*Electronic Supplementary Information*

# Chiral Copper(I)-Organic Frameworks for Dye Degradations and Enantioselective Recognition of Amino Acids

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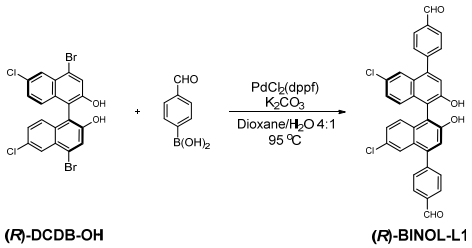
## 1. Instruments and methods.

Starting materials, reagents, and solvents were purchased from commercial sources and used without further purification. Powder X-ray diffraction (PXRD) data was collected at 40 kV, 30 mA using microcrystalline samples on a Rigaku Ultima IV diffractometer using Cu-Kα radiation (λ = 1.5418 Å). The measurement parameters include a scan speed of 0.5 °/min, a step size of 0.02°, and a scan range of 2$\theta$ from 1.5°to 30°. For temperature-dependent PXRD, the measurement parameters include a scan speed of 2 °C/min, a step size of 0.02°, and a scan range of 2$\theta$ from 1.5° to 30°. Thermogravimetric analysis was performed on a Mettler-Toledo (TGA/DSC1) thermal analyzer. Measurement were made on approximately 5 mg of dried samples under a $N_2$ flow with a heating rate of 10 °C/min. The scanning electron microscopy (SEM) and Energy Dispersive X-ray Spectroscopy (EDS) images were obtained on a Helios Nanolab G3 CX microscope. Transmission electron microscopy (TEM) analysis was performed on a JEM-2100F. Fourier transform infrared (FT-IR) spectrum was measured using a Nicolet Avatar 360 FT-IR spectrophotometer. X-ray photoelectron spectroscopy (XPS) experiments were performed by a Thermo ESCALAB 250XI system. GC-MS analysis was carried out on an Agilent 7890B GC analyzer. Liquid $^{1}H$ and $^{13}C$ NMR spectra were recorded on a Bruker Biospin Avance (400 MHz) equipment using tetramethylsilane (TMS) as an internal standard. Solid-state NMR experiments were performed on a Bruker WB Avance II 400 MHz NMR spectrometer. The $^{13}C$ CP/MAS NMR spectra were recorded with a 4-mm double-resonance MAS probe and with a sample spinning rate of 10.0 kHz; a contact time of 2 ms (ramp 100) and a pulse delay of 3 s was applied. Gas sorption analyses were conducted using an ASAP 2020 PLUS Analyzer (Micromeritics) with extra-high pure gases. Surface areas were calculated from the adsorption data using Brunauer-Emmett-Teller (BET) methods. The pore size distribution curves were obtained from the adsorption branches using density functional theory (DFT) method. Circular dichroism (CD) spectra were obtained on a Bio-Logic MOS-500 at room temperature.

## 2. Synthetic procedures

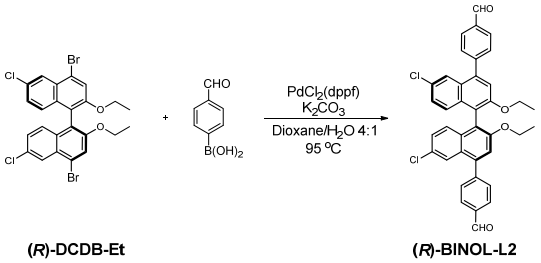
### 2-1. Synthesis of monomers




(*R*)-DCDB-OH (*R*)-BINOL-L1

(*R*)-DCDB-OH, (*S*)-DCDB-OH, (*R*)-DCDB-Et and (*S*)-DCDB-Et were synthesized according to the published procedure. (*Chem. Commun.* 2010, 46, 4911).

(*R*)-DCDB-OH (1.02 g, 2 mmol), 4-Formylphenylboronic acid (0.72 g, 4.8 mmol), $K_2CO_3$ (1.38 g, 10 mmol) and $PdCl_2$(dppf) (0.163 g, 0.2 mmol) were added in Dioxane/$H_2O$ (100 mL, 4:1, v/v). After the solution was stirred for 48 hours at 95 ℃ and filtered after cooling to room temperature. After the filtrate was concentrated, water (50 mL) was added, and the mixture was extracted with ethyl acetate, organic phase was dried over anhydrous $Na_2SO_4$ and then concentrated under reduced pressure to remove the solvent. The crude product was purified by silica gel column chromatography (hexanes/ethyl acetate, 3:1 v/v) to afford (*R*)-BINOL-L1. Yield: (0.506 g, 45%). $^1$H NMR (400 MHz, $CDCl_3$): δ 10.17 (s, 2H), 8.11 (d, $J$ = 8.0 Hz, 4H), δ 7.76-7.83 (m, 6H), 7.42 (s, 2H), 7.31-7.34 (m, 2H), 7.21-7.23 (m, 2H).$^{13}$C NMR (100 MHz, $CDCl_3$): δ 191.79, 152.25, 145.22, 141.88, 135.97, 132.24, 130.89, 130.54, 130.07, 128.67, 128.25, 126.30, 125.25, 119.87, 111.04. (*S*)-BINOL-L1 was synthesized following the same method mentioned above except that (*S*)-DCDB-OH was used instead of (*R*)-DCDB-OH.

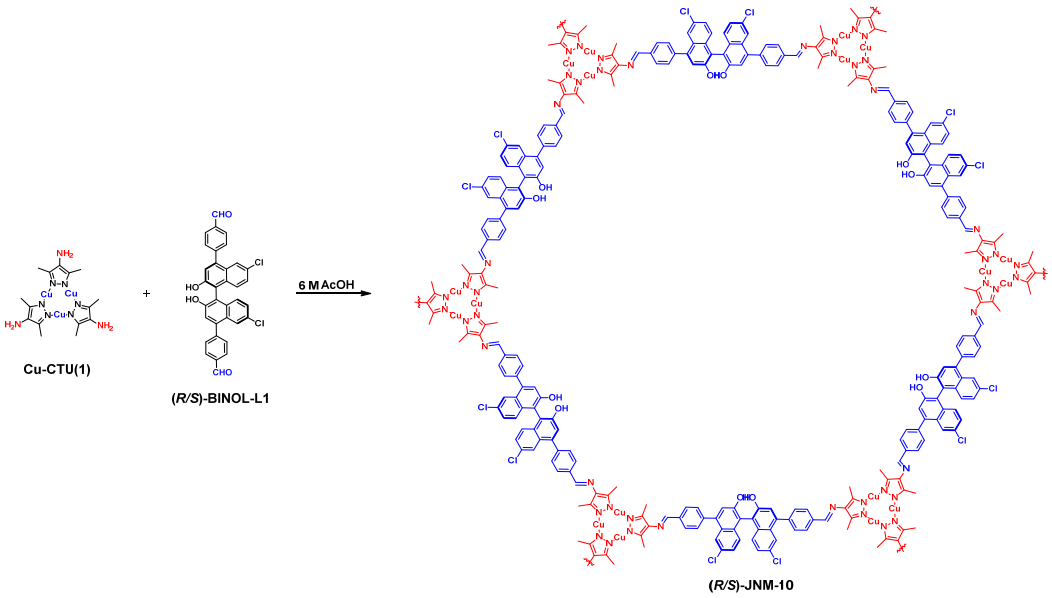



(*R*)-DCDB-Et (*R*)-BINOL-L2

(*R*)-DCDB-Et (1.13 g, 2 mmol), 4-Formylphenylboronic acid (0.72 g, 4.8 mmol), $K_2CO_3$ (1.38 g, 10 mmol) and $PdCl_2$(dppf) (0.163 g, 0.2 mmol) were added in Dioxane/$H_2O$ (100 mL, 4:1, v/v). After the solution was stirred for 48 hours at 95 ℃ and filtered after cooling to room temperature. After the filtrate was concentrated, water

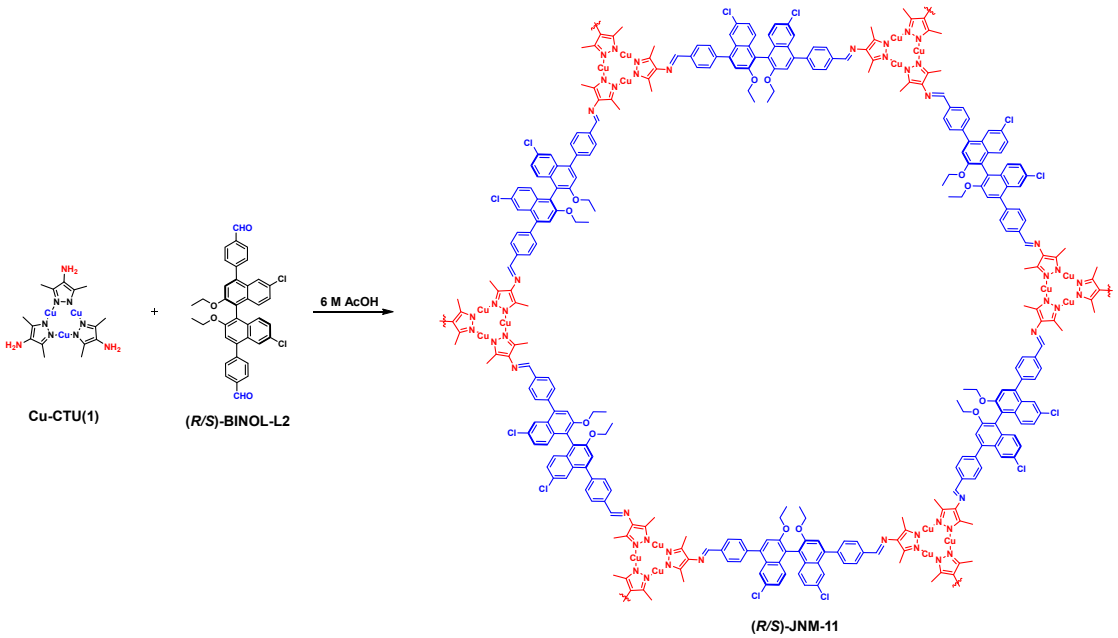
(50 mL) was added, and the mixture was extracted with ethyl acetate, organic phase was dried over anhydrous $Na_2SO_4$ and then concentrated under reduced pressure to remove the solvent. The crude product was purified by silica gel column chromatography (hexanes/ethyl acetate, 5:1 v/v) to afford (*R*)-BINOL-L2. Yield: (0.878 g, 71%). $^1$H NMR (400 MHz, $CDCl_3$): δ 10.18 (s, 2H), 8.10 (d, *J* = 8.0 Hz, 4H), δ 7.81-7.89 (m, 6H), 7.40 (s, 2H), 7.18-7.23 (m, 4H), 4.11-4.13 (m, 4H), 1.08 (t, *J* = 8.0 Hz, 6H).$^{13}$C NMR (100 MHz, $CDCl_3$): δ 191.89, 153.79, 146.39, 139.66, 135.67, 132.77, 130.79, 130.12, 129.97, 127.60, 127.47, 127.37, 124.50, 120.07, 117.35, 65.19, 14.96. (*S*)-BINOL-L2 was synthesized following the same method mentioned above except that (*S*)-DCDB-Et was used instead of (*R*)-DCDB-Et.

**2-2. Synthesis of (*R/S*)-JNM-10**




A 10 mL Schlenk tube was charged with **Cu-CTU(1)** (10.4 mg, 0.02 mmol), **(*R/S*)-BINOL-L1** (16.9 mg, 0.03 mmol), 0.75 mL of mesitylene, 0.25 mL of 1,4-dioxane and 0.10 mL of 6 M aqueous acetic acid (AcOH). The mixture was flash frozen at 77 K in liquid nitrogen bath and degassed with three freeze-pump-thaw cycles. Upon warming to room temperature, the mixture was heated at 120 °C for 72 h. The yellowish brown powders were isolated by filtration, washed and solvent exchanged with EtOH, DMF and acetone. The resultants were dried under vacuum at 100 °C for 8 h. Yield: 11.05 mg (40.5%, based on **1**). Elemental analysis calcd (%): C 57.3, H 4.0, N 10.7; Found: C 56.9, H 4.0, N 10.7.

**2-3. Synthesis of JNM-11**




A 10 mL Schlenk tube was charged with **Cu-CTU(1)** (10.4 mg, 0.02 mmol), **(*R/S*)-BINOL-L2** (18.5 mg, 0.03 mmol), 0.75 mL of mesitylene, 0.25 mL of 1,4-dioxane and 0.10 mL of 6 M aqueous acetic acid (AcOH). The mixture was flash frozen at 77 K in liquid nitrogen bath and degassed with three freeze-pump-thaw cycles. Upon warming to room temperature, the mixture was heated at 120 °C for 72 h. The yellowish brown powders were isolated by filtration, washed and solvent exchanged with EtOH, DMF and acetone. The resultants were dried under vacuum at 100 °C for 8 h. Yield: 14.9 mg (51.5%, based on **1**). Elemental analysis calcd (%): C 58.8, H 4.5, N 10.2; Found: C 57.9, H 4.4, N 10.2.

## 2-4. Optimization of synthetic condition

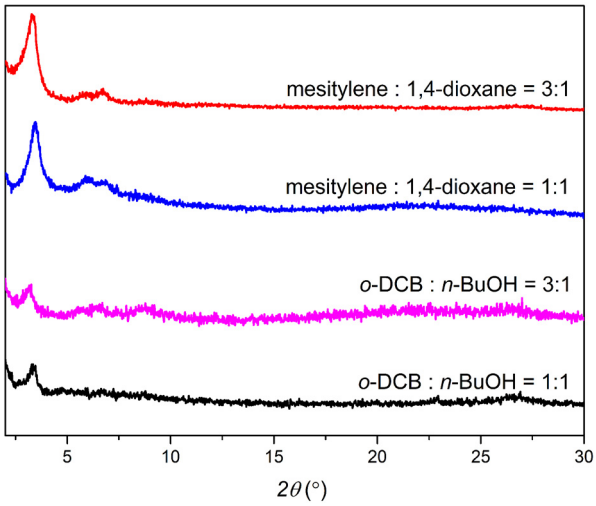



**Figure S1.** Optimization of **(*R/S*)-JNM-10** reaction condition, showing the best condition is mesitylene (0.75 mL), 1,4-dioxane (0.25 mL) and AcOH (6 M, 0.12 mL) for 3 days.

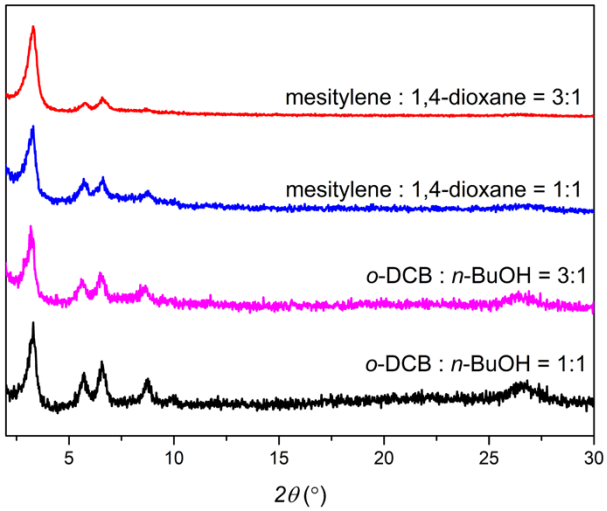



**Figure S2.** Optimization of **(*R/S*)-JNM-11** reaction condition, showing the best condition is mesitylene (0.75 mL), 1,4-dioxane (0.25 mL) and AcOH (6 M, 0.12 mL) for 3 days.

