Supplementary Information

Fabrication of Multi-functional Molecular Tunnelling Junctions by Click Chemistry

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1 Materials and Synthesis

1.1 Materials and Characterizations

All commercial reagents and solvents were used as received without further purification unless otherwise mentioned. Column chromatography was performed with silica gel (pore size 60 Å, 230-400 mesh particle size) and thin layer chromatography (TLC) was performed on silica gel with GF254 indicator. All yields given refer to isolated yields unless otherwise noted. Nuclear magnetic resonance (NMR) spectra were recorded on a 400 MHz Bruker spectrometer. Chemical shifts were reported in ppm. Coupling constants (J values) were reported in Hertz. ^{1}H NMR chemical shifts were referenced to $CHCl_3$ (7.26 ppm).

1.2 Synthesis and characterization of $N_3(CH_2)_{11}SH$

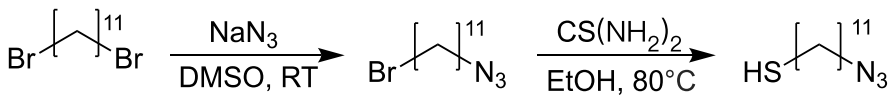
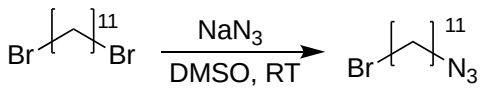


Figure S1. The synthetic route of target molecule $N_3(CH_2)_{11}SH$.

Synthesis

Compound $N_3(CH_2)_{11}Br$



We synthesized $N_3(CH_2)_{11}Br$ according to a procedure reported in the literature[1]. A round-bottom flask was used to add with 1,11-dibromoundecane (2.0 g, 6.37 mmol) and sodium azide (0.42 g, 6.37 mmol). To the solid mixture was added DMSO (35 mL).

The solution was stirred vigorously at room temperature for 8 h. The solution was diluted with water (30 mL). The aqueous phase was extracted with ether (3 × 30 mL) and the combined organic phase was washed with water (2 × 20 mL), dried over $MgSO_4$, filtered, and concentrated under reduced pressure. The reaction mixture was purified by flash chromatography to afford the desired product as a colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.41 (t, J = 6.9 Hz, 2H), 3.26 (s, 2H), 1.65 – 1.54 (m, 4H), 1.48 – 1.23 (m, 14H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 51.48, 33.93, 32.83, 29.40, 29.39, 29.37, 29.11, 28.83, 28.73, 28.15, 26.70. TOF-MS m/z calc for $C_{11}H_{23}N_3Br$ $[M+H]^+$ 276.1075, found 276.1061.

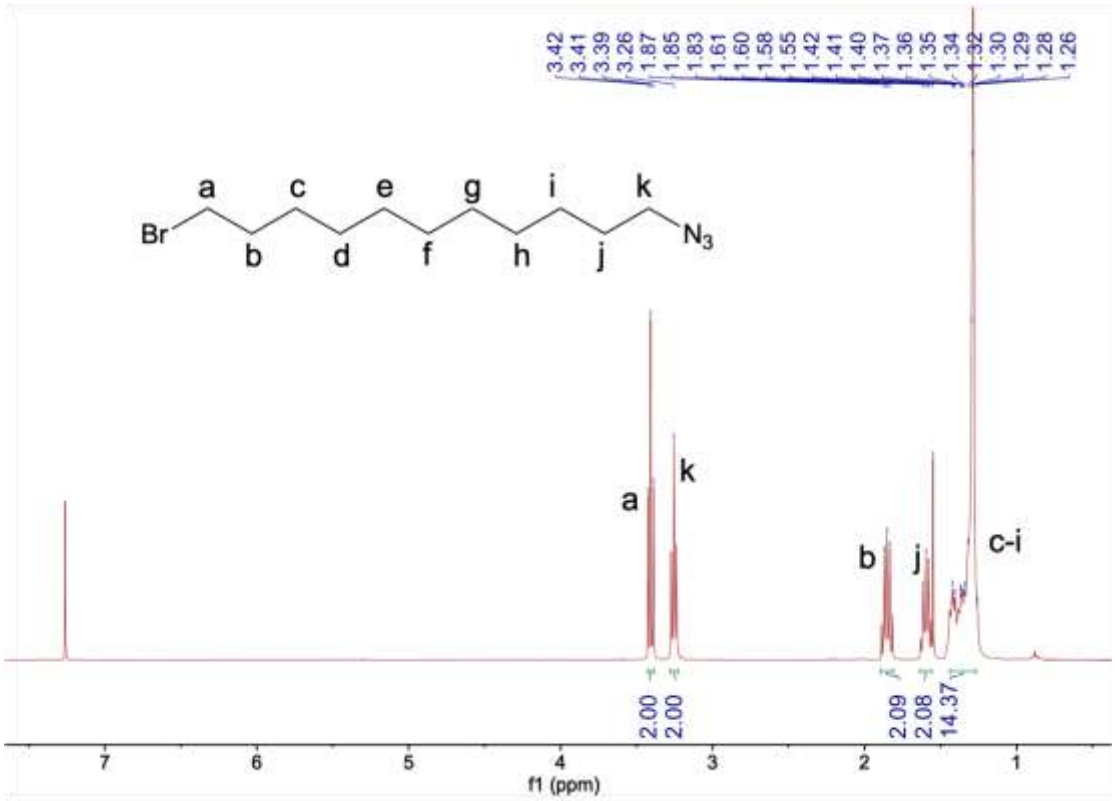


Figure S2 The ^{1}H-NMR spectrum of $N_3(CH_2)_{11}Br$.

