	0.68362	**C126**	0.38501	0.70126	0.22189	**H245**	0.55117	0.34585	0.22189
N72	1.78776	-0.0056	0.68362	**C127**	0.35086	0.72163	0.22189	**H246**	0.79167	0.44772	0.22189
C73	0.98266	-0.25804	0.68363	**C128**	0.29601	0.68755	0.22189	**H247**	0.6536	0.20776	0.22189
C74	0.92842	-0.29209	0.68363	**O129**	0.26186	0.70792	0.22189	**H248**	0.79215	0.33715	0.22189
N75	0.88966	-0.27728	0.68363	**C130**	0.37105	0.77639	0.22189	**H249**	0.54237	0.20708	0.22189
C76	0.84024	-0.32305	0.68363	**O131**	0.4396	0.73549	0.22189	**H250**	0.42908	0.01844	0.22189
C77	0.84808	-0.36643	0.68363	**C132**	0.39872	0.62628	0.22189	**H251**	0.59219	0.04385	0.22189
N78	0.90233	-0.34749	0.68363	**O133**	0.28953	0.55781	0.22189	**H252**	0.62969	0.1441	0.22189
N79	0.80875	-0.41934	0.68363	**N134**	0.37827	0.57167	0.22189	**H253**	0.56648	0.98252	0.22189
C80	1.34417	-0.07391	0.68363	**C135**	0.41242	0.5513	0.22189	**H254**	0.40341	0.95688	0.22189
C81	1.39879	-0.03981	0.68363	**N136**	0.42558	0.8101	0.22189	**H255**	0.36591	0.85663	0.22189
N82	1.43717	-0.05468	0.68363	**C137**	0.39198	0.49669	0.22189	**H256**	0.98077	0.4127	0.22189
C83	1.48697	-0.00885	0.68363	**C138**	0.42613	0.47632	0.22189	**H257**	0.95517	0.55005	0.22189
C84	1.4786	0.03407	0.68363	**C139**	0.48073	0.51055	0.22189	**H258**	0.85529	0.48769	0.22189
N85	1.42435	0.01514	0.68363	**C140**	0.50117	0.56516	0.22189	**H259**	0.03867	0.65158	0.22189
N86	1.51846	0.08744	0.68363	**C141**	0.46702	0.58553	0.22189	**H260**	0.18951	0.76114	0.22189
C87	1.07161	-0.57874	0.68363	**C142**	0.51488	0.49018	0.22189	**H261**	0.20304	0.86106	0.22189
C88	1.03743	-0.55831	0.68363	**C143**	0.49443	0.43557	0.22189	**O262**	0.04763	0.84407	0.22095
C89	1.25583	-0.75592	0.68363	**C144**	0.52858	0.4152	0.22189	**O263**	0.13166	0.90429	0.22298
C90	1.29	-0.77636	0.68363	**C145**	0.58318	0.44943	0.22189	**H264**	0.34599	0.39127	0.22189
N91	1.05261	-0.50459	0.68363	**C146**	0.60362	0.50404	0.22189	**H265**	0.65006	0.60999	0.22189
C92	1.0064	-0.50112	0.68363	**C147**	0.56947	0.52441	0.22189	**H266**	0.3892	0.04223	0.22189
C93	0.96308	-0.55238	0.68363	**N148**	0.61733	0.42906	0.22189	**H267**	0.95693	0.34915	0.22189
N94	0.98213	-0.58761	0.68363	**C149**	0.59688	0.37445	0.22189	**H268**	0.13613	0.34607	0.22189
N95	1.27483	-0.83008	0.68363	**C150**	0.63104	0.35408	0.22189	**H269**	0.75991	0.56849	0.22189
C96	1.32066	-0.8336	0.68362	**C151**	0.61059	0.29947	0.22189	**H270**	0.85965	0.65499	0.22189
C97	1.36398	-0.78235	0.68362	**C152**	0.64499	0.27895	0.22189	**H271**	0.43055	0.19312	0.22189
N98	1.34493	-0.74712	0.68362	**C153**	0.69959	0.31318	0.22189	**H272**	0.34418	0.20661	0.22189
C99	1.57615	-0.34689	0.68362	**C154**	0.72003	0.36779	0.22189	**H273**	0.80609	0.23959	0.22189