## 3. Fourier-transform infrared (FT-IR) spectra

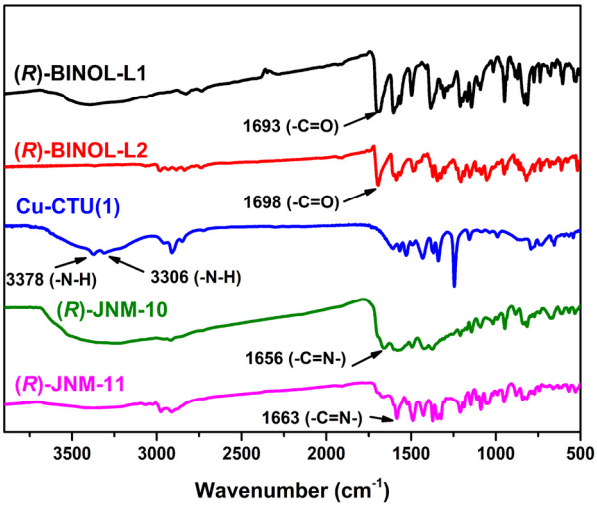



**Figure S3.** FT-IR spectra of **(*R*)-BINOL-L1**, **(*R*)-BINOL-L2**, **Cu-CTU(1)**, **(*R*)-JNM-10** and **(*R*)-JNM-11**.

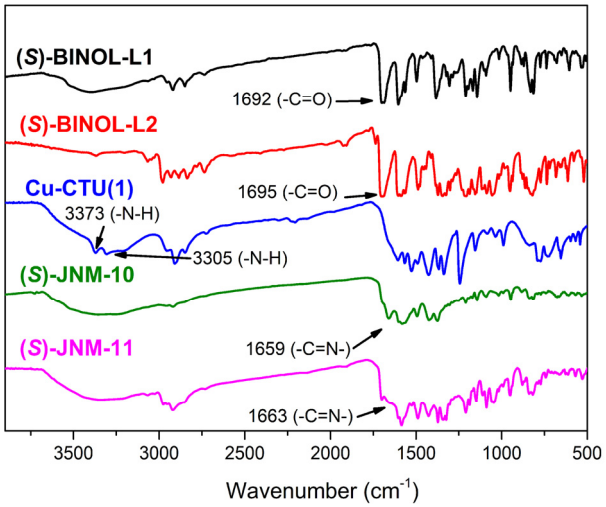



**Figure S4.** FT-IR spectra of **(*S*)-BINOL-L1**, **(*S*)-BINOL-L2**, **Cu-CTU(1)**, **(*S*)-JNM-10** and **(*S*)-JNM-11**.

## 4. Solid-state 13C CP/MAS NMR spectra

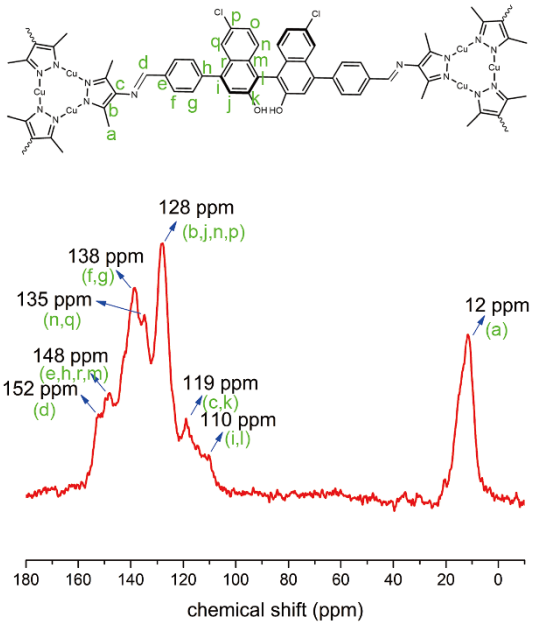



**Figure S5.** Solid-state $^{13}$C CP/MAS NMR spectra and peak assignments of **(*R*)-JNM-10**.

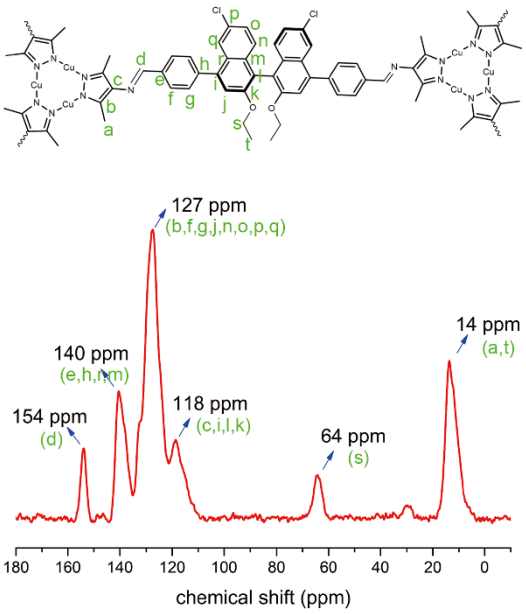



**Figure S6.** Solid-state $^{13}$C CP/MAS NMR spectra and peak assignments of **(*R*)-JNM-11**.

## 5. Scanning electron microscopy (SEM)

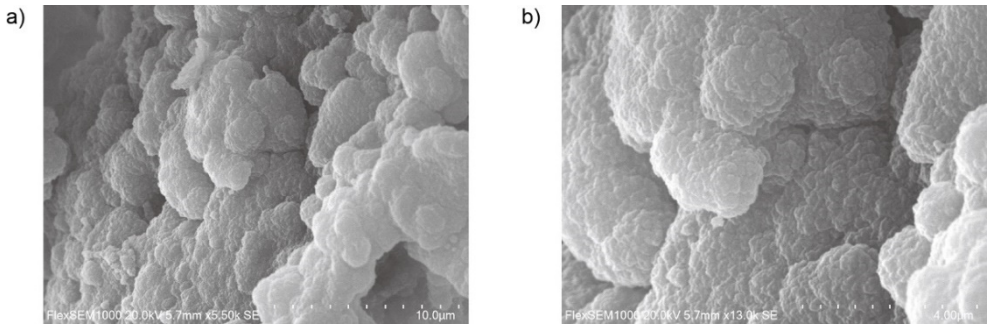



**Figure S7.** SEM images of **(*R*)-JNM-10.**

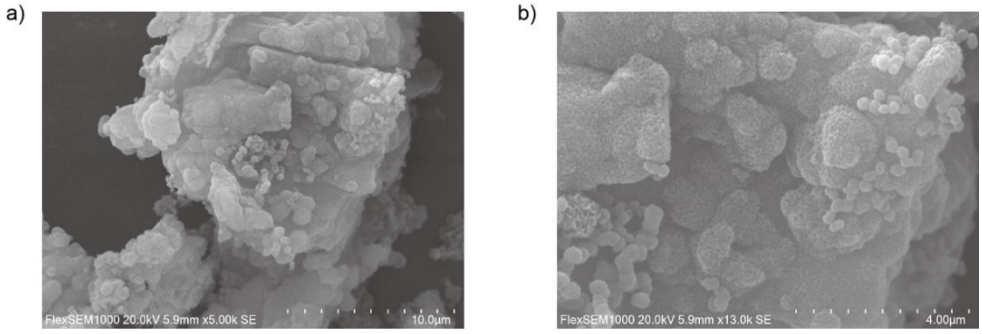



**Figure S8.** SEM images of **(*R*)-JNM-11.**

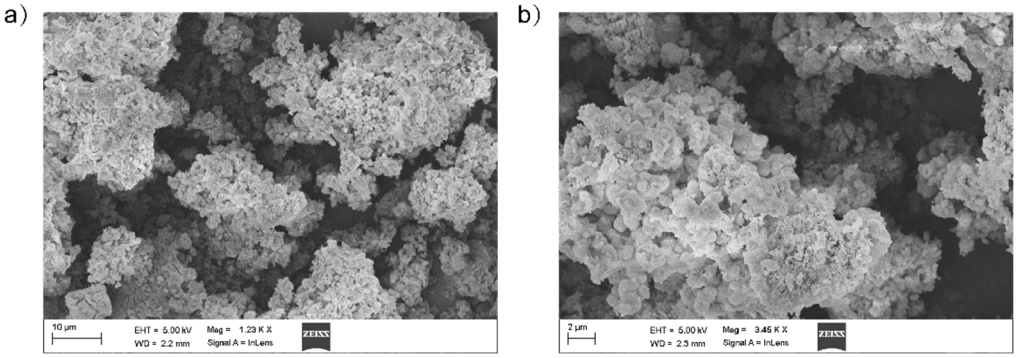



**Figure S9.** SEM images of **(*S*)-JNM-10.**

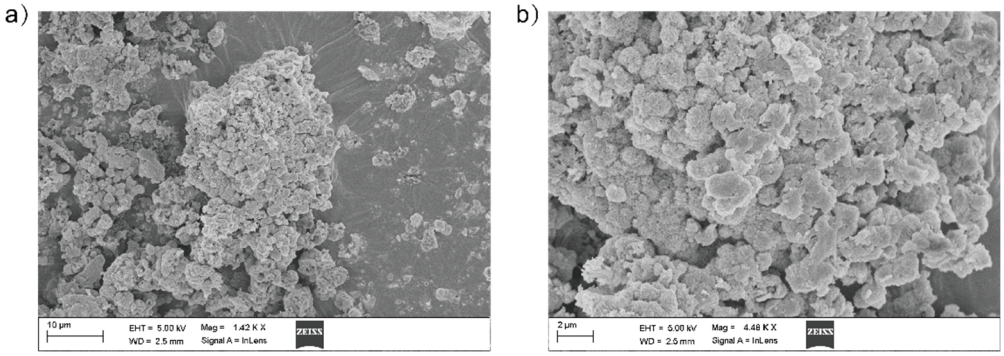



**Figure S10.** SEM images of **(*S*)-JNM-11.**

## 6. Energy Dispersive X-ray Spectroscopy (EDS)

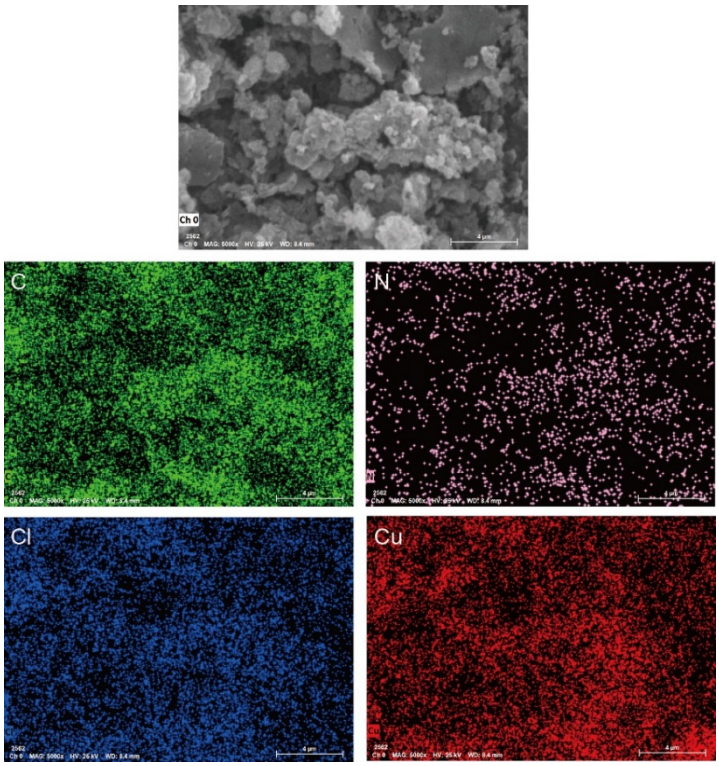



**Figure S11**. EDS of **(*R*)-JNM-10** showing the uniform distribution of element C, N, Cl and Cu.

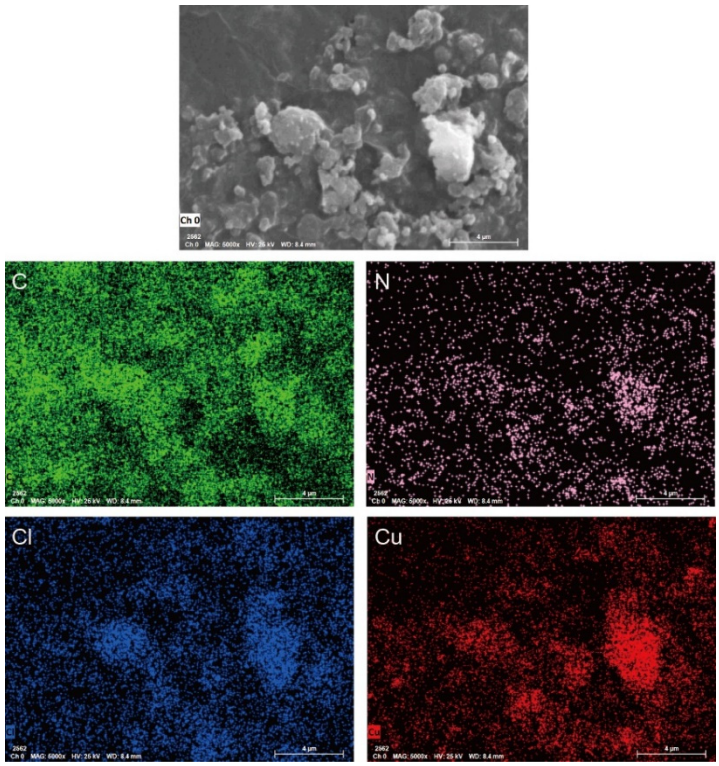



**Figure S12**. EDS of **(*R*)-JNM-11** showing the uniform distribution of element C, N, Cl and Cu.

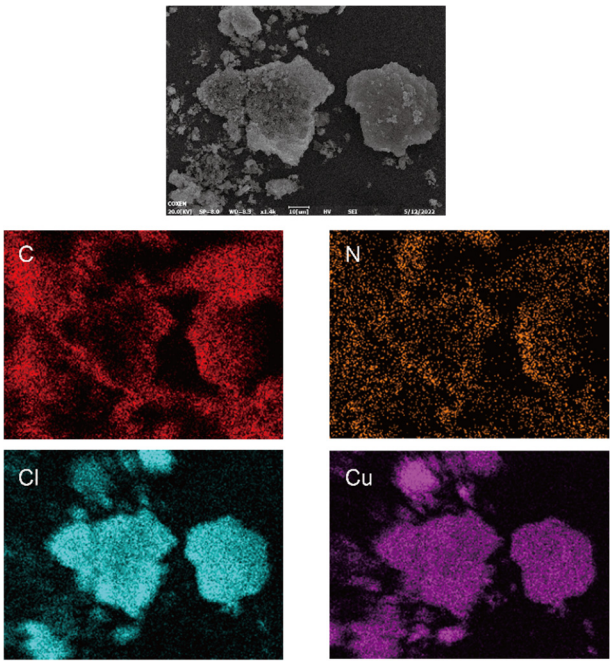



**Figure S13**. EDS of **(*S*)-JNM-10** showing the uniform distribution of element C, N, Cl and Cu.

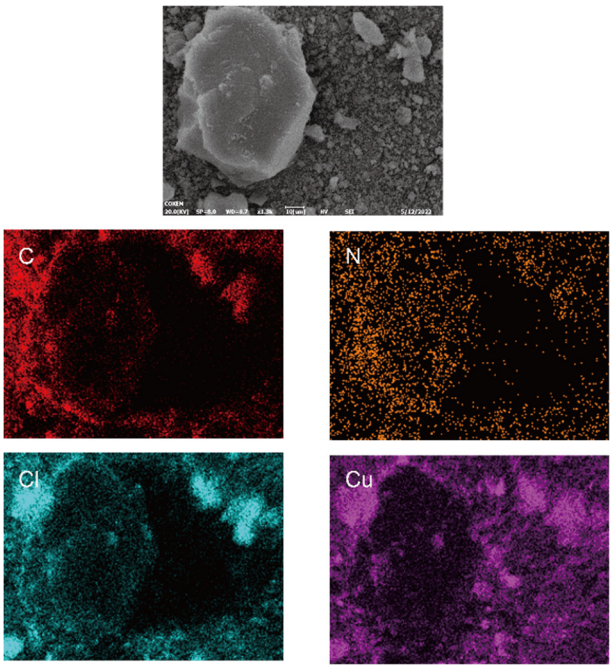



**Figure S14**. EDS of **(*S*)-JNM-11** showing the uniform distribution of element C, N, Cl and Cu.

## 7. Structural Simulation of (*R*)-JNM-10

Theoretical simulations of **(*R*)-JNM-10** were carried out in Accelrys Materials Studio 2019 software package. The relative total energies were calculated by molecular mechanics calculation using DMol$^3$ energy task, after which the simulated PXRD patterns were determined by the Reflex module. The Pawley refinement of the experimental PXRD was conducted with the Reflex module.[1]

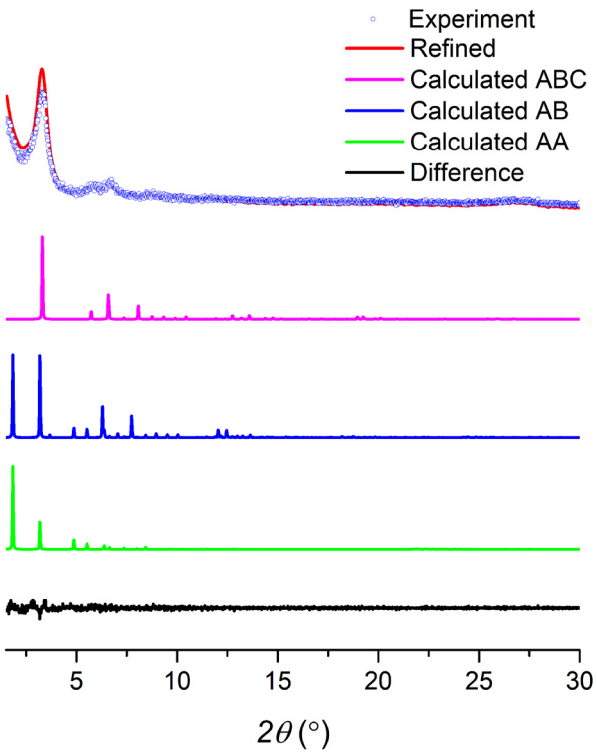



**Figure S15.** PXRD patterns of **(*R*)-JNM-10** with the experimental profiles in black, difference curve in light orange, and calculated profiles of AA (green), AB (blue) and ABC (magenta) packing modes. (refinement parameters of *Rp* = 6.75% and *Rwp* = 9.19%).