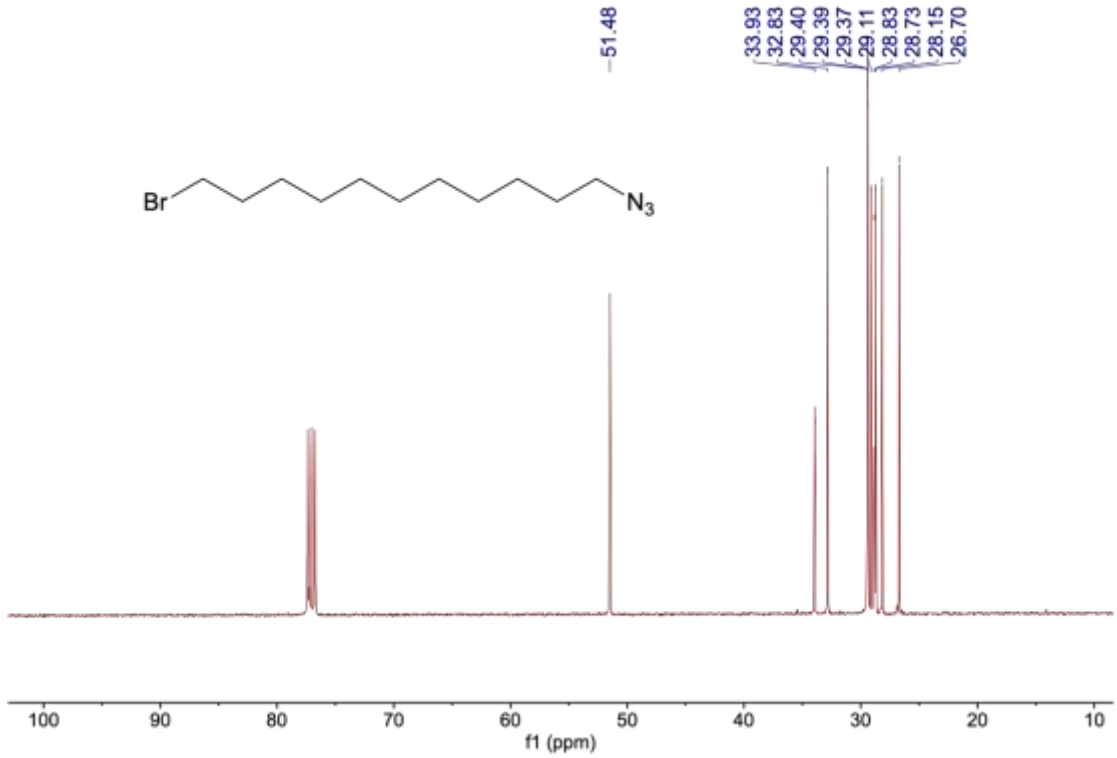


Figure S3 The ^{13}C-NMR spectrum of $N_3(CH_2)_{11}Br$.

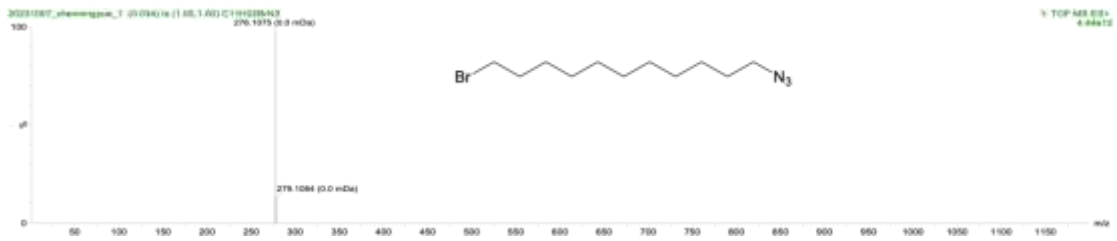


Figure S4 The HRMS spectrum of $N_3(CH_2)_{11}Br$.

Compound $N_3(CH_2)_{11}SH$

We synthesized $N_3(CH_2)_{11}SH$ according to a procedure reported in the literature[2]. The compound $Br(CH_2)_{11}N_3$ (6.5 g, 23 mmol) was added to a solution of $CS(NH_2)_2$ (1.75 g, 24 mmol) in ethanol (50 mL). The mixture was stirred for 16 h at 80 °C. To

this mixture was then added a NaOH solution (10 mL, 3 M). After stirring for 5 min at ambient temperature, the final mixture was neutralized with H_2SO_4 solution (20 mL, 3M), and was stirred for 20 min at ambient temperature. All volatiles were removed. The crude was extracted with CH_2Cl_2 (4×50 mL), and the extract was dried to give $N_3(CH_2)_{11}SH$ as a transparent liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.26 (t, J = 7.0 Hz, 2H), 2.52 (q, J = 7.4 Hz, 2H), 1.66 – 1.55 (m, 4H), 1.41 – 1.26 (m, 14H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 51.47, 34.02, 29.43, 29.43, 29.42, 29.11, 29.03, 28.83, 28.34, 26.70, 24.61. TOF-MS m/z calc for $C_{11}H_{22}N_3S$ $[M-H]^+$ 228.1534, found 228.1528.

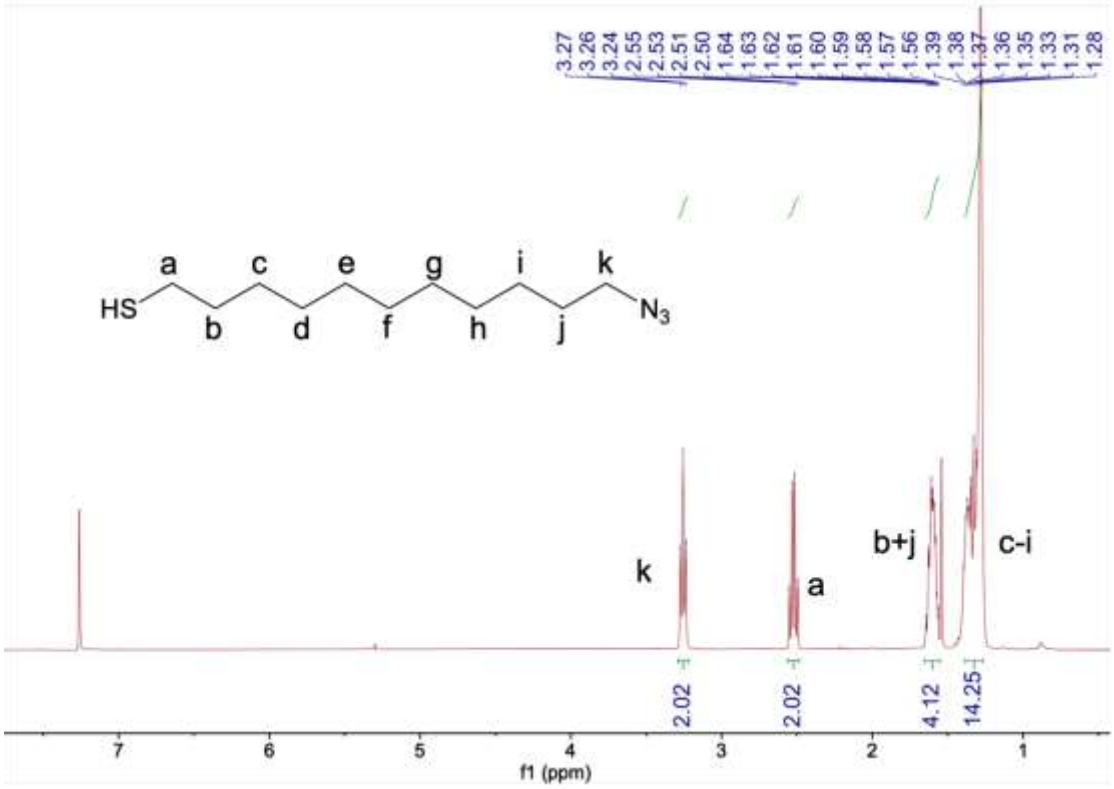


Figure S5 The ^{1}H-NMR spectrum of $N_3(CH_2)_{11}SH$.