C100	1.5557	-0.40143	0.68362	**C155**	0.68563	0.38831	0.22189	**H274**	0.79256	0.13967	0.22189
C101	1.75358	0.01483	0.68362	**O156**	0.55632	0.26561	0.22189	**H275**	0.60641	0.9585	0.22189
C102	1.77403	0.06936	0.68362	**O157**	0.70607	0.44292	0.22189	**H276**	0.56505	0.80761	0.22189
N103	1.82744	0.10781	0.68362	**C158**	0.77463	0.40202	0.22189	**H277**	0.65142	0.79412	0.22189
C104	1.83103	0.15711	0.68362	**O159**	0.73374	0.29281	0.22189	**O278**	0.76678	0.86472	0.2274
C105	1.77986	0.14923	0.68362	**C160**	0.62487	0.22471	0.22189	**O279**	0.78801	0.9499	0.22574
N106	1.74467	0.09507	0.68362	**N161**	0.80878	0.38165	0.22189	**O280**	0.15245	0.20628	0.22109
N107	1.50229	-0.43988	0.68362	**N162**	0.57027	0.19048	0.22189	**O281**	0.09252	0.23319	0.21954
C108	1.4987	-0.48917	0.68362	**C163**	0.54983	0.13587	0.22189	**O282**	0.90229	0.76574	0.21791
C109	1.54987	-0.48129	0.68362	**C164**	0.49523	0.10164	0.22189	**O283**	0.84444	0.79528	0.21851
N110	1.58506	-0.42713	0.68362	**C165**	0.47479	0.04703	0.22189	**O284**	0.20636	0.05008	0.22754
N111	1.76645	0.18911	0.68362	**C166**	0.50894	0.02666	0.22189	**O285**	0.22932	0.13621	0.21638
N112	1.56343	-0.52077	0.68362	**C167**	0.56354	0.06089	0.22189	**O286**	0.86311	0.09469	0.22636
N113	0.91018	-0.56581	0.68363	**C168**	0.58398	0.1155	0.22189	**O287**	0.94857	0.15866	0.22677
N114	1.41688	-0.76891	0.68362	**C169**	0.44577	0.86486	0.22189	**H288**	0.23591	0.43208	0.22189
H289	2.01145	0.12746	0.68362	**C170**	0.86337	0.41588	0.22189	**C115**	1.02336	0.51676	0.22189
H290	2.12244	0.12771	0.68361	**C171**	0.50062	0.89894	0.22189	**C166**	0.50894	1.02666	0.22189
O291	1.56625	0.10073	0.68315	**C172**	0.52081	0.9537	0.22189	**C173**	0.48666	-0.02593	0.22189
O292	1.50045	0.11823	0.68423	**C173**	0.48666	0.97407	0.22189	**C178**	-0.02776	0.48397	0.22189
H293	1.70787	-0.01378	0.68362	**C174**	0.43206	0.93984	0.22189				

References

1 J. H. Chong, M. Sauer, B. O. Patrick and M. J. MacLachlan, *Org. Lett.*, 2003, **5**, 3823–3826.

2 A. Baliani, V. Peal, L. Gros, R. Brun, M. Kaiser, M. P. Barrett and I. H. Gilbert, *Org. Biomol. Chem.*, 2009, **7**, 1154–1166.

3 B. G. Lawhorn, R. a Mehl and T. P. Begley, *Org. Biomol. Chem.*, 2004, **2**, 2538–2546.

4 B. P. Biswal, S. Kandambeth, S. Chandra, D. B. Shinde, S. Bera, S. Karak, B. Garai, U. K. Kharul and R. Banerjee, *J. Mater. Chem. A*, 2015, **3**, 23664–23669.

5 S. P. S. Fernandes, P. Kovar, M. Psenicka, A. M. S. Silva, L. M. Salonen and B. Espina, *ACS Appl. Mater. Interfaces*, 2021, **13**, 15053–15063.

6 K. Okuda, Y. Okabe, T. Kadonosono, T. Ueno, B. G. M. Youssif, S. Kizaka-Kondoh and H. Nagasawa, *Bioconjug. Chem.*, 2012, **23**, 324–329.