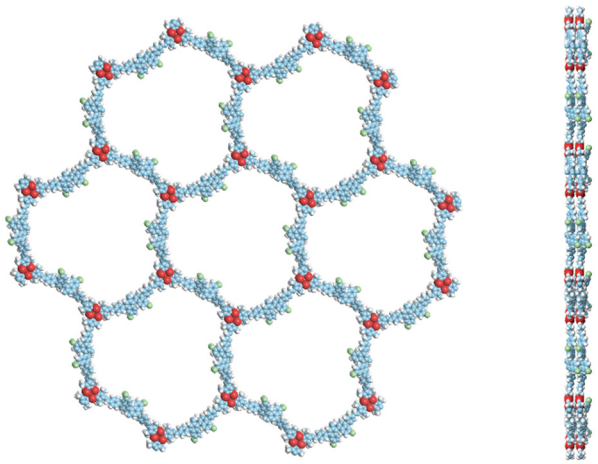


**Figure S16.** Space-filling mode of **(*R*)-JNM-10** in AA stacking model viewed from (left) c axis and (right) *a* axis.

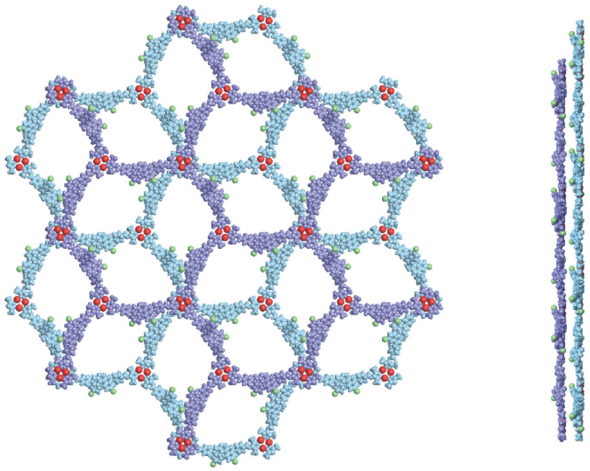


**Figure S17.** Space-filling mode of **(*R*)-JNM-10** in AB stacking model viewed from (left) c axis and (right) *a* axis.

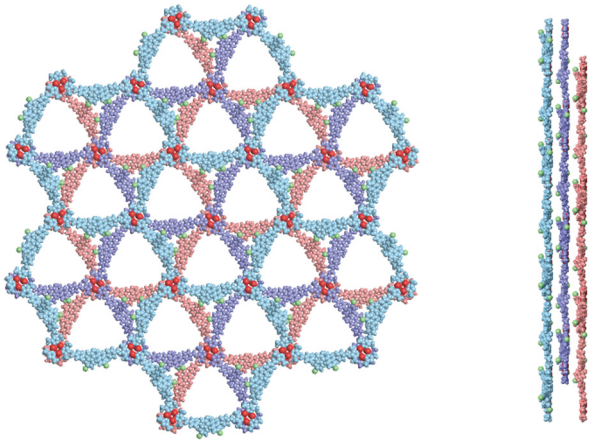


**Figure S18.** Space-filling mode of **(*R*)-JNM-10** in ABC stacking model viewed from (left) c axis and (right) *a* axis.

**Table S1.** AA stacking model for **(*R*)-JNM-10**.

| Space group: *P3*<br>a = b = 55.44210 Å, and c = 4.0898 Å<br>α =β = 90°, and γ = 120° | | | |
|---|---|---|---|
| | X | Y | Z |
| Cu | 0.32217 | 0.62743 | 0.08994 |
| C | 0.37285 | 0.62215 | 0.13298 |
| Cu | 0.69463 | 0.37263 | 0.74183 |
| C | 0.44301 | 0.60459 | 0.36606 |
| C | 0.46912 | 0.62249 | 0.22523 |
| C | 0.49041 | 0.61599 | 0.23974 |
| C | 0.48608 | 0.59158 | 0.39562 |
| C | 0.45997 | 0.57381 | 0.5373 |
| C | 0.4387 | 0.58031 | 0.52402 |
| C | 0.50058 | 0.55787 | 0.24884 |
| C | 0.50759 | 0.58296 | 0.39562 |
| C | 0.53258 | 0.59689 | 0.56906 |
| C | 0.54839 | 0.58337 | 0.62813 |
| C | 0.54173 | 0.55726 | 0.47353 |
| C | 0.51635 | 0.54437 | 0.28422 |
| C | 0.5487 | 0.51478 | 0.58506 |
| C | 0.59115 | 0.55894 | 0.46861 |
| C | 0.60692 | 0.54481 | 0.49718 |
| C | 0.59366 | 0.51676 | 0.59648 |
| C | 0.56541 | 0.50322 | 0.65847 |
| C | 0.59551 | 0.4734 | 0.47431 |
| C | 0.60764 | 0.49975 | 0.6247 |
| C | 0.63153 | 0.50837 | 0.81761 |
| C | 0.64325 | 0.49134 | 0.85627 |
| C | 0.6308 | 0.46492 | 0.71067 |
| C | 0.60685 | 0.45611 | 0.51806 |
| C | 0.64265 | 0.44667 | 0.76827 |
| C | 0.41994 | 0.61056 | 0.34702 |
| N | 0.36164 | -0.27697 | 0.09378 |
| N | 0.33522 | -0.2836 | 0.09137 |
| N | 0.6189 | 0.28347 | 0.7424 |
| C | 0.62725 | 0.24918 | 0.72246 |
| C | 0.59859 | 0.23756 | 0.71744 |
| N | 0.57905 | 0.20856 | 0.67113 |
| C | 0.2604 | 0.59394 | 0.1271 |
| C | 0.23801 | 0.59837 | 0.15832 |
| N | 0.2095 | 0.57696 | 0.1969 |
| N | -0.27697 | 0.36182 | 0.74141 |
| C | -0.26005 | 0.33386 | 0.72623 |

| | | | |
|---|---|---|---|
| C | -0.01695 | 0.43923 | 0.50887 |
| C | 0.57036 | 0.59638 | 0.84925 |
| C | 0.58031 | 0.62371 | 0.95658 |
| C | 0.56622 | 0.63758 | 0.87519 |
| C | 0.5421 | 0.62404 | 0.68995 |
| C | 0.63575 | 0.55913 | 0.42404 |
| C | 0.64967 | 0.58707 | 0.33906 |
| C | 0.63533 | 0.60146 | 0.33109 |
| C | 0.60693 | 0.58774 | 0.39673 |
| Cl | 0.5783 | 0.67168 | 1.01377 |
| Cl | 0.68534 | 0.60414 | 0.24605 |
| O | 0.50672 | 0.51805 | 0.13722 |
| O | 0.51986 | 0.49648 | 0.5957 |
| C | 0.76588 | 0.40909 | 0.69846 |
| C | 0.43312 | 0.69318 | 0.14787 |
| C | 0.35636 | 0.59103 | 0.13642 |
| C | 0.56704 | 0.2599 | 0.68523 |
| H | 0.47301 | 0.64244 | 0.09834 |
| H | 0.51152 | 0.63056 | 0.12431 |
| H | 0.45601 | 0.55385 | 0.66465 |
| H | 0.41768 | 0.56584 | 0.64209 |
| H | 0.48116 | 0.54694 | 0.08917 |
| H | 0.5558 | 0.48168 | 0.77488 |
| H | 0.57621 | 0.46598 | 0.31467 |
| H | 0.64158 | 0.52949 | 0.94491 |
| H | 0.66305 | 0.4989 | 1.00695 |
| H | 0.59658 | 0.43474 | 0.39653 |
| H | 0.6635 | 0.45514 | 0.89909 |
| H | 0.39903 | 0.59575 | 0.46523 |
| H | 0.58026 | 0.58396 | 0.94296 |
| H | 0.60005 | 0.63455 | 1.11117 |
| H | 0.52965 | 0.63483 | 0.63331 |
| H | 0.64752 | 0.54717 | 0.43624 |
| H | 0.64678 | 0.62465 | 0.2706 |
| H | 0.59518 | 0.59975 | 0.3943 |
| H | 0.76992 | 0.41553 | 0.4304 |
| H | 0.78658 | 0.41809 | 0.83396 |
| H | 0.75265 | 0.41733 | 0.81267 |
| H | 0.43913 | 0.70311 | -0.10497 |
| H | 0.44998 | 0.68888 | 0.24147 |
| H | 0.43091 | 0.70797 | 0.32296 |
| H | 0.36835 | 0.58257 | 0.27613 |
| H | 0.35268 | 0.58288 | -0.12535 |
| H | 0.33546 | 0.58391 | 0.26112 |

| | | | |
|---|---|---|---|
| H | 0.54896 | 0.23846 | 0.75204 |
| H | 0.5648 | 0.26483 | 0.42014 |
| H | 0.56687 | 0.27628 | 0.85221 |
| H | 0.48371 | 0.50549 | 0.16071 |
| H | 0.51035 | 0.504 | 0.77876 |

**Table S2.** AB stacking model for **(*R*)-JNM-10**.

Space group: *P3*

a = b = 55.4210 Å, and c = 15.2174 Å

α =β = 90°, and γ = 120°

| | X | Y | Z |
|---|---|---|---|
| Cu | 0.32217 | 0.62743 | 0.13672 |
| C | 0.37285 | 0.62215 | 0.14828 |
| Cu | 0.69463 | 0.37263 | 0.31191 |
| C | 0.44301 | 0.60459 | 0.21093 |
| C | 0.46912 | 0.62249 | 0.17308 |
| C | 0.49041 | 0.61599 | 0.17698 |
| C | 0.48608 | 0.59158 | 0.21887 |
| C | 0.45997 | 0.57381 | 0.25695 |
| C | 0.4387 | 0.58031 | 0.25338 |
| C | 0.50058 | 0.55787 | 0.17942 |
| C | 0.50759 | 0.58296 | 0.21887 |
| C | 0.53258 | 0.59689 | 0.26548 |
| C | 0.54839 | 0.58337 | 0.28136 |
| C | 0.54173 | 0.55726 | 0.23981 |
| C | 0.51635 | 0.54437 | 0.18893 |
| C | 0.5487 | 0.51478 | 0.26978 |
| C | 0.59115 | 0.55894 | 0.23849 |
| C | 0.60692 | 0.54481 | 0.24616 |
| C | 0.59366 | 0.51676 | 0.27285 |
| C | 0.56541 | 0.50322 | 0.28951 |
| C | 0.59551 | 0.4734 | 0.24002 |
| C | 0.60764 | 0.49975 | 0.28044 |
| C | 0.63153 | 0.50837 | 0.33228 |
| C | 0.64325 | 0.49134 | 0.34267 |
| C | 0.6308 | 0.46492 | 0.30354 |
| C | 0.60685 | 0.45611 | 0.25178 |
| C | 0.64265 | 0.44667 | 0.31902 |
| C | 0.41994 | 0.61056 | 0.20581 |
| N | 0.36164 | 0.72303 | 0.13775 |
| N | 0.33522 | 0.7164 | 0.1371 |
| N | 0.6189 | 0.28347 | 0.31207 |
| C | 0.62725 | 0.24918 | 0.30671 |
| C | 0.59859 | 0.23756 | 0.30536 |

| | | | |
|---|---|---|---|
| N | 0.57905 | 0.20856 | 0.29292 |
| C | 0.2604 | 0.59394 | 0.1467 |
| C | 0.23801 | 0.59837 | 0.1551 |
| N | 0.2095 | 0.57696 | 0.16546 |
| N | 0.72303 | 0.36182 | 0.3118 |
| C | 0.73995 | 0.33386 | 0.30772 |
| C | 0.98305 | 0.43923 | 0.24931 |
| C | 0.57036 | 0.59638 | 0.34079 |
| C | 0.58031 | 0.62371 | 0.36963 |
| C | 0.56622 | 0.63758 | 0.34776 |
| C | 0.5421 | 0.62404 | 0.29797 |
| C | 0.63575 | 0.55913 | 0.22651 |
| C | 0.64967 | 0.58707 | 0.20367 |
| C | 0.63533 | 0.60146 | 0.20153 |
| C | 0.60693 | 0.58774 | 0.21917 |
| Cl | 0.5783 | 0.67168 | 0.385 |
| Cl | 0.68534 | 0.60414 | 0.17867 |
| O | 0.50672 | 0.51805 | 0.14942 |
| O | 0.51986 | 0.49648 | 0.27264 |
| C | 0.76588 | 0.40909 | 0.30026 |
| C | 0.43312 | 0.69318 | 0.15229 |
| C | 0.35636 | 0.59103 | 0.14921 |
| C | 0.56704 | 0.2599 | 0.2967 |
| H | 0.47301 | 0.64244 | 0.13897 |
| H | 0.51152 | 0.63056 | 0.14596 |
| H | 0.45601 | 0.55385 | 0.29117 |
| H | 0.41768 | 0.56584 | 0.28511 |
| H | 0.48116 | 0.54694 | 0.13651 |
| H | 0.5558 | 0.48168 | 0.3208 |
| H | 0.57621 | 0.46598 | 0.19711 |
| H | 0.64158 | 0.52949 | 0.36649 |
| H | 0.66305 | 0.4989 | 0.38317 |
| H | 0.59658 | 0.43474 | 0.21911 |
| H | 0.6635 | 0.45514 | 0.35418 |
| H | 0.39903 | 0.59575 | 0.23758 |
| H | 0.58026 | 0.58396 | 0.36597 |
| H | 0.60005 | 0.63455 | 0.41118 |
| H | 0.52965 | 0.63483 | 0.28275 |
| H | 0.64752 | 0.54717 | 0.22979 |
| H | 0.64678 | 0.62465 | 0.18527 |
| H | 0.59518 | 0.59975 | 0.21851 |
| H | 0.76992 | 0.41553 | 0.22822 |
| H | 0.78658 | 0.41809 | 0.33668 |
| H | 0.75265 | 0.41733 | 0.33095 |