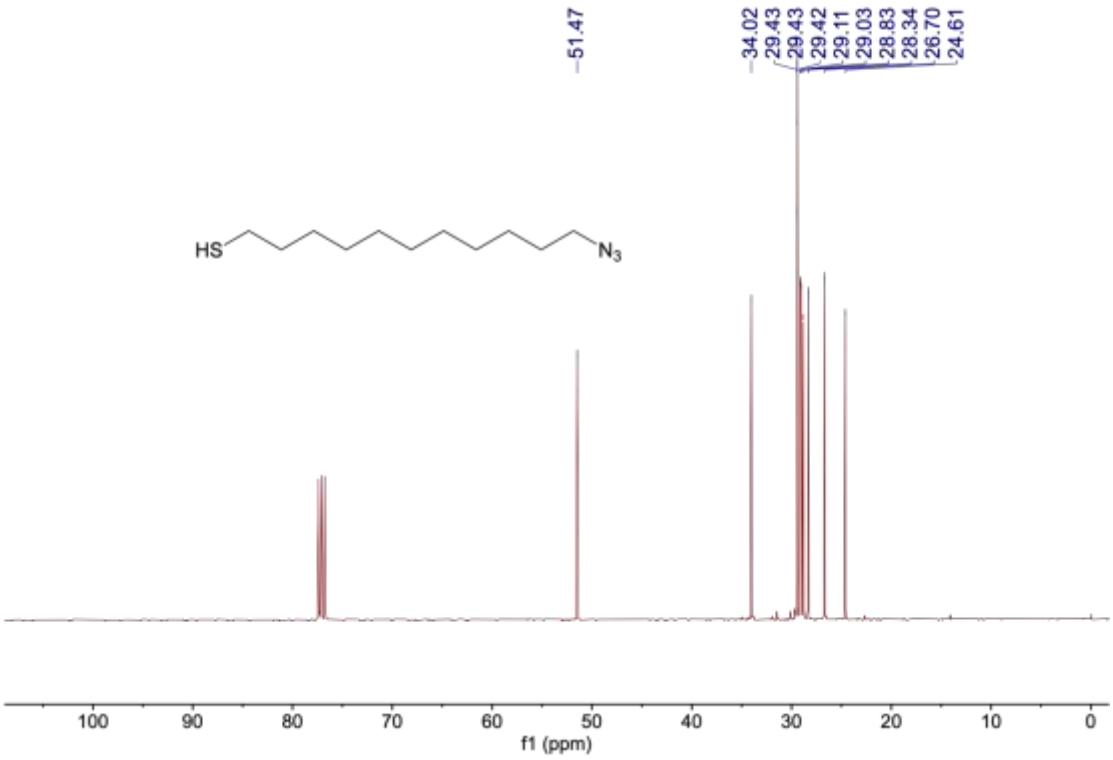


Figure S6 The ^{13}C-NMR spectrum of $N_3(CH_2)_{11}SH$.

Figure S7 The HRMS spectrum of $N_3(CH_2)_{11}SH$.

1.3 Synthesis and characterization of FcC_3-CC

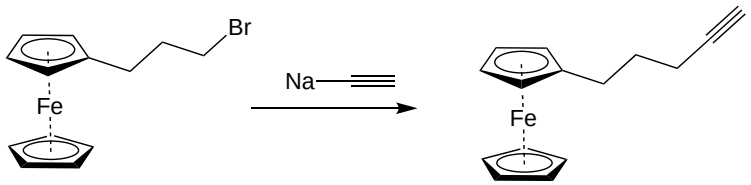


Figure S8. The synthetic route of target molecule FcC_3-CC.

Synthesis

FcC_3Br (307 mg, 1 mmol) was dissolved in 10 mL dimethylformamide. At 0°C sodium acetylide (410ml (18 weight-% slurry in xylene), 1.3 mmol, 1.3 eq.) was slowly added, and the mixture was stirred for1h. After complete conversion, monitored by TLC, 2 mL water was added. The solvent was removed in vacuo, and the residue was dissolved in water (100 mL) and hexane (30 mL). Layers were separated, and the aqueous layer was extracted three times with hexane (20 mL). After drying the solution over Na_2SO_4, filtration through silica gel (pentane/toluene, 9/1) and evaporation of the solvent, the product was obtained as an orange oil. ^{1}H NMR (400 MHz, CDCl3) δ 4.11 (s, 5H), 4.09 – 4.06 (m, 2H), 4.06 – 4.04 (m, 2H), 2.45 (t, J = 7.7 Hz, 2H), 2.21 (td, J = 7.1, 2.6 Hz, 2H), 1.98 (d, J = 2.7 Hz, 1H), 1.73 (p, J = 7.3 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 88.18, 84.43, 68.56, 68.14, 67.24, 29.71, 28.51, 18.21. TOF-MS m/z calc for $C_{15}H_{16}Fe$ $[M]^+$ 252.0601, found 252.062.

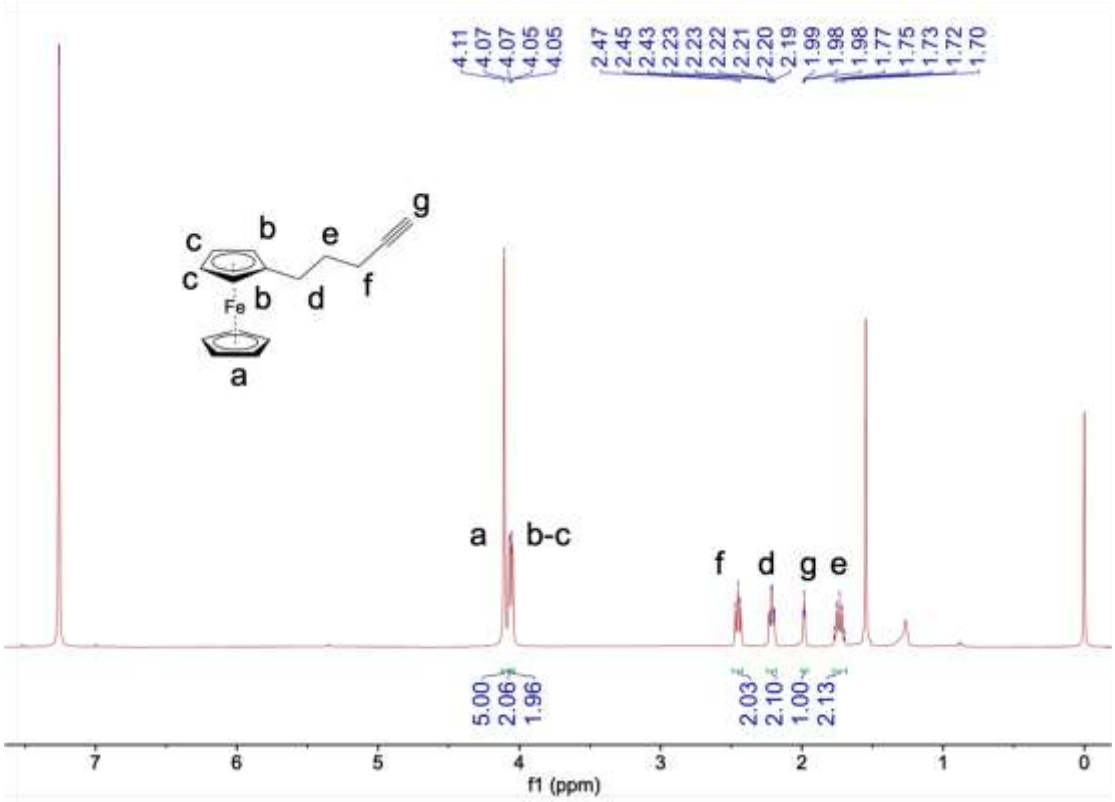


Figure S9. The ^{1}H-NMR spectrum of FcC_3-CC.

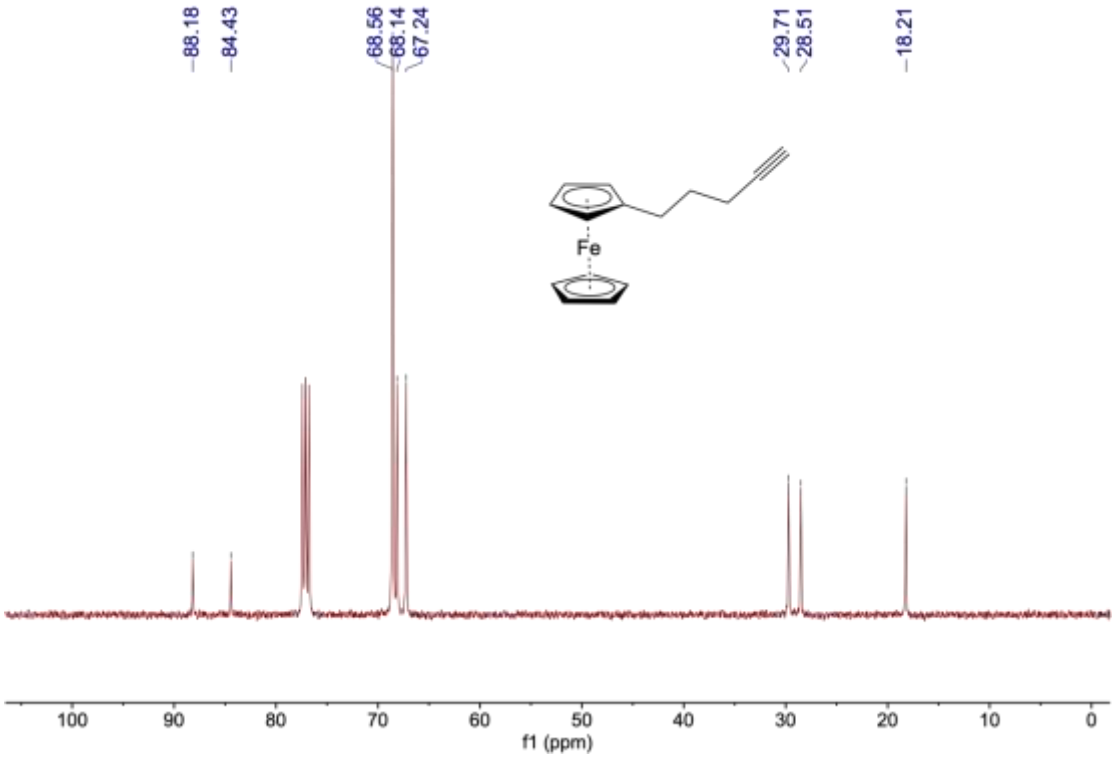


Figure S10. The ^{13}C-NMR spectrum of FcC_3-CC.

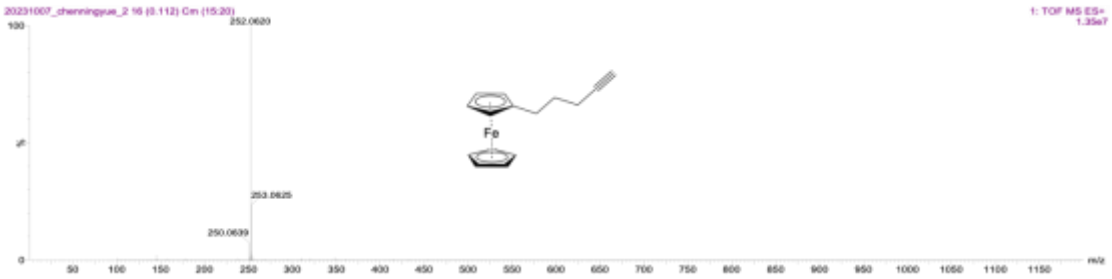


Figure S11 The HRMS spectrum of FcC_3-CC.

1.4 Synthesis and characterization of exTTF-CC[3]

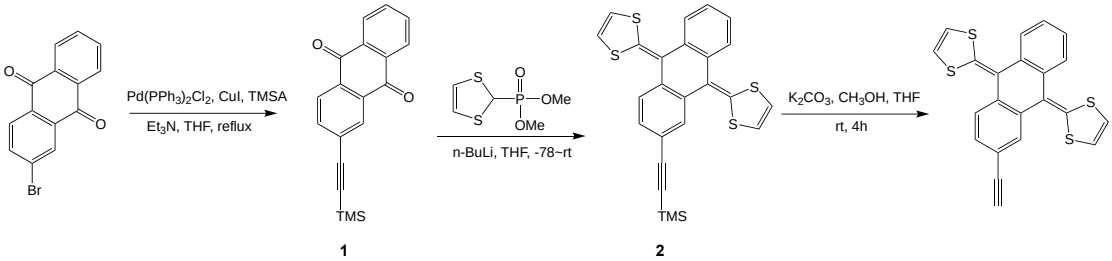
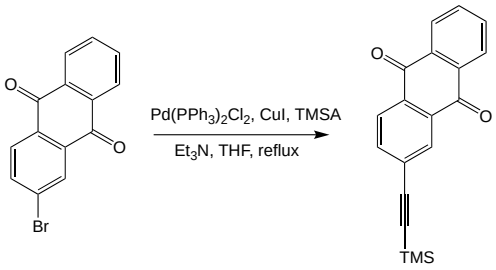


Figure S12. The synthetic route of target molecule exTTF-CC.

Synthesis

Compound 1



2-bro-moanthraquinone (0.29 g, 1.0 mmol), trimethylsilylacetylene (0.22 mL, 1.5 mmol), $Pd(PPh_3)_2Cl_2$ (55 mg, 0.05 mmol), and CuI (30 mg, 0.05 mmol), anhydrous triethylamine (15 mL), anhydrous THF (15 mL) were added into a 100 mL Schlenk tube. After degassing by bubbling with N_2 for 15 min, the mixture was then heated at 85 °C for 12 h under N_2 atmosphere. After the mixture was cooled down to room temperature, the solvents were removed in vacuo. The crude product was then purified by column chromatography (silica gel, CH_2Cl_2/petroleum ether = 1/4 v/v) and recrystallized from $CHCl_3$/CH_3OH to obtain pure product as light-yellow solids. Yield:

274 mg, 90%.^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 (d, J = 1.6 Hz, 1H), 8.34 – 8.30 (m, 2H), 8.25 (d, J = 8.0 Hz, 1H), 7.85 – 7.79 (m, 3H), 0.29 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 182.54, 182.50, 136.92, 134.37, 134.28, 133.58, 133.46, 133.40, 132.57, 130.74, 129.44, 127.41, 127.37, 127.33, 103.31, 100.24, 0.11. TOF-MS m/z calc for $C_{19}H_{16}O_2Si$ $[M+H]^+$ 305.0998, found 305.1017.