| | | | |
|---|---|---|---|
| H | 0.43913 | 0.70311 | 0.08433 |
| H | 0.44998 | 0.68888 | 0.17744 |
| H | 0.43091 | 0.70797 | 0.19934 |
| H | 0.36835 | 0.58257 | 0.18676 |
| H | 0.35268 | 0.58288 | 0.07886 |
| H | 0.33546 | 0.58391 | 0.18272 |
| H | 0.54896 | 0.23846 | 0.31466 |
| H | 0.5648 | 0.26483 | 0.22546 |
| H | 0.56687 | 0.27628 | 0.34158 |
| H | 0.48371 | 0.50549 | 0.15574 |
| H | 0.51035 | 0.504 | 0.32184 |
| Cu | 0.6555 | 0.2941 | 0.63672 |
| C | 0.70619 | 0.28881 | 0.64828 |
| Cu | 0.02796 | 0.0393 | 0.81191 |
| C | 0.77634 | 0.27126 | 0.71093 |
| C | 0.80245 | 0.28916 | 0.67308 |
| C | 0.82374 | 0.28265 | 0.67698 |
| C | 0.81941 | 0.25825 | 0.71887 |
| C | 0.79331 | 0.24048 | 0.75695 |
| C | 0.77203 | 0.24698 | 0.75338 |
| C | 0.83391 | 0.22454 | 0.67942 |
| C | 0.84093 | 0.24963 | 0.71887 |
| C | 0.86592 | 0.26356 | 0.76548 |
| C | 0.88173 | 0.25003 | 0.78136 |
| C | 0.87506 | 0.22393 | 0.73981 |
| C | 0.84969 | 0.21103 | 0.68893 |
| C | 0.88203 | 0.18144 | 0.76978 |
| C | 0.92449 | 0.22561 | 0.73849 |
| C | 0.94025 | 0.21148 | 0.74616 |
| C | 0.927 | 0.18343 | 0.77285 |
| C | 0.89874 | 0.16989 | 0.78951 |
| C | 0.92885 | 0.14007 | 0.74002 |
| C | 0.94097 | 0.16641 | 0.78044 |
| C | 0.96486 | 0.17504 | 0.83228 |
| C | 0.97658 | 0.15801 | 0.84267 |
| C | 0.96414 | 0.13159 | 0.80354 |
| C | 0.94019 | 0.12278 | 0.75178 |
| C | 0.97598 | 0.11334 | 0.81902 |
| C | 0.75328 | 0.27722 | 0.70581 |
| N | 0.69497 | 0.3897 | 0.63775 |
| N | 0.66855 | 0.38307 | 0.6371 |
| N | 0.95224 | 0.95013 | 0.81207 |
| C | 0.96059 | 0.91585 | 0.80671 |
| C | 0.93193 | 0.90423 | 0.80536 |

| | | | |
|---|---|---|---|
| N | 0.91238 | 0.87523 | 0.79292 |
| C | 0.59373 | 0.2606 | 0.6467 |
| C | 0.57134 | 0.26504 | 0.6551 |
| N | 0.54284 | 0.24363 | 0.66546 |
| N | 0.05636 | 0.02848 | 0.8118 |
| C | 0.07328 | 0.00052 | 0.80772 |
| C | 0.31639 | 0.1059 | 0.74931 |
| C | 0.90369 | 0.26305 | 0.84079 |
| C | 0.91365 | 0.29038 | 0.86963 |
| C | 0.89956 | 0.30424 | 0.84776 |
| C | 0.87544 | 0.29071 | 0.79797 |
| C | 0.96908 | 0.2258 | 0.72651 |
| C | 0.98301 | 0.25374 | 0.70367 |
| C | 0.96867 | 0.26813 | 0.70153 |
| C | 0.94026 | 0.25441 | 0.71917 |
| Cl | 0.91164 | 0.33835 | 0.885 |
| Cl | 0.01867 | 0.27081 | 0.67867 |
| O | 0.84005 | 0.18472 | 0.64942 |
| O | 0.8532 | 0.16315 | 0.77264 |
| C | 0.09921 | 0.07575 | 0.80026 |
| C | 0.76645 | 0.35985 | 0.65229 |
| C | 0.68969 | 0.2577 | 0.64921 |
| C | 0.90037 | 0.92656 | 0.7967 |
| H | 0.80635 | 0.30911 | 0.63897 |
| H | 0.84486 | 0.29723 | 0.64596 |
| H | 0.78934 | 0.22052 | 0.79117 |
| H | 0.75101 | 0.23251 | 0.78511 |
| H | 0.81449 | 0.21361 | 0.63651 |
| H | 0.88913 | 0.14835 | 0.8208 |
| H | 0.90955 | 0.13265 | 0.69711 |
| H | 0.97492 | 0.19616 | 0.86649 |
| H | 0.99638 | 0.16557 | 0.88317 |
| H | 0.92991 | 0.10141 | 0.71911 |
| H | 0.99683 | 0.12181 | 0.85418 |
| H | 0.73236 | 0.26242 | 0.73758 |
| H | 0.91359 | 0.25063 | 0.86597 |
| H | 0.93338 | 0.30122 | 0.91118 |
| H | 0.86299 | 0.30149 | 0.78275 |
| H | 0.98085 | 0.21384 | 0.72979 |
| H | 0.98012 | 0.29132 | 0.68527 |
| H | 0.92851 | 0.26641 | 0.71851 |
| H | 0.10325 | 0.0822 | 0.72822 |
| H | 0.11991 | 0.08476 | 0.83668 |
| H | 0.08599 | 0.084 | 0.83095 |

| | | | |
|---|---|---|---|
| H | 0.77246 | 0.36978 | 0.58433 |
| H | 0.78331 | 0.35555 | 0.67744 |
| H | 0.76424 | 0.37464 | 0.69934 |
| H | 0.70168 | 0.24924 | 0.68676 |
| H | 0.68601 | 0.24955 | 0.57886 |
| H | 0.6688 | 0.25058 | 0.68272 |
| H | 0.88229 | 0.90513 | 0.81466 |
| H | 0.89813 | 0.9315 | 0.72546 |
| H | 0.9002 | 0.94295 | 0.84158 |
| H | 0.81705 | 0.17216 | 0.65574 |
| H | 0.84368 | 0.17067 | 0.82184 |

**Table S3.** ABC stacking model for **(*R*)-JNM-10**.

| Space group: *R3*<br>a = b = 53.4210 Å, and c = 14.0391 Å<br>α =β = 90°, and γ = 120° | | | |
|---|---|---|---|
| | X | Y | Z |
| Cu | -0.32244 | -0.62748 | 0.09725 |
| C | -0.37346 | -0.62261 | 0.10299 |
| Cu | -0.69426 | -0.37276 | 0.11351 |
| C | -0.44487 | -0.60553 | 0.13538 |
| C | -0.47071 | -0.62434 | 0.1093 |
| C | -0.4925 | -0.61853 | 0.10955 |
| C | -0.48895 | -0.59391 | 0.13589 |
| C | -0.46306 | -0.5751 | 0.16165 |
| C | -0.44129 | -0.58093 | 0.16175 |
| C | -0.50555 | -0.56232 | 0.10362 |
| C | -0.51129 | -0.58648 | 0.13401 |
| C | -0.53678 | -0.60127 | 0.16514 |
| C | -0.55428 | -0.58922 | 0.17193 |
| C | -0.54829 | -0.56397 | 0.14066 |
| C | -0.52406 | -0.55208 | 0.10407 |
| C | -0.55174 | -0.51922 | 0.15668 |
| C | -0.59554 | -0.56236 | 0.13481 |
| C | -0.60943 | -0.54631 | 0.133 |
| C | -0.59464 | -0.5176 | 0.14644 |
| C | -0.5665 | -0.50512 | 0.15942 |
| C | -0.59395 | -0.47391 | 0.11365 |
| C | -0.60719 | -0.49921 | 0.14581 |
| C | -0.6312 | -0.50578 | 0.17961 |
| C | -0.64228 | -0.48801 | 0.17956 |
| C | -0.62904 | -0.46283 | 0.14736 |
| C | -0.60465 | -0.45584 | 0.11464 |
| C | -0.64088 | -0.44421 | 0.14854 |

| | | | |
|---|---|---|---|
| C | -0.4214 | -0.61096 | 0.13508 |
| N | -0.3613 | -0.72306 | 0.09779 |
| N | -0.33483 | -0.71622 | 0.09751 |
| N | -0.6193 | -0.28312 | 0.11415 |
| C | -0.62822 | -0.2492 | 0.11699 |
| C | -0.59958 | -0.23732 | 0.12102 |
| N | -0.58012 | -0.208 | 0.12301 |
| C | -0.2606 | -0.59358 | 0.10227 |
| C | -0.23799 | -0.59774 | 0.10662 |
| N | -0.20942 | -0.57605 | 0.11041 |
| N | -0.72304 | -0.36246 | 0.11356 |
| C | -0.74046 | -0.33496 | 0.11844 |
| C | -0.98331 | -0.43443 | 0.14543 |
| C | -0.57704 | -0.60279 | 0.21073 |
| C | -0.58549 | -0.62924 | 0.23425 |
| C | -0.56955 | -0.64169 | 0.22404 |
| C | -0.54502 | -0.62757 | 0.19098 |
| C | -0.63782 | -0.55927 | 0.11585 |
| C | -0.65314 | -0.58761 | 0.10398 |
| C | -0.64059 | -0.60365 | 0.1091 |
| C | -0.61252 | -0.59129 | 0.12411 |
| Cl | -0.57995 | -0.67481 | 0.25393 |
| Cl | -0.68822 | -0.60299 | 0.0823 |
| O | -0.51748 | -0.52892 | 0.06897 |
| O | -0.52309 | -0.50134 | 0.16486 |
| C | -0.7656 | -0.41009 | 0.11812 |
| C | -0.43343 | -0.69385 | 0.10469 |
| C | -0.35719 | -0.59149 | 0.10175 |
| C | -0.56719 | -0.25879 | 0.1169 |
| H | -0.47408 | -0.64349 | 0.08852 |
| H | -0.51215 | -0.63343 | 0.08968 |
| H | -0.45967 | -0.55579 | 0.18155 |
| H | -0.42157 | -0.56612 | 0.18213 |
| H | -0.48637 | -0.55134 | 0.07798 |
| H | -0.55508 | -0.48305 | 0.17015 |
| H | -0.57538 | -0.46823 | 0.08723 |
| H | -0.64141 | -0.5247 | 0.20596 |
| H | -0.66094 | -0.49371 | 0.20564 |
| H | -0.59401 | -0.4366 | 0.08912 |
| H | -0.66004 | -0.45075 | 0.17312 |
| H | -0.40226 | -0.59623 | 0.15731 |
| H | -0.58915 | -0.59324 | 0.21945 |
| H | -0.60449 | -0.64018 | 0.26037 |
| H | -0.53301 | -0.63779 | 0.18489 |

| | | | |
|---|---|---|---|
| H | -0.64856 | -0.54771 | 0.11065 |
| H | -0.65243 | -0.62582 | 0.10016 |
| H | -0.60457 | -0.60516 | 0.12487 |
| H | -0.78117 | -0.41854 | 0.08106 |
| H | -0.7766 | -0.41775 | 0.16192 |
| H | -0.75053 | -0.41758 | 0.11243 |
| H | -0.43681 | -0.70518 | 0.06134 |
| H | -0.45105 | -0.69008 | 0.1126 |
| H | -0.43275 | -0.70697 | 0.14181 |
| H | -0.36702 | -0.58341 | 0.06999 |
| H | -0.33556 | -0.58427 | 0.08635 |
| H | -0.35621 | -0.5831 | 0.14786 |
| H | -0.55285 | -0.24256 | 0.08464 |
| H | -0.57029 | -0.27929 | 0.10201 |
| H | -0.5578 | -0.25433 | 0.16281 |
| H | -0.49703 | -0.51823 | 0.05731 |
| H | -0.51005 | -0.50871 | 0.16013 |

## 8. Structural Simulation of (*R*)-JNM-11

Theoretical simulations of **(*R*)-JNM-11** were carried out in Accelrys Materials Studio 2019 software package. The relative total energies were calculated by molecular mechanics calculation using DMol$^3$ energy task, after which the simulated PXRD patterns were determined by the Reflex module. The Pawley refinement of the experimental PXRD was conducted with the Reflex module.[1]

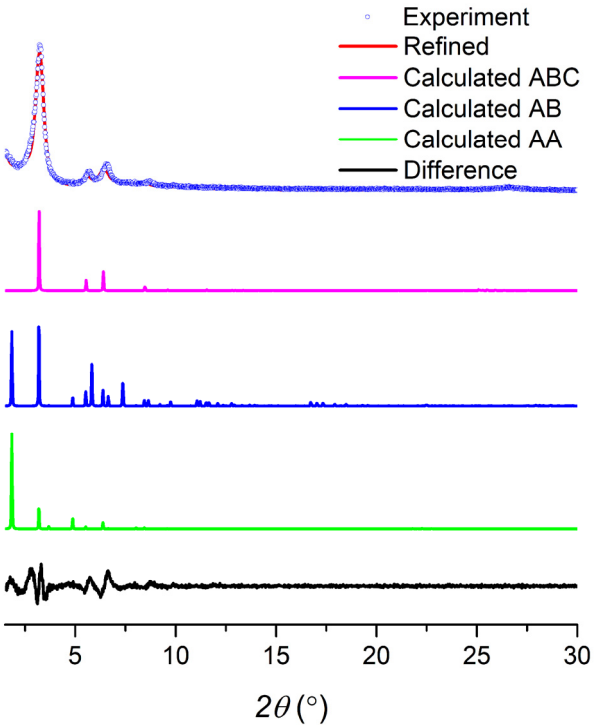



**Figure S19.** PXRD patterns of **(*R*)-JNM-11** with the experimental profiles in black, difference curve in light orange, and calculated profiles of AA (green), AB (blue) and ABC (magenta) packing modes. (refinement parameters of *Rp* = 7.24% and *Rwp* = 9.11%).

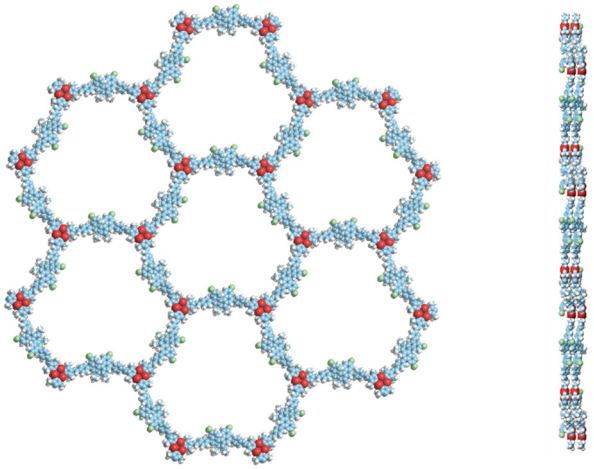


**Figure S20.** Space-filling mode of **(*R*)-JNM-11** in AA stacking model viewed from (left) c axis and (right) a axis.

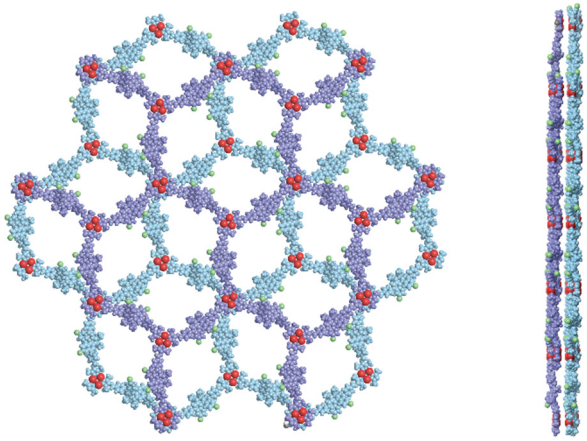


**Figure S21.** Space-filling mode of **(*R*)-JNM-11** in AB stacking model viewed from (left) c axis and (right) a axis.