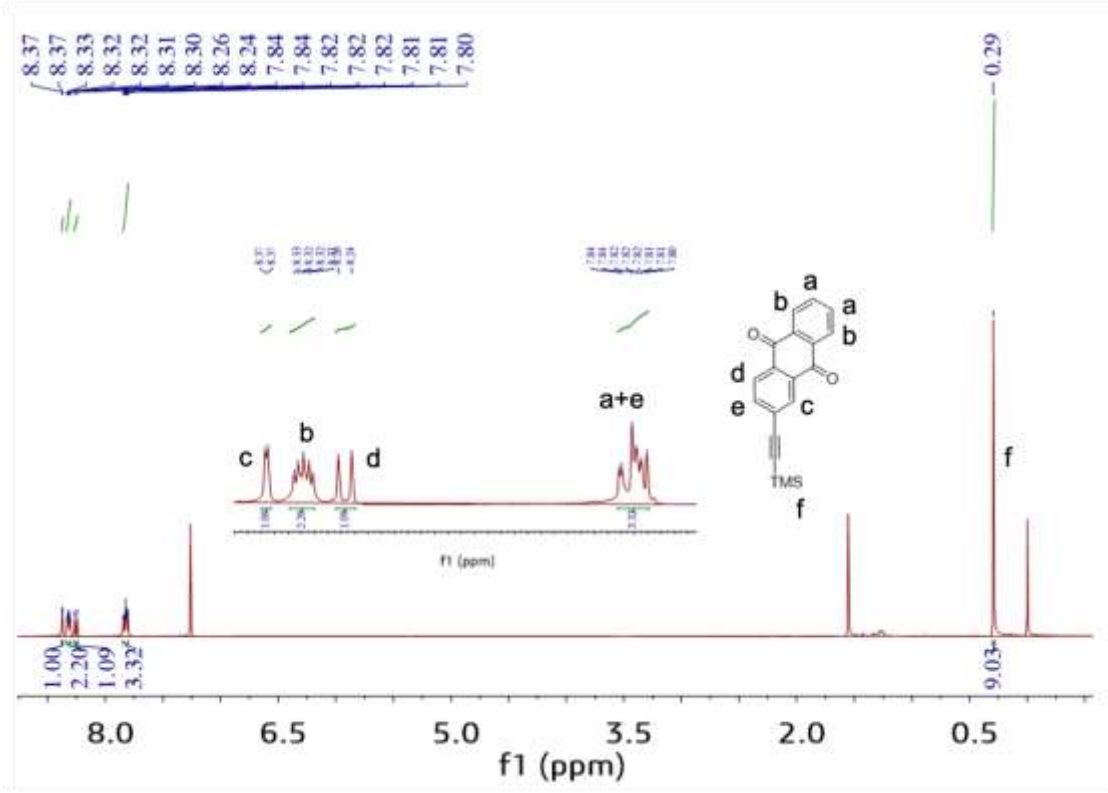


Figure S13 The ^{1}H-NMR spectrum of compound **1**.

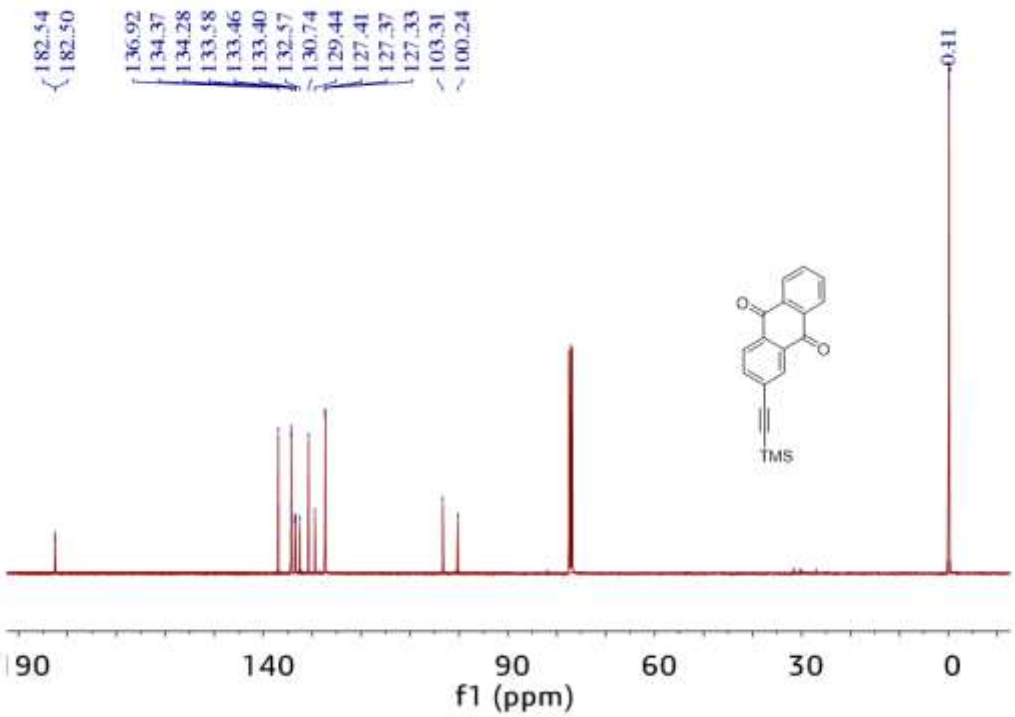


Figure S14. The ^{13}C-NMR spectrum of compound **1**.

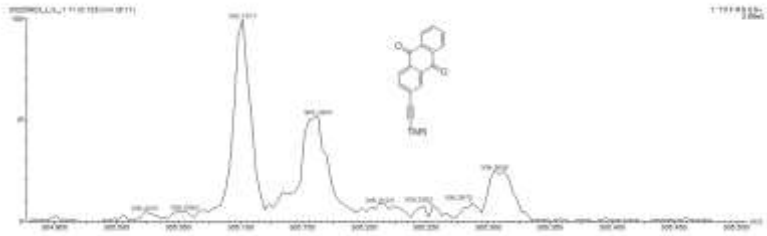
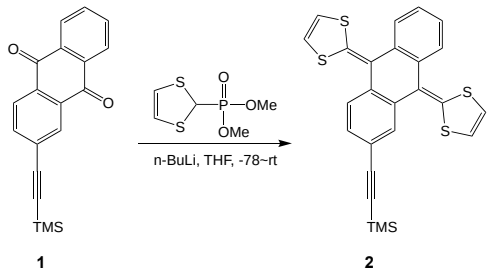


Figure S15. The HRMS spectrum of compound **1**.

Compound 2



To a solution of dimethyl 1,3-dithiol-2-yl-2-phosphonate (1.00 g, 4.72 mmol) in dry THF (50 mL) at -78°C under N_2 atmosphere, n-BuLi (1.6 M, 1.90 ml, 4.72 mmol) was added over a period of 10 min. After 0.5h at -78°C, the compound **1** (0.57 g, 1.89 mmol), suspended in dry THF (50 mL), was added dropwise into the solution of the phosphonate. The mixture was stirred for an additional hour at -78°C, then allowed to warm to room temperature, and then left to stand overnight at room temperature. The THF was evaporated under reduced pressure and water (100 mL) was added. The residue was extracted with CH_2Cl_2, (3×100 ml) and the combined organic layers were dried over Na_2SO_4, filtered and the solvent was removed under reduced pressure. The crude product was then purified by column chromatography (silica gel, CH_2Cl_2/ hexanes = 1/4 v/v) and obtained a pure product as yellow solids (586 mg, 65%). ^{1}H NMR (400 MHz, CDCl3) δ 7.77 (s, 1H), 7.71 – 7.65 (m, 2H), 7.62 (d, J = 8.0 Hz, 1H), 7.37 (dd, J = 8.0, 1.4 Hz, 1H), 7.28 (dd, J = 5.6, 3.3 Hz, 2H), 6.30 (s, 4H), 0.26 (s, 9H). ^{13}C NMR (101 MHz, CDCl3) δ 136.81, 136.68, 135.66, 135.50, 135.33, 129.66, 128.31, 126.20, 126.18, 125.11, 125.02, 124.97, 121.83, 121.37, 120.64, 117.43, 117.40, 117.30, 105.46, 94.47, 0.19. TOF-MS m/z calc for $C_{25}H_{20}S_4Si$ $[M]^+$ 476.0217, found 476.0194.

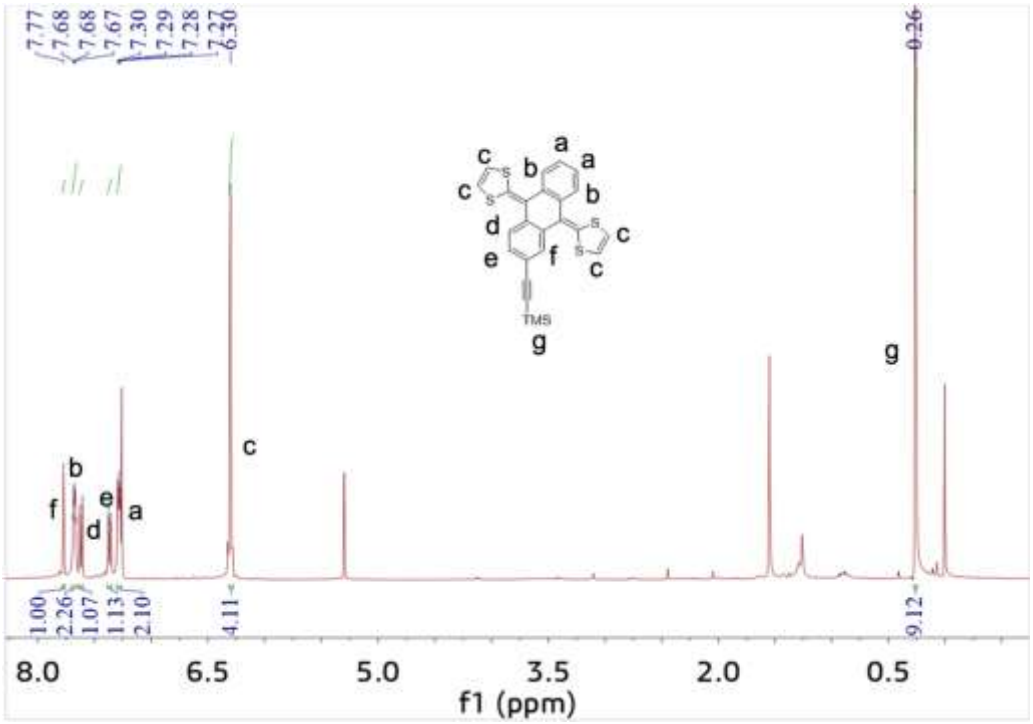


Figure S16. The ^{1}H-NMR spectrum of compound **2**.

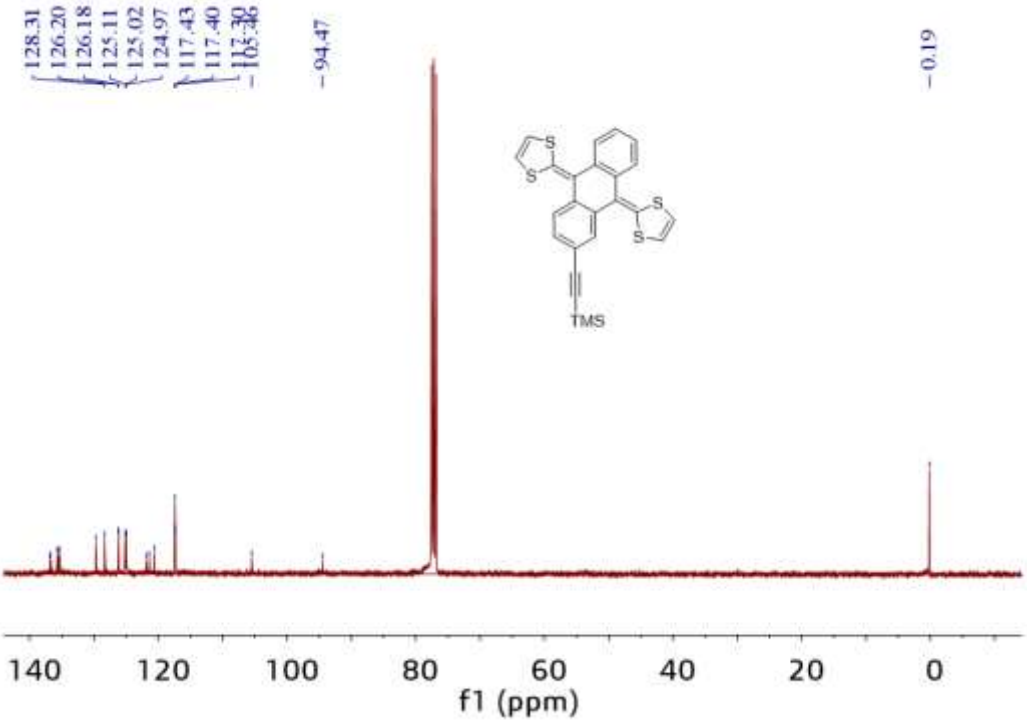


Figure S17. The ^{13}C-NMR spectrum of compound **2**.