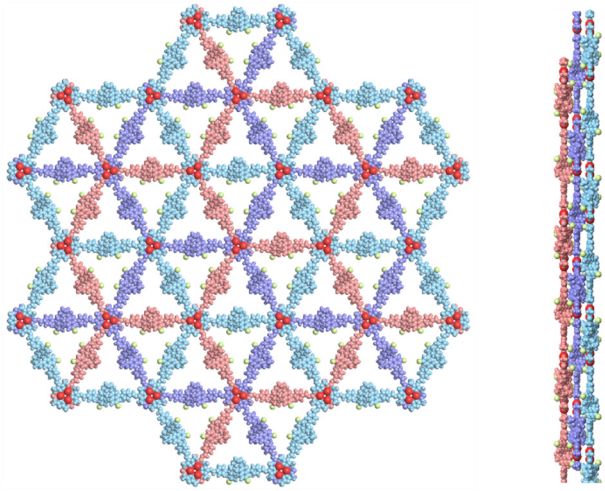


**Figure S22.** Space-filling mode of **(*R*)-JNM-11** in ABC stacking model viewed from (left) c axis and (right) a axis.

**Table S4.** AA stacking model for **(*R*)-JNM-11**.

Space group: *P3*
a = b = 55.4210 Å, and c = 4.0898 Å
α =β = 90°, and γ = 120°

| | X | Y | Z |
|---|---|---|---|
| Cu | 0.32217 | 0.62743 | 0.08994 |
| C | 0.37285 | 0.62215 | 0.13298 |
| Cu | 0.69463 | 0.37263 | 0.74183 |
| C | 0.44301 | 0.60459 | 0.36606 |
| C | 0.46912 | 0.62249 | 0.22523 |
| C | 0.49041 | 0.61599 | 0.23974 |
| C | 0.48608 | 0.59158 | 0.39562 |
| C | 0.45997 | 0.57381 | 0.5373 |
| C | 0.4387 | 0.58031 | 0.52402 |
| C | 0.50058 | 0.55787 | 0.24884 |
| C | 0.50759 | 0.58296 | 0.39562 |
| C | 0.53258 | 0.59689 | 0.56906 |
| C | 0.54839 | 0.58337 | 0.62813 |
| C | 0.54173 | 0.55726 | 0.47353 |
| C | 0.51635 | 0.54437 | 0.28422 |
| C | 0.5487 | 0.51478 | 0.58506 |
| C | 0.59115 | 0.55894 | 0.46861 |
| C | 0.60692 | 0.54481 | 0.49718 |
| C | 0.59366 | 0.51676 | 0.59648 |
| C | 0.56541 | 0.50322 | 0.65847 |
| C | 0.59551 | 0.4734 | 0.47431 |
| C | 0.60764 | 0.49975 | 0.6247 |
| C | 0.63153 | 0.50837 | 0.81761 |
| C | 0.64325 | 0.49134 | 0.85627 |
| C | 0.6308 | 0.46492 | 0.71067 |
| C | 0.60685 | 0.45611 | 0.51806 |
| C | 0.64265 | 0.44667 | 0.76827 |
| C | 0.41994 | 0.61056 | 0.34702 |
| N | 0.36164 | -0.27697 | 0.09378 |
| N | 0.33522 | -0.2836 | 0.09137 |
| N | 0.6189 | 0.28347 | 0.7424 |
| C | 0.62725 | 0.24918 | 0.72246 |
| C | 0.59859 | 0.23756 | 0.71744 |
| N | 0.57905 | 0.20856 | 0.67113 |
| C | 0.2604 | 0.59394 | 0.1271 |
| C | 0.23801 | 0.59837 | 0.15832 |
| N | 0.2095 | 0.57696 | 0.1969 |
| N | -0.27697 | 0.36182 | 0.74141 |
| C | -0.26005 | 0.33386 | 0.72623 |

| | | | |
|---|---|---|---|
| C | -0.01695 | 0.43923 | 0.50887 |
| C | 0.57036 | 0.59638 | 0.84925 |
| C | 0.58031 | 0.62371 | 0.95658 |
| C | 0.56622 | 0.63758 | 0.87519 |
| C | 0.5421 | 0.62404 | 0.68995 |
| C | 0.63575 | 0.55913 | 0.42404 |
| C | 0.64967 | 0.58707 | 0.33906 |
| C | 0.63533 | 0.60146 | 0.33109 |
| C | 0.60693 | 0.58774 | 0.39673 |
| Cl | 0.5783 | 0.67168 | 1.01377 |
| Cl | 0.68534 | 0.60414 | 0.24605 |
| O | 0.50672 | 0.51805 | 0.13722 |
| C | 0.48018 | 0.50434 | -0.03089 |
| C | 0.45462 | 0.49223 | 0.19243 |
| C | 0.50985 | 0.4709 | 0.41264 |
| O | 0.51986 | 0.49648 | 0.5957 |
| C | 0.4962 | 0.44506 | 0.62843 |
| C | 0.76588 | 0.40909 | 0.69846 |
| C | 0.43312 | 0.69318 | 0.14787 |
| C | 0.35636 | 0.59103 | 0.13642 |
| C | 0.56704 | 0.2599 | 0.68523 |
| H | 0.47306 | 0.6414 | 0.10153 |
| H | 0.51023 | 0.63013 | 0.13076 |
| H | 0.456 | 0.55471 | 0.65633 |
| H | 0.41877 | 0.56622 | 0.63494 |
| H | 0.48179 | 0.549 | 0.10596 |
| H | 0.55558 | 0.48203 | 0.74757 |
| H | 0.57712 | 0.46617 | 0.32299 |
| H | 0.64109 | 0.52825 | 0.9392 |
| H | 0.66162 | 0.49851 | 1.00762 |
| H | 0.5969 | 0.43591 | 0.40027 |
| H | 0.66162 | 0.45463 | 0.90902 |
| H | 0.40055 | 0.59653 | 0.46733 |
| H | 0.58098 | 0.58567 | 0.91529 |
| H | 0.59908 | 0.63436 | 1.10147 |
| H | 0.53142 | 0.63534 | 0.63784 |
| H | 0.648 | 0.549 | 0.4293 |
| H | 0.64612 | 0.62343 | 0.27062 |
| H | 0.59789 | 0.60057 | 0.38468 |
| H | 0.47819 | 0.48613 | -0.16193 |
| H | 0.47927 | 0.51805 | -0.21966 |
| H | 0.45464 | 0.47648 | 0.35875 |
| H | 0.43559 | 0.48146 | 0.03901 |
| H | 0.45299 | 0.50831 | 0.33451 |

| | | | |
|---|---|---|---|
| H | 0.52643 | 0.47056 | 0.26351 |
| H | 0.4937 | 0.46895 | 0.24159 |
| H | 0.48809 | 0.42624 | 0.47147 |
| H | 0.47834 | 0.44391 | 0.76386 |
| H | 0.5114 | 0.44463 | 0.79989 |
| H | 0.77716 | 0.41566 | 0.46282 |
| H | 0.78125 | 0.41827 | 0.89943 |
| H | 0.75096 | 0.41688 | 0.7137 |
| H | 0.43728 | 0.70455 | -0.08687 |
| H | 0.45051 | 0.68927 | 0.20095 |
| H | 0.43194 | 0.70634 | 0.34425 |
| H | 0.35468 | 0.58324 | 0.38962 |
| H | 0.36643 | 0.5824 | -0.02258 |
| H | 0.33497 | 0.58378 | 0.04392 |
| H | 0.5545 | 0.2524 | 0.91173 |
| H | 0.55509 | 0.24614 | 0.4787 |
| H | 0.57115 | 0.2813 | 0.63386 |

**Table S5.** AB stacking model for **(*R*)-JNM-11**.

Space group: *P3*
a = b = 55.4210 Å, and c = 15.9888 Å
α =β = 90°, and γ = 120°

| | X | Y | Z |
|---|---|---|---|
| Cu | 0.32217 | 0.62743 | 0.15425 |
| C | 0.37285 | 0.62215 | 0.16525 |
| Cu | 0.69463 | 0.37263 | 0.32099 |
| C | 0.44301 | 0.60459 | 0.22487 |
| C | 0.46912 | 0.62249 | 0.18885 |
| C | 0.49041 | 0.61599 | 0.19256 |
| C | 0.48608 | 0.59158 | 0.23243 |
| C | 0.45997 | 0.57381 | 0.26867 |
| C | 0.4387 | 0.58031 | 0.26528 |
| C | 0.50058 | 0.55787 | 0.19489 |
| C | 0.50759 | 0.58296 | 0.23243 |
| C | 0.53258 | 0.59689 | 0.2768 |
| C | 0.54839 | 0.58337 | 0.29191 |
| C | 0.54173 | 0.55726 | 0.25236 |
| C | 0.51635 | 0.54437 | 0.20394 |
| C | 0.5487 | 0.51478 | 0.28089 |
| C | 0.59115 | 0.55894 | 0.2511 |
| C | 0.60692 | 0.54481 | 0.25841 |
| C | 0.59366 | 0.51676 | 0.28381 |
| C | 0.56541 | 0.50322 | 0.29967 |

| | | | |
|---|---|---|---|
| C | 0.59551 | 0.4734 | 0.25256 |
| C | 0.60764 | 0.49975 | 0.29103 |
| C | 0.63153 | 0.50837 | 0.34037 |
| C | 0.64325 | 0.49134 | 0.35026 |
| C | 0.6308 | 0.46492 | 0.31302 |
| C | 0.60685 | 0.45611 | 0.26375 |
| C | 0.64265 | 0.44667 | 0.32775 |
| C | 0.41994 | 0.61056 | 0.22 |
| N | 0.36164 | 0.72303 | 0.15523 |
| N | 0.33522 | 0.7164 | 0.15461 |
| N | 0.6189 | 0.28347 | 0.32114 |
| C | 0.62725 | 0.24918 | 0.31604 |
| C | 0.59859 | 0.23756 | 0.31475 |
| N | 0.57905 | 0.20856 | 0.30291 |
| C | 0.2604 | 0.59394 | 0.16375 |
| C | 0.23801 | 0.59837 | 0.17174 |
| N | 0.2095 | 0.57696 | 0.1816 |
| N | 0.72303 | 0.36182 | 0.32088 |
| C | 0.73995 | 0.33386 | 0.317 |
| C | 0.98305 | 0.43923 | 0.2614 |
| C | 0.57036 | 0.59638 | 0.34847 |
| C | 0.58031 | 0.62371 | 0.37592 |
| C | 0.56622 | 0.63758 | 0.3551 |
| C | 0.5421 | 0.62404 | 0.30772 |
| C | 0.63575 | 0.55913 | 0.2397 |
| C | 0.64967 | 0.58707 | 0.21797 |
| C | 0.63533 | 0.60146 | 0.21593 |
| C | 0.60693 | 0.58774 | 0.23272 |
| Cl | 0.5783 | 0.67168 | 0.39055 |
| Cl | 0.68534 | 0.60414 | 0.19418 |
| O | 0.50672 | 0.51805 | 0.16634 |
| C | 0.48018 | 0.50434 | 0.12334 |
| C | 0.45462 | 0.49223 | 0.18046 |
| C | 0.50985 | 0.4709 | 0.23679 |
| O | 0.51986 | 0.49648 | 0.28361 |
| C | 0.4962 | 0.44506 | 0.29198 |
| C | 0.76588 | 0.40909 | 0.3099 |
| C | 0.43312 | 0.69318 | 0.16906 |
| C | 0.35636 | 0.59103 | 0.16614 |
| C | 0.56704 | 0.2599 | 0.30651 |
| H | 0.47306 | 0.6414 | 0.15721 |
| H | 0.51023 | 0.63013 | 0.16469 |
| H | 0.456 | 0.55471 | 0.29912 |
| H | 0.41877 | 0.56622 | 0.29365 |

| | | | |
|---|---|---|---|
| H | 0.48179 | 0.549 | 0.15834 |
| H | 0.55558 | 0.48203 | 0.32246 |
| H | 0.57712 | 0.46617 | 0.21386 |
| H | 0.64109 | 0.52825 | 0.37147 |
| H | 0.66162 | 0.49851 | 0.38898 |
| H | 0.5969 | 0.43591 | 0.23362 |
| H | 0.66162 | 0.45463 | 0.36376 |
| H | 0.40055 | 0.59653 | 0.25078 |
| H | 0.58098 | 0.58567 | 0.36536 |
| H | 0.59908 | 0.63436 | 0.41298 |
| H | 0.53142 | 0.63534 | 0.29439 |
| H | 0.648 | 0.549 | 0.24105 |
| H | 0.64612 | 0.62343 | 0.20046 |
| H | 0.59789 | 0.60057 | 0.22964 |
| H | 0.47819 | 0.48613 | 0.08982 |
| H | 0.47927 | 0.51805 | 0.07505 |
| H | 0.45464 | 0.47648 | 0.223 |
| H | 0.43559 | 0.48146 | 0.14122 |
| H | 0.45299 | 0.50831 | 0.2168 |
| H | 0.52643 | 0.47056 | 0.19864 |
| H | 0.4937 | 0.46895 | 0.19303 |
| H | 0.48809 | 0.42624 | 0.25183 |
| H | 0.47834 | 0.44391 | 0.32663 |
| H | 0.5114 | 0.44463 | 0.33584 |
| H | 0.77716 | 0.41566 | 0.24962 |
| H | 0.78125 | 0.41827 | 0.3613 |
| H | 0.75096 | 0.41688 | 0.31379 |
| H | 0.43728 | 0.70455 | 0.10902 |
| H | 0.45051 | 0.68927 | 0.18264 |
| H | 0.43194 | 0.70634 | 0.21929 |
| H | 0.35468 | 0.58324 | 0.2309 |
| H | 0.36643 | 0.5824 | 0.12546 |
| H | 0.33497 | 0.58378 | 0.14247 |
| H | 0.5545 | 0.2524 | 0.36445 |
| H | 0.55509 | 0.24614 | 0.25368 |
| H | 0.57115 | 0.2813 | 0.29337 |
| Cu | 0.6555 | 0.2941 | 0.65425 |
| C | 0.70619 | 0.28881 | 0.66525 |
| Cu | 0.02796 | 0.0393 | 0.82099 |
| C | 0.77634 | 0.27126 | 0.72487 |
| C | 0.80245 | 0.28916 | 0.68885 |
| C | 0.82374 | 0.28265 | 0.69256 |
| C | 0.81941 | 0.25825 | 0.73243 |
| C | 0.79331 | 0.24048 | 0.76867 |

| | | | |
|---|---|---|---|
| C | 0.77203 | 0.24698 | 0.76528 |
| C | 0.83391 | 0.22454 | 0.69489 |
| C | 0.84093 | 0.24963 | 0.73243 |
| C | 0.86592 | 0.26356 | 0.7768 |
| C | 0.88173 | 0.25003 | 0.79191 |
| C | 0.87506 | 0.22393 | 0.75236 |
| C | 0.84969 | 0.21103 | 0.70394 |
| C | 0.88203 | 0.18144 | 0.78089 |
| C | 0.92449 | 0.22561 | 0.7511 |
| C | 0.94025 | 0.21148 | 0.75841 |
| C | 0.927 | 0.18343 | 0.78381 |
| C | 0.89874 | 0.16989 | 0.79967 |
| C | 0.92885 | 0.14007 | 0.75256 |
| C | 0.94097 | 0.16641 | 0.79103 |
| C | 0.96486 | 0.17504 | 0.84037 |
| C | 0.97658 | 0.15801 | 0.85026 |
| C | 0.96414 | 0.13159 | 0.81302 |
| C | 0.94019 | 0.12278 | 0.76375 |
| C | 0.97598 | 0.11334 | 0.82775 |
| C | 0.75328 | 0.27722 | 0.72 |
| N | 0.69497 | 0.3897 | 0.65523 |
| N | 0.66855 | 0.38307 | 0.65461 |
| N | 0.95224 | 0.95013 | 0.82114 |
| C | 0.96059 | 0.91585 | 0.81604 |
| C | 0.93193 | 0.90423 | 0.81475 |
| N | 0.91238 | 0.87523 | 0.80291 |
| C | 0.59373 | 0.2606 | 0.66375 |
| C | 0.57134 | 0.26504 | 0.67174 |
| N | 0.54284 | 0.24363 | 0.6816 |
| N | 0.05636 | 0.02848 | 0.82088 |
| C | 0.07328 | 0.00052 | 0.817 |
| C | 0.31639 | 0.1059 | 0.7614 |
| C | 0.90369 | 0.26305 | 0.84847 |
| C | 0.91365 | 0.29038 | 0.87592 |
| C | 0.89956 | 0.30424 | 0.8551 |
| C | 0.87544 | 0.29071 | 0.80772 |
| C | 0.96908 | 0.2258 | 0.7397 |
| C | 0.98301 | 0.25374 | 0.71797 |
| C | 0.96867 | 0.26813 | 0.71593 |
| C | 0.94026 | 0.25441 | 0.73272 |
| Cl | 0.91164 | 0.33835 | 0.89055 |
| Cl | 0.01867 | 0.27081 | 0.69418 |
| O | 0.84005 | 0.18472 | 0.66634 |
| C | 0.81352 | 0.171 | 0.62334 |