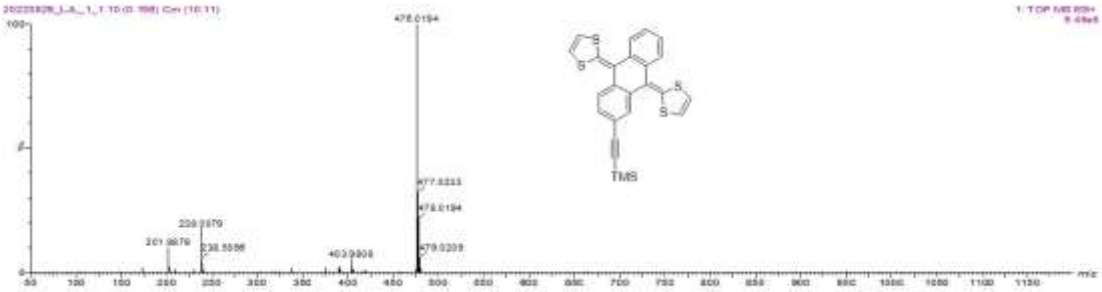
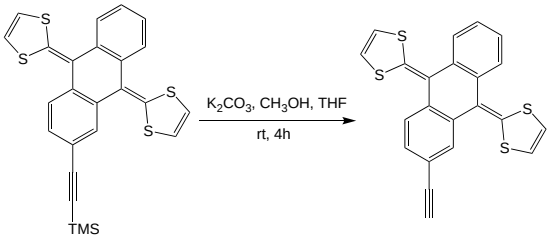


Figure S18. The HRMS spectrum of compound **2**.

exTTF-CC



2

A solution of compound **2** (143 mg, 0.3 mmol) in THF/CH_3OH (1:1, 20 mL) and K_2CO_3 (40 mg, 0.3 mmol) was stirred at room temperature for 4 h. The mixture was then extracted with CH_2Cl_2 (3×25 mL), and the combined organic layers were washed with water (2×50 mL) and dried with Na_2SO_4. The residue was purified by flash chromatography on silica gel using PE/CH_2Cl_2 (3:1) as the eluent to give compound exTTF-CC (122 mg, 100%) as a yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (brs, 1H), 7.73 – 7.68 (m, 2H), 7.65 (d, J = 8.0 Hz, 1H), 7.40 (d, J = 8.0 Hz, 1H), 7.33 – 7.28 (m, 2H), 6.31 (s, 4H), 3.10 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.08, 136.91, 135.98, 135.60, 135.30, 129.73, 128.57, 126.25, 126.23, 125.11, 125.06, 125.04, 121.68, 121.20, 119.49, 117.45, 117.38, 117.31, 84.02, 77.38. TOF-MS m/z calc for $C_{22}H_{12}S_4$ $[M]^+$ 403.9822, found 403.9808.

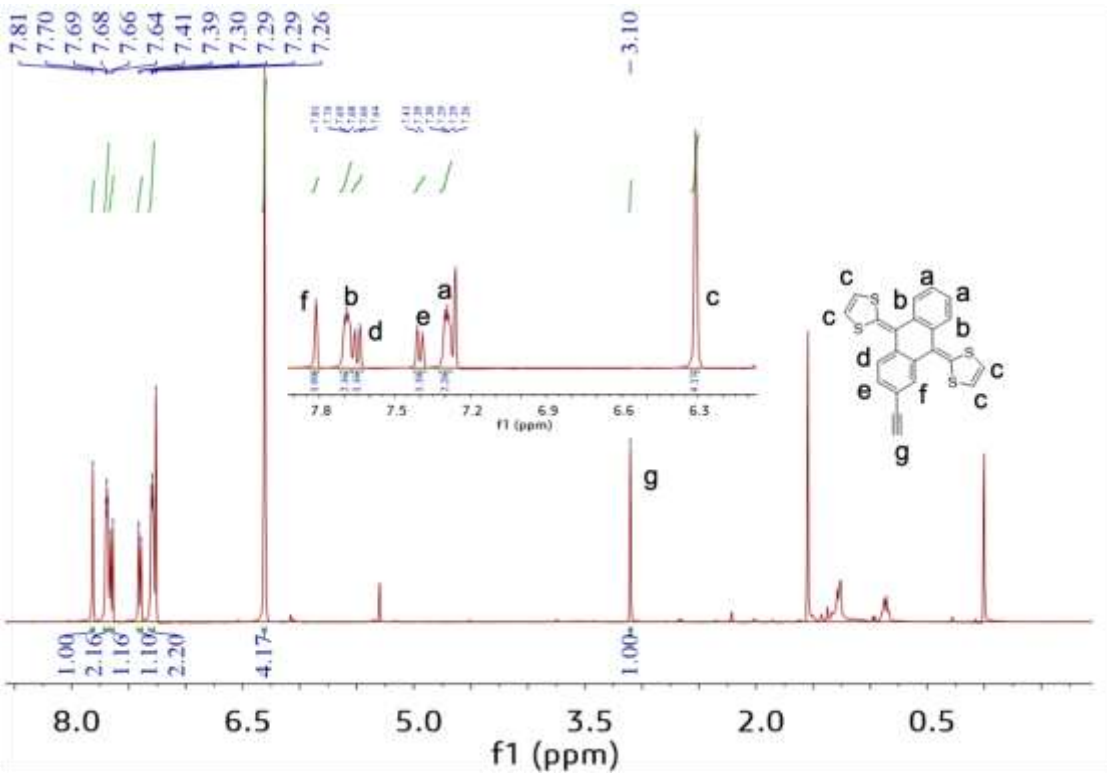


Figure S19. The ^{1}H-NMR spectrum of exTTF-CC.

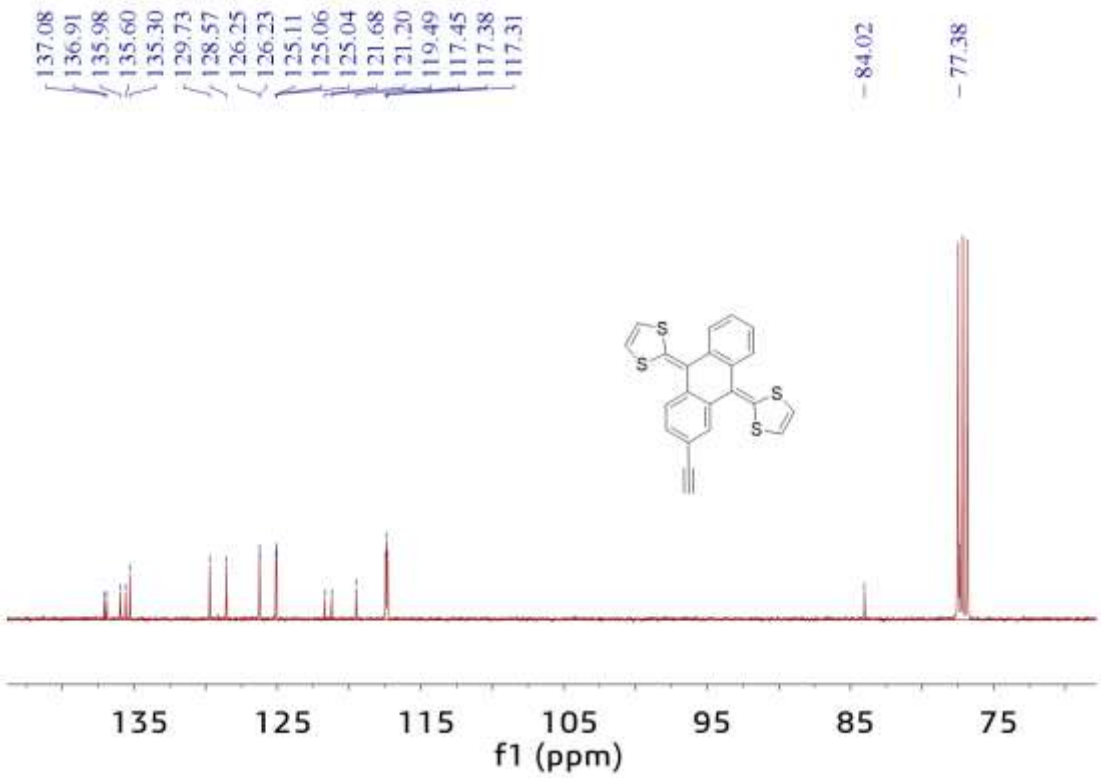


Figure S20. The ^{13}C-NMR spectrum of exTTF-CC.