| | | | |
|---|---|---|---|
| C | 0.78796 | 0.15889 | 0.68046 |
| C | 0.84318 | 0.13757 | 0.73679 |
| O | 0.8532 | 0.16315 | 0.78361 |
| C | 0.82953 | 0.11173 | 0.79198 |
| C | 0.09921 | 0.07575 | 0.8099 |
| C | 0.76645 | 0.35985 | 0.66906 |
| C | 0.68969 | 0.2577 | 0.66614 |
| C | 0.90037 | 0.92656 | 0.80651 |
| H | 0.80639 | 0.30807 | 0.65721 |
| H | 0.84356 | 0.2968 | 0.66469 |
| H | 0.78933 | 0.22138 | 0.79912 |
| H | 0.7521 | 0.23289 | 0.79365 |
| H | 0.81513 | 0.21567 | 0.65834 |
| H | 0.88891 | 0.1487 | 0.82246 |
| H | 0.91046 | 0.13283 | 0.71386 |
| H | 0.97443 | 0.19492 | 0.87147 |
| H | 0.99496 | 0.16517 | 0.88898 |
| H | 0.93023 | 0.10257 | 0.73362 |
| H | 0.99495 | 0.12129 | 0.86376 |
| H | 0.73388 | 0.26319 | 0.75078 |
| H | 0.91432 | 0.25234 | 0.86536 |
| H | 0.93242 | 0.30103 | 0.91298 |
| H | 0.86475 | 0.30201 | 0.79439 |
| H | 0.98134 | 0.21567 | 0.74105 |
| H | 0.97946 | 0.2901 | 0.70046 |
| H | 0.93122 | 0.26724 | 0.72964 |
| H | 0.81152 | 0.15279 | 0.58982 |
| H | 0.81261 | 0.18471 | 0.57505 |
| H | 0.78797 | 0.14314 | 0.723 |
| H | 0.76892 | 0.14813 | 0.64122 |
| H | 0.78633 | 0.17497 | 0.7168 |
| H | 0.85977 | 0.13723 | 0.69864 |
| H | 0.82704 | 0.13561 | 0.69303 |
| H | 0.82142 | 0.0929 | 0.75183 |
| H | 0.81167 | 0.11058 | 0.82663 |
| H | 0.84474 | 0.11129 | 0.83584 |
| H | 0.1105 | 0.08233 | 0.74962 |
| H | 0.11458 | 0.08494 | 0.8613 |
| H | 0.08429 | 0.08355 | 0.81379 |
| H | 0.77061 | 0.37122 | 0.60902 |
| H | 0.78385 | 0.35594 | 0.68264 |
| H | 0.76527 | 0.373 | 0.71929 |
| H | 0.68801 | 0.24991 | 0.7309 |
| H | 0.69977 | 0.24906 | 0.62546 |

| | | | |
|---|---|---|---|
| H | 0.66831 | 0.25045 | 0.64247 |
| H | 0.88784 | 0.91907 | 0.86445 |
| H | 0.88843 | 0.91281 | 0.75368 |
| H | 0.90448 | 0.94796 | 0.79337 |

**Table S6.** ABC stacking model for **(*R*)-JNM-11**.

Space group: *R3*

a = b = 55.4540 Å, and c = 15.0000 Å

α =β = 90°, and γ = 120°

| | X | Y | Z |
|---|---|---|---|
| N | 0.62815 | 0.3482 | 0.17371 |
| N | 0.62835 | 0.27935 | 0.17516 |
| C | 0.64647 | 0.25573 | 0.17272 |
| C | 0.62019 | 0.23822 | 0.17407 |
| C | 0.61011 | 0.25471 | 0.17578 |
| Cu | 0.62828 | 0.31395 | 0.17405 |
| N | 0.61046 | 0.21114 | 0.17234 |
| C | 0.46756 | 0.49699 | 0.13696 |
| C | 0.45307 | 0.51006 | 0.13544 |
| C | 0.46231 | 0.5347 | 0.17369 |
| C | 0.48611 | 0.54374 | 0.20854 |
| C | 0.50021 | 0.53082 | 0.21031 |
| C | 0.49209 | 0.50686 | 0.17607 |
| C | 0.44714 | 0.55009 | 0.17615 |
| C | 0.4573 | 0.57572 | 0.15505 |
| C | 0.44408 | 0.58898 | 0.15665 |
| C | 0.41857 | 0.57843 | 0.17927 |
| C | 0.40859 | 0.55296 | 0.20103 |
| C | 0.42177 | 0.53978 | 0.20022 |
| C | 0.39863 | 0.58904 | 0.18286 |
| N | 0.37223 | 0.65192 | 0.17774 |
| N | 0.37154 | 0.72097 | 0.18032 |
| C | 0.35331 | 0.74451 | 0.17627 |
| C | 0.37959 | 0.76209 | 0.17846 |
| C | 0.38974 | 0.74568 | 0.18156 |
| Cu | 0.37177 | 0.68644 | 0.17936 |
| N | 0.38925 | 0.78933 | 0.17568 |
| C | 0.50753 | 0.49172 | 0.17894 |
| C | 0.5303 | 0.49905 | 0.13548 |
| C | 0.54349 | 0.48523 | 0.13588 |
| C | 0.53603 | 0.46268 | 0.17946 |
| C | 0.51286 | 0.45448 | 0.22746 |
| C | 0.49935 | 0.46853 | 0.22654 |
| C | 0.55181 | 0.44798 | 0.17691 |

| | | | |
|---|---|---|---|
| C | 0.57792 | 0.45975 | 0.18804 |
| C | 0.59191 | 0.44739 | 0.18699 |
| C | 0.58219 | 0.42147 | 0.17482 |
| C | 0.55607 | 0.40962 | 0.16282 |
| C | 0.54204 | 0.42201 | 0.16319 |
| C | 0.6023 | 0.41137 | 0.17686 |
| C | 0.66646 | 0.24956 | 0.17086 |
| C | 0.58374 | 0.24785 | 0.17726 |
| H | 0.49493 | 0.56175 | 0.23975 |
| O | 0.52344 | 0.54228 | 0.25037 |
| H | 0.47648 | 0.58621 | 0.13411 |
| H | 0.45449 | 0.6083 | 0.13778 |
| H | 0.3893 | 0.54235 | 0.22081 |
| H | 0.41144 | 0.5206 | 0.22098 |
| H | 0.38083 | 0.57216 | 0.1947 |
| O | 0.54009 | 0.52113 | 0.08809 |
| H | 0.56035 | 0.4932 | 0.09694 |
| H | 0.58821 | 0.47951 | 0.19992 |
| H | 0.6117 | 0.45904 | 0.19695 |
| H | 0.54576 | 0.38984 | 0.15183 |
| H | 0.5224 | 0.41043 | 0.15089 |
| H | 0.62032 | 0.42829 | 0.18442 |
| C | 0.33293 | 0.75011 | 0.17412 |
| C | 0.41617 | 0.75254 | 0.18481 |
| C | 0.42973 | 0.49801 | 0.09307 |
| C | 0.42045 | 0.47503 | 0.0557 |
| C | 0.43347 | 0.46226 | 0.05716 |
| C | 0.45649 | 0.47335 | 0.09654 |
| C | 0.47738 | 0.45866 | 0.27778 |
| C | 0.46821 | 0.43711 | 0.32642 |
| C | 0.48134 | 0.42444 | 0.3266 |
| C | 0.50291 | 0.43274 | 0.27987 |
| Cl | 0.46932 | 0.39616 | 0.39186 |
| Cl | 0.39049 | 0.46066 | 0.00075 |
| C | 0.56488 | 0.53229 | 0.04927 |
| C | 0.57128 | 0.55777 | 0.01786 |
| C | 0.5349 | 0.56796 | 0.28065 |
| C | 0.5611 | 0.57561 | 0.30697 |
| H | 0.57723 | 0.09007 | 0.28391 |
| H | 0.5312 | 0.99877 | 0.27873 |
| H | 0.56997 | 0.02123 | 0.36428 |
| H | 0.75129 | 0.35158 | 0.84055 |
| H | 0.76 | 0.33245 | 0.78122 |
| H | 0.76066 | 0.33294 | 0.89923 |

| | | | |
|---|---|---|---|
| H | 0.74337 | 0.42161 | 0.23031 |
| H | 0.74265 | 0.42082 | 0.11157 |
| H | 0.77048 | 0.42852 | 0.16938 |
| H | 0.76296 | 0.3374 | 0.2371 |
| H | 0.76329 | 0.33724 | 0.11858 |
| H | 0.73564 | 0.31761 | 0.17706 |
| H | 0.89819 | 0.18756 | 0.65995 |
| H | 0.91122 | 0.19994 | 0.76732 |
| H | 0.90407 | 0.23525 | 0.7411 |
| H | 0.89149 | 0.22332 | 0.63391 |
| H | 0.92315 | 0.23385 | 0.65563 |
| H | 0.85785 | 0.23583 | 1.0045 |
| H | 0.8679 | 0.24609 | 0.89226 |
| H | 0.90391 | 0.26139 | 0.99702 |
| H | 0.90442 | 0.24078 | 0.91611 |
| H | 0.89459 | 0.2305 | 1.02747 |
| H | 0.09403 | 0.1044 | 0.54581 |
| H | 0.09002 | 0.08566 | 0.45124 |
| H | 0.08528 | 0.073 | 0.56062 |
| H | 0.75893 | 0.11086 | 0.69358 |
| H | 0.80022 | 0.13047 | 0.76301 |
| H | 0.75266 | 0.17417 | 0.75511 |

## 8. Gas adsorption isotherms and the pore size distribution

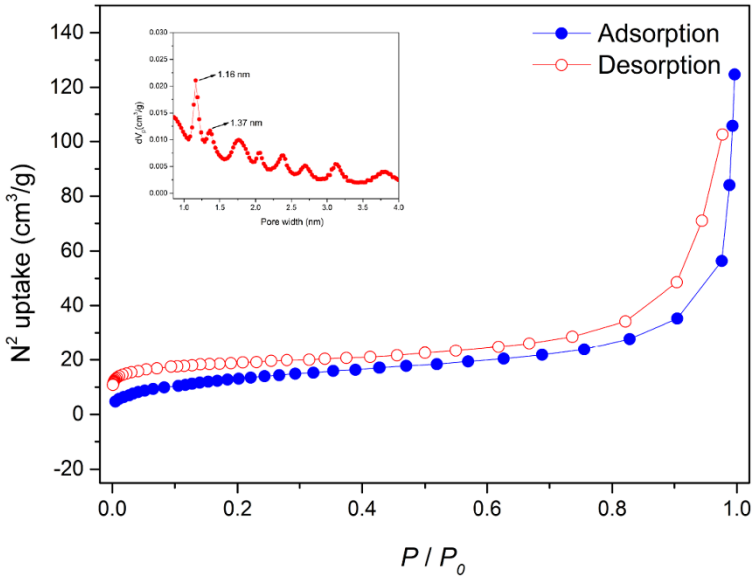



**Figure S23.** The $N_2$ adsorption and desorption isotherm profiles of **(*R*)-JNM-10** at 77 K and the Brunauer−Emmett−Teller (BET) surface areas of **(*R*)-JNM-10** are calculated to be 47.24 $m^2\ g^{-1}$. Inset, the pore size distribution profiles of **(*R*)-JNM-10** calculated by nonlocal DFT modeling based on $N_2$ adsorption data, showing the pore size at 1.16 and 1.37 nm.

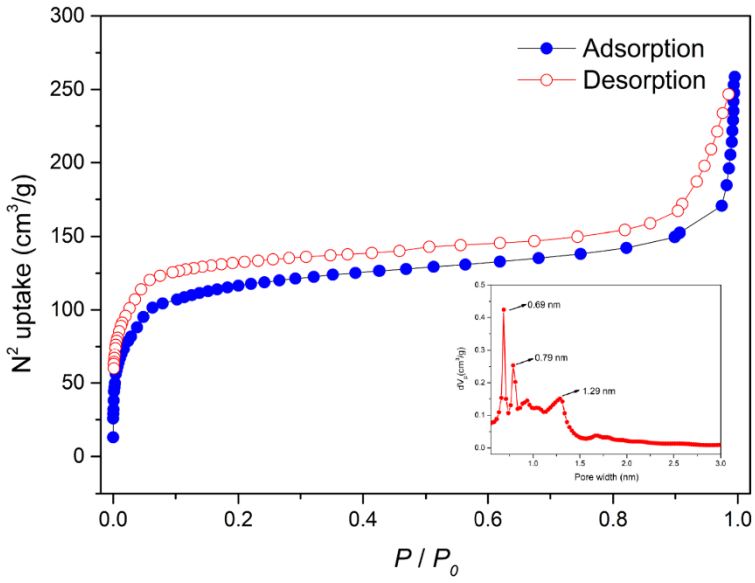



**Figure S24.** The $N_2$ adsorption and desorption isotherm profiles of **(*R*)-JNM-11** at 77 K and the Brunauer−Emmett−Teller (BET) surface areas of **(*R*)-JNM-11** are calculated to be 416.43 $m^2\ g^{-1}$. Inset, the pore size distribution profiles of **(*R*)-JNM-11** calculated by nonlocal DFT modeling based on $N_2$ adsorption data, showing the pore size at 0.69, 0.79 and 1.29 nm.

## 9. Transmission electron microscopy (TEM)

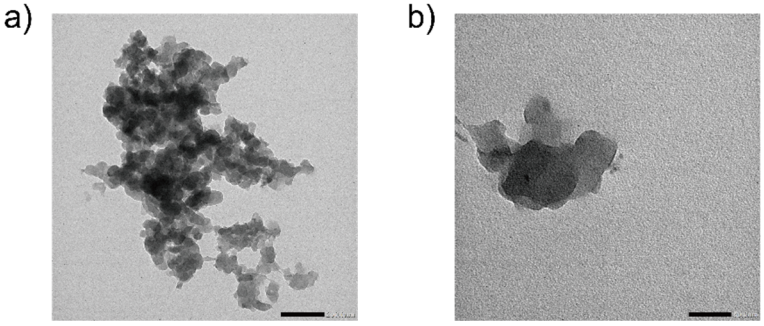



**Figure S25.** TEM images of **(*R*)-JNM-10**.

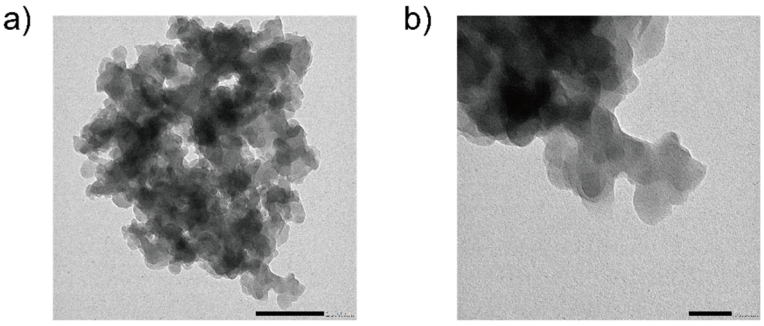



**Figure S26.** TEM images of **(*R*)-JNM-11**.

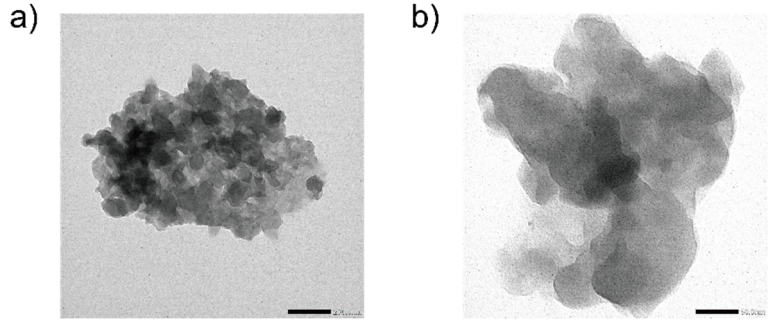



**Figure S27.** TEM images of **(*S*)-JNM-10**.

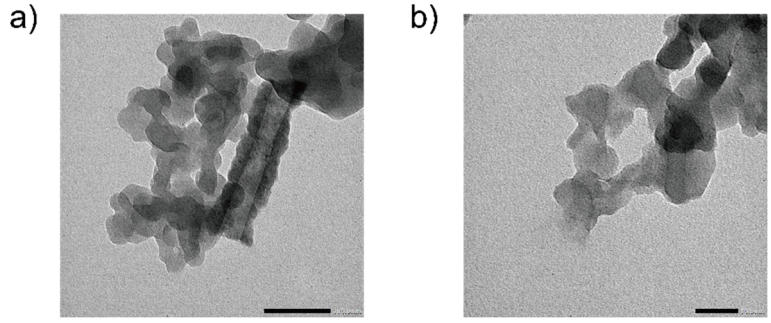



**Figure S28.** TEM images of **(*S*)-JNM-11**.

## 10. Thermogravimetric analysis (TGA)

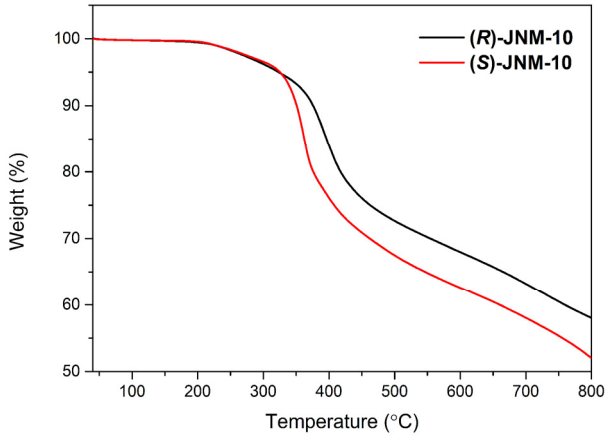



**Figure S29.** TGA curve of **(*R*)-JNM-10** and **(*S*)-JNM-10** under $N_2$ atmosphere.

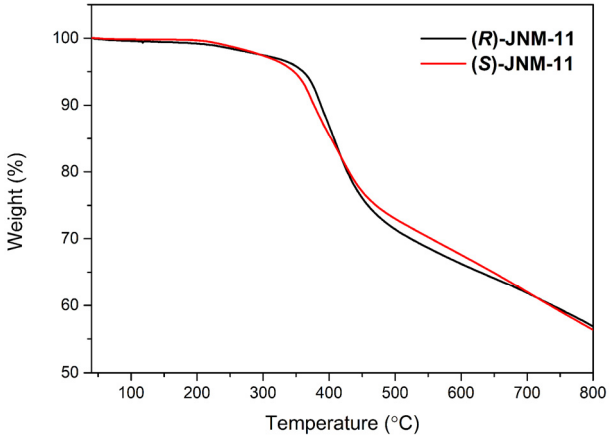



**Figure S30.** TGA curve of **(*R*)-JNM-11** and **(*S*)-JNM-11** under $N_2$ atmosphere.

## 11. Various-Temperature PXRD

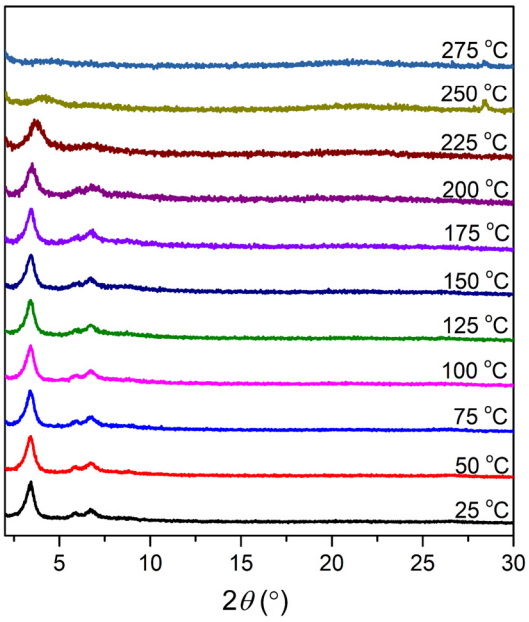



**Figure S31.** *In-situ* variable-temperature PXRD patterns of **(*R*)-JNM-10** under air atmosphere.

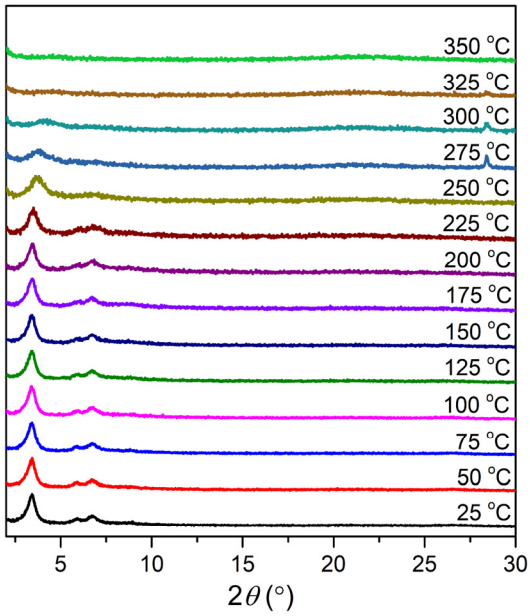



**Figure S32.** *In-situ* variable-temperature PXRD patterns of **(*R*)-JNM-11** under air atmosphere.

## 12. X-ray photoelectron spectroscopy (XPS)

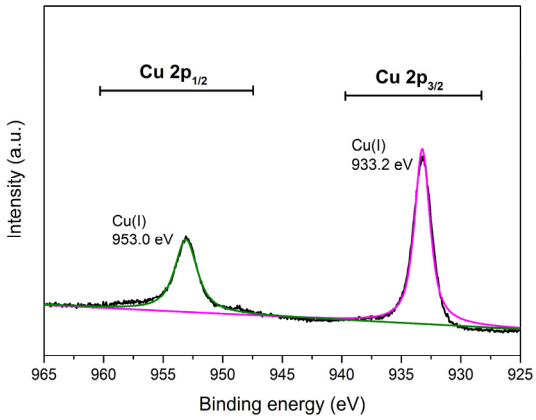



**Figure S33.** XPS spectrum of **(*R*)-JNM-10** exposed to air for over one month.

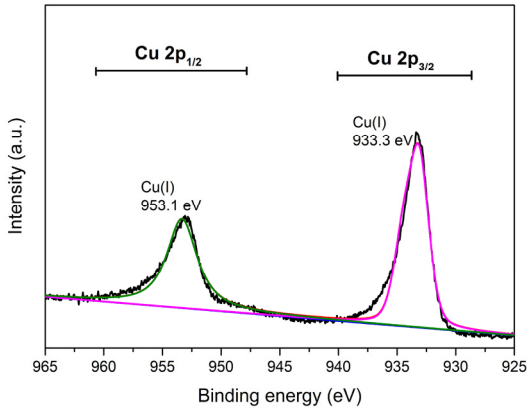



**Figure S34.** XPS spectrum of **(*R*)-JNM-11** exposed to air for over one month.

## 13. Stability in various solvents

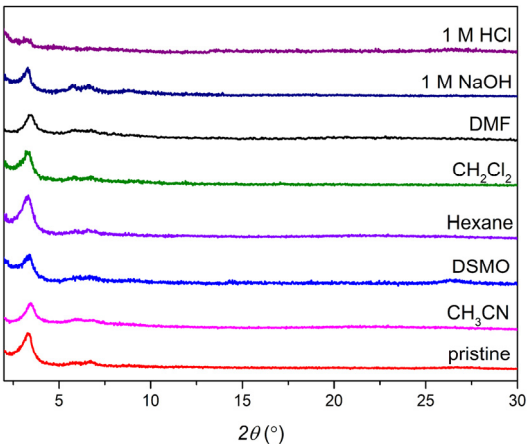



**Figure S35.** PXRD patterns for samples of **(*R*)-JNM-10** after treatment with different solvents for 3 d.

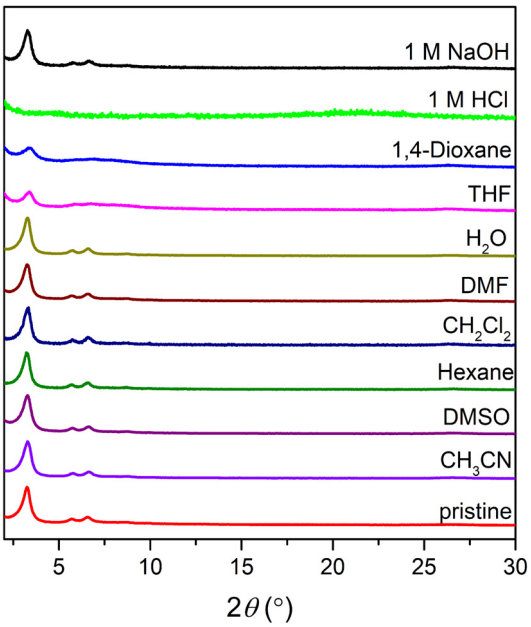



**Figure S36.** PXRD patterns for samples of **(*R*)-JNM-11** after treatment with different solvents for 3 d.

## 14. Solid-state UV−vis absorption spectra

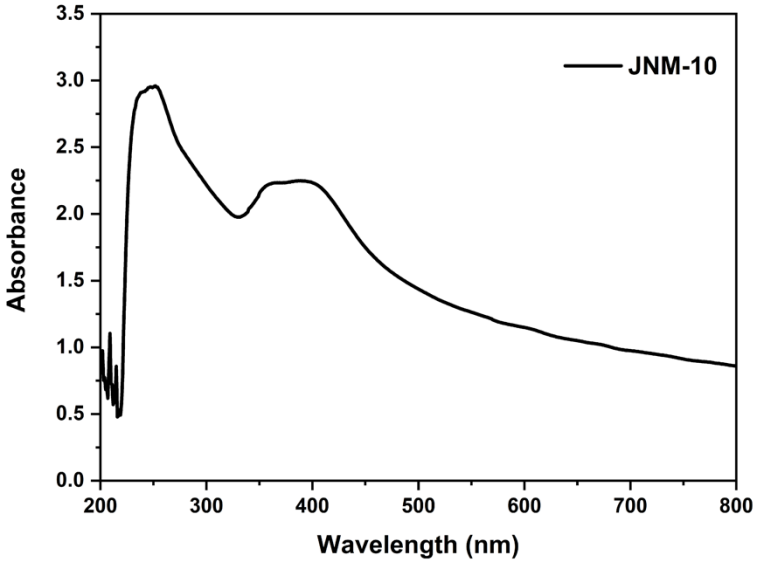



**Figure S37.** Solid-state UV−vis absorption spectra of **JNM-10**.

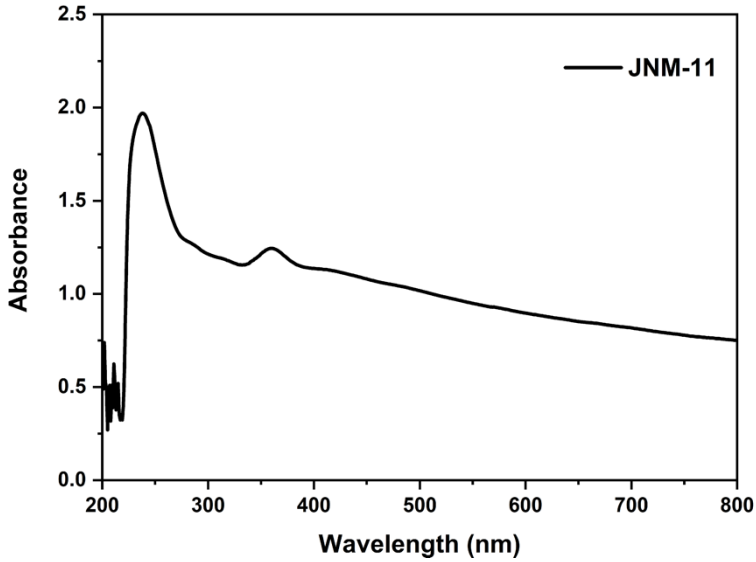



**Figure S38.** Solid-state UV−vis absorption spectra of **JNM-11**.

## 15. CD spectra of ligands and JNMs

For chiral ligands, 1.0 mg of samples were dissolved in $CH_3CN$ (10 mL). For JNM-10 and JNM-11, 5.0 mg of samples were dispersed in $CH_3CN$ (10 mL).

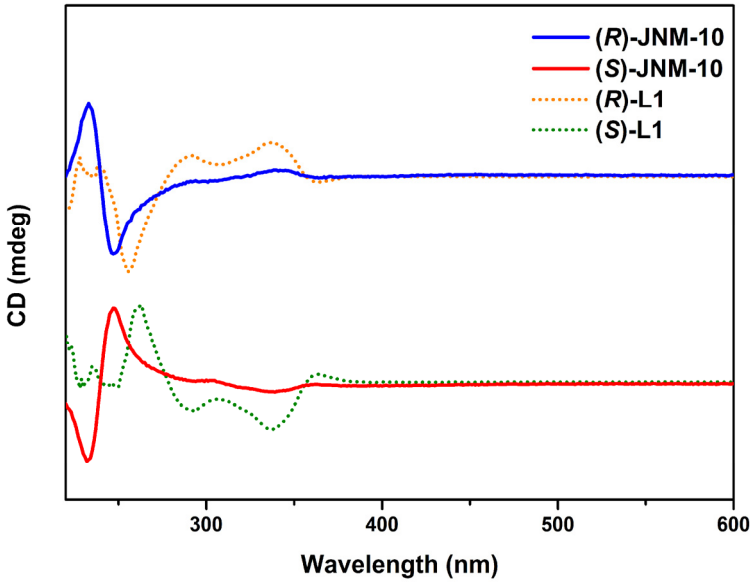



**Figure S39.** CD spectra of **L1** and **JNM-10**.

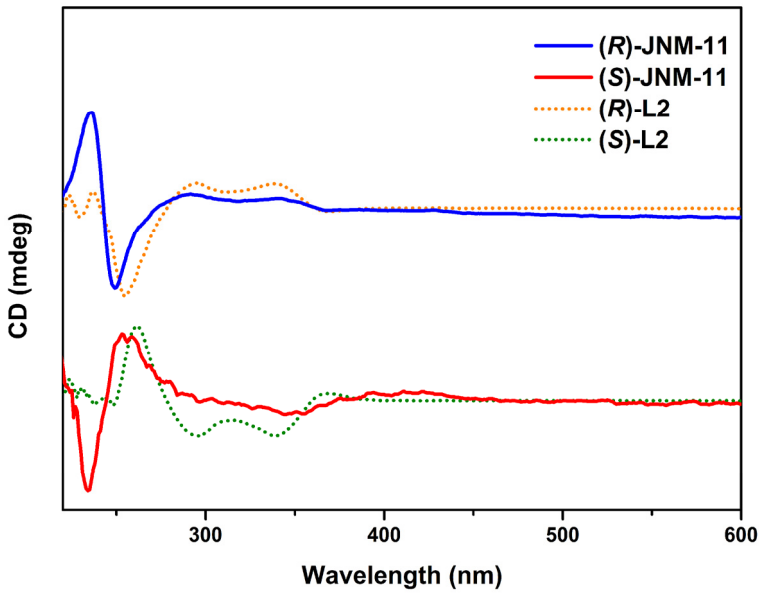



**Figure S40.** CD spectra of **L2** and **JNM-11**.

## 16. Dye adsorption and degradation

The adsorption experiments were conducted at r.t. in a dark condition. Initial concentrations of Methylene Blue (MB), Chrome azurol S (CA) and Rhodamine B (RhB) were fixed to be 10 μM. Typically 10 mg of **(*R*)-JNM-10** or **(*R*)-JNM-11** was added into aqueous solution of Methylene Blue (MB) or Rhodamine B (RB) (10 mL), then the mixture was stirred at rt. At appropriate time interval, the mixture was filtered and detected using an ultraviolet-visible spectrometer.

The removal efficiency of dye was calculated as following equation (1):

$$\text{Removal efficiency (\%)} = (C_0 - C_t) / C_0 \times 100 \quad (1)$$

Where $C_0$ and $C_t$ are the concentration of dyes at initial condition and in the filtrate, respectively.

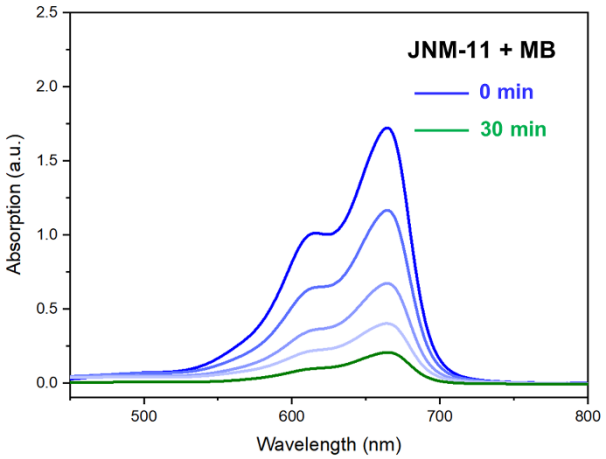



**Figure S41.** UV−vis absorption spectra of an aqueous solution of MB after treatment with **JNM-11** at different intervals.

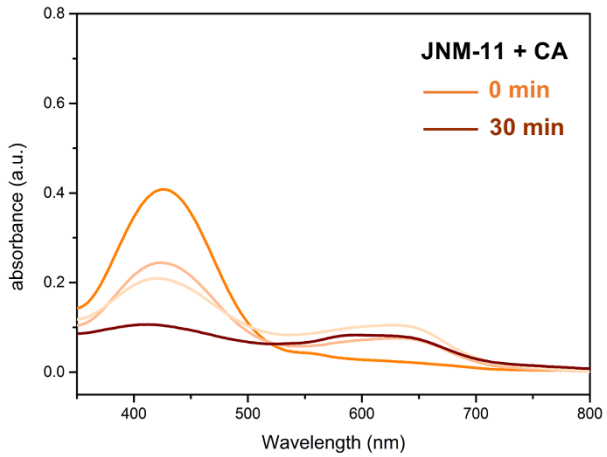



**Figure S42.** UV−vis absorption spectra of an aqueous solution of CA after treatment with **JNM-11** at different intervals.

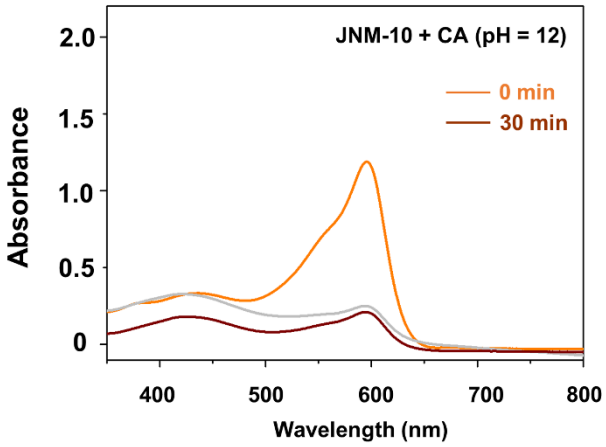



**Figure S43.** UV−vis absorption spectra of a pH = 12 aqueous solution of CA after treatment with **JNM-10** at different intervals.

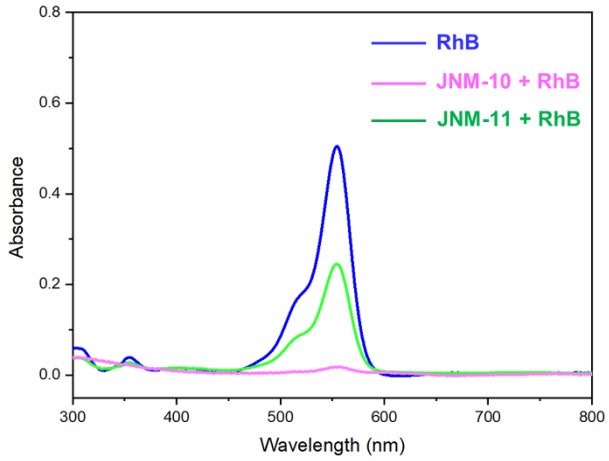
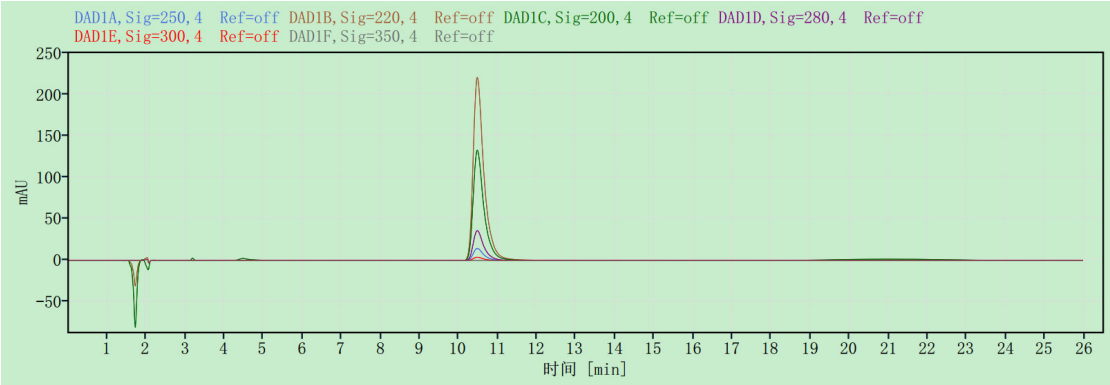



**Figure S44.** UV-vis absorption spectra of an aqueous solution of RhB after mixing with **JNM-10** or **JNM-11** for 30 min.

The dye degradation chose 300 W xenon lamp as light source. Initial concentrations of Rhodamine B (RhB) was fixed to be 100 μM. Typically 10 mg of **(*R*)-JNM-10** or **(*R*)-JNM-11** was added into RhB aqueous solution (10 mL) and 250 uL $H_2O_2$ then injected, the mixture was stirred at r.t. At appropriate time interval, the mixture was filtered and the solution was detected using an ultraviolet-visible spectrometer. The degradation efficiency of dye was calculated as equation (1).

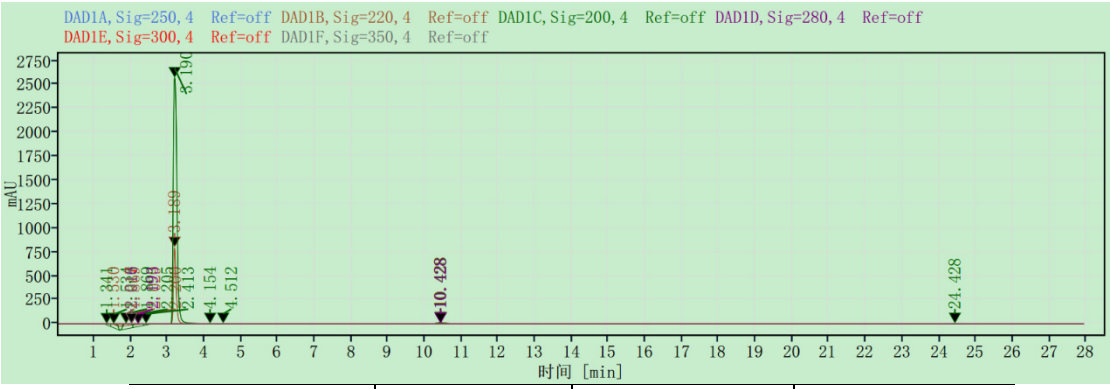
## 17. Chiral recognition.

The chiral recognition was conducted at r.t.. Initial concentrations of amino acids were fixed to be 1 × $10^{-4}$ moL/L. Typically 10 mg of **(*R*)-JNM-10** or **(*R*)-JNM-11** was added into 10 mL amino acids aqueous solutions and the mixture was stirred at r.t. At appropriate time interval, the mixture was filtered and the solution was detected using HPLC.



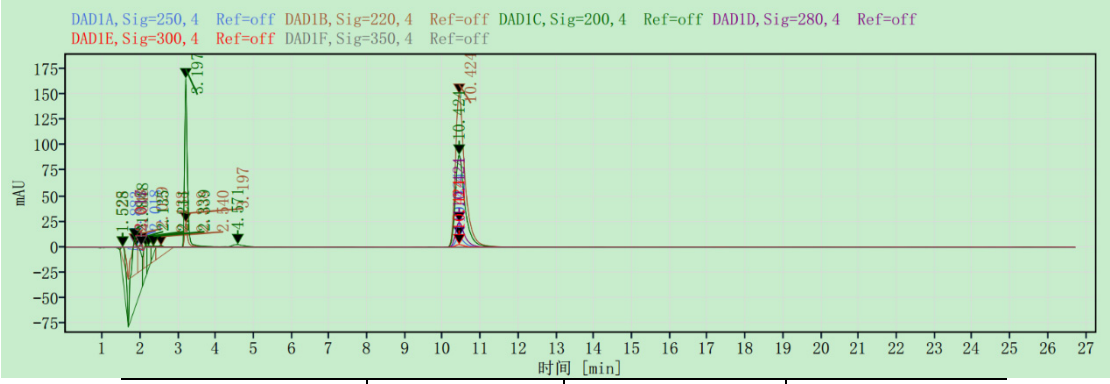

| name | Ret. Time | Height | Area |
|---|---|---|---|
| D/L-Tryptophan | 10.475 | 220.62 | 4284.03 |

**Figure S45.** D/L-Tryptophan standard sample (Sig=220).



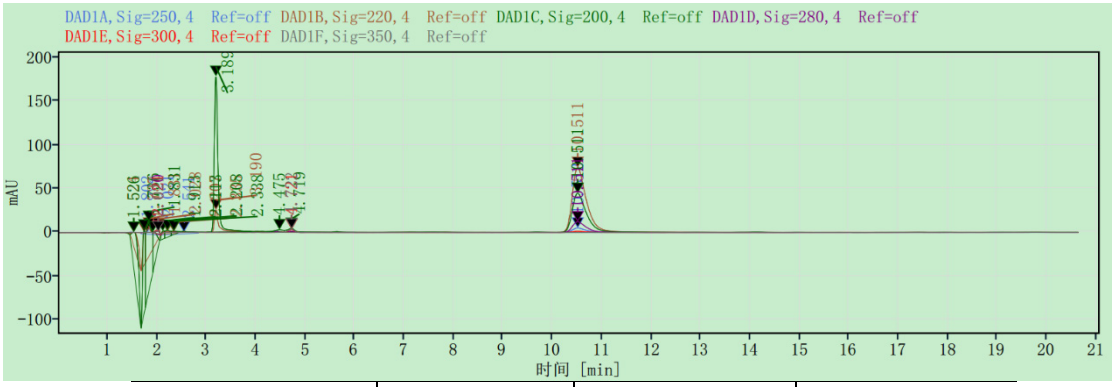

| name | Ret. Time | Height | Area |
|---|---|---|---|
| L-Tryptophan | 10.428 | 14.28 | 278.45 |

**Figure S46.** L-Tryptophan + (*R*)-JNM-10, 2 h. (Sig=220).



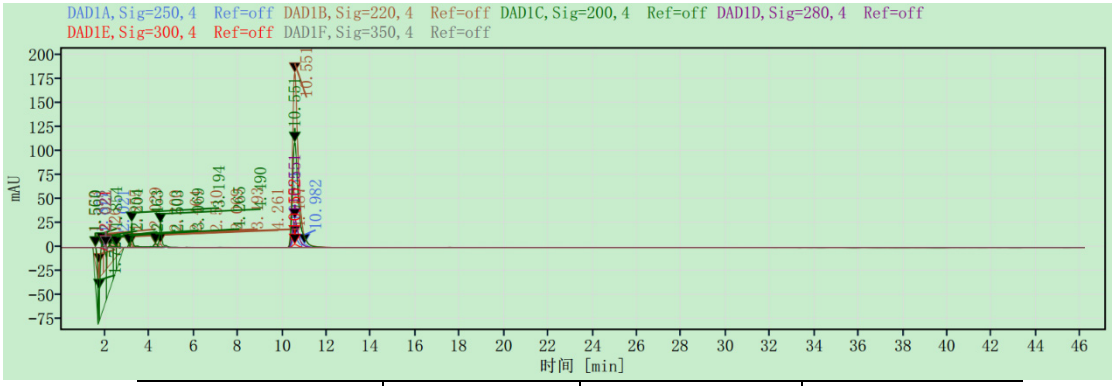

| name | Ret. Time | Height | Area |
|---|---|---|---|
| D-Tryptophan | 10.424 | 150.10 | 2656.83 |

**Figure S47.** D-Tryptophan + (*R*)-JNM-10, 2 h. (Sig=220).



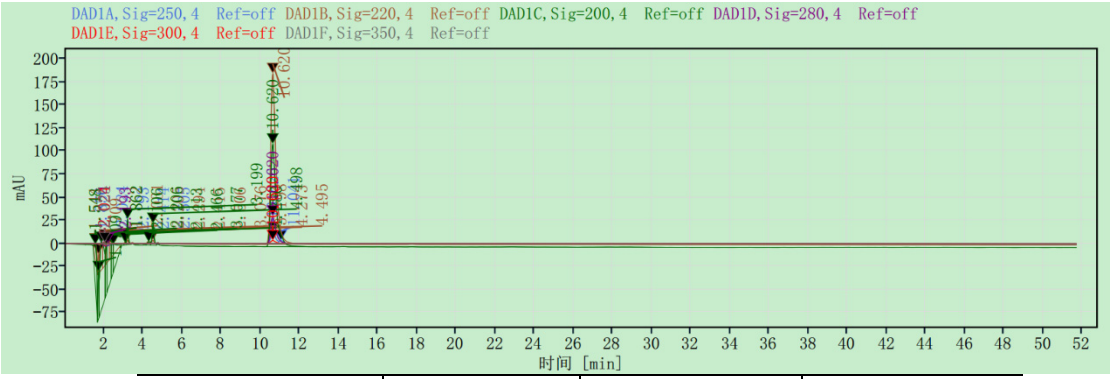

| name | Ret. Time | Height | Area |
|---|---|---|---|
| D-Tryptophan | 10.511 | 74.16 | 1495.55 |

**Figure S48.** D-Tryptophan + (*R*)-JNM-10, 24 h. (Sig=220).




| name | Ret. Time | Height | Area |
|---|---|---|---|
| L-Tryptophan | 10.551 | 181.34 | 3383.45 |

**Figure S49.** L-Tryptophan + (*R*)-JNM-11, 24 h. (Sig=220).




| name | Ret. Time | Height | Area |
|---|---|---|---|
| D-Tryptophan | 10.620 | 185.51 | 3533.54 |

**Figure S50.** D-Tryptophan + (*R*)-JNM-11, 24 h. (Sig=220).