Figure S21. The HRMS spectrum of exTTF-CC.

1.5 Synthesis and characterization of I+MPP-CC

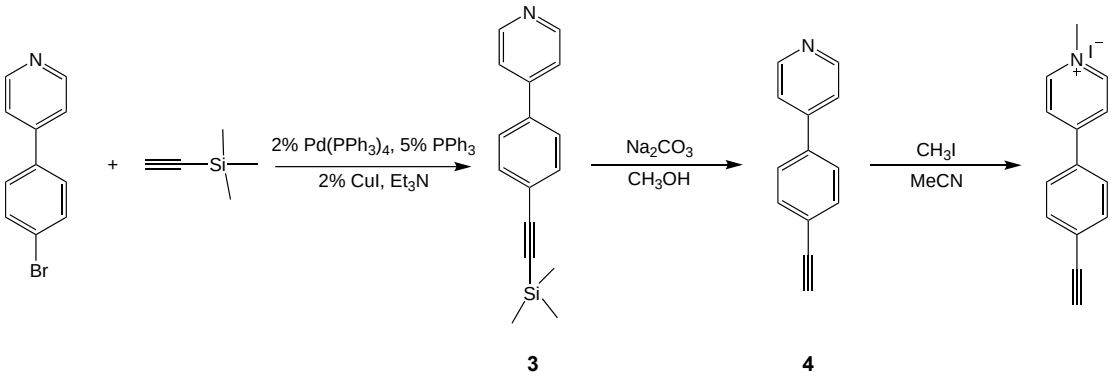
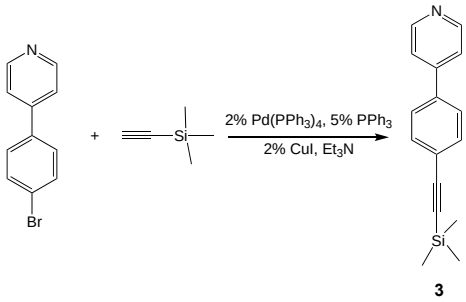


Figure S22. The synthetic route of target molecule I+MPP-CC

Compound 3



Ethynyltrimethylsilane (0.66 g, 6.7 mmol) in dry Et_3N was added dropwise to a suspension of 4-(4-bromophenyl) pyridine (1.31 g, 5.6 mmol), $Pd(PPh_3)_4$ (0.13 g, 0.11 mmol), CuI (0.02 g, 0.11 mmol) and PPh_3 (0.07 g, 0.28 mmol) in dry Et_3N (50 mL) at room temperature. The solution was heated at 60 °C and stirred for 8 h. The mixture was then cooled and filtered, and DCM was added and the organic layer was washed

with saturated ammonium chloride solution, dried over anhydrous $MgSO_4$ and the solvents were evaporated. The crude product was purified by column chromatography using PE as eluent, to give a pale-yellow solid, yield 85%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.66 (d, *J* = 4.2 Hz, 2H), 7.58 (d, *J* = 1.8 Hz, 4H), 7.50 (d, *J* = 4.3 Hz, 2H), 0.27 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.32, 147.46, 137.94, 132.67, 126.77, 124.06, 121.42, 104.36, 96.14, -0.08. TOF-MS m/z calc for $C_{16}H_{18}NSi$ $[M+H]^+$ 252.1209, found 252.1205.

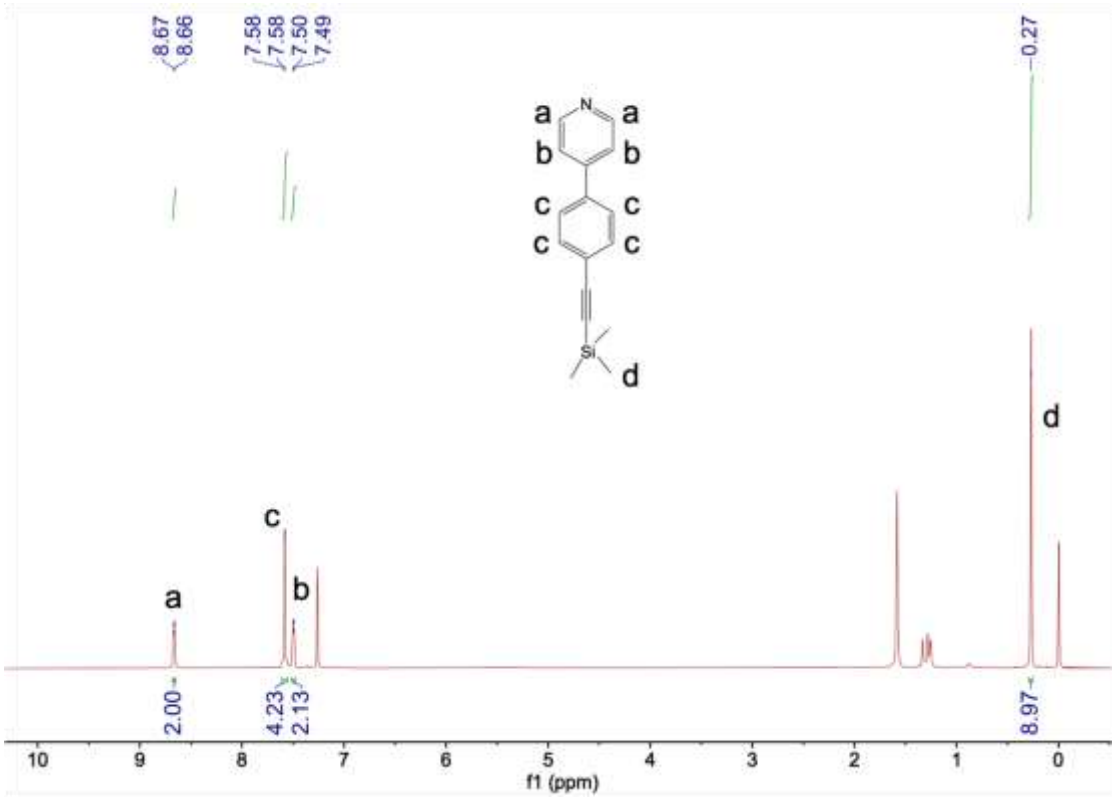


Figure S23. The ^{1}H-NMR spectrum of compound **3**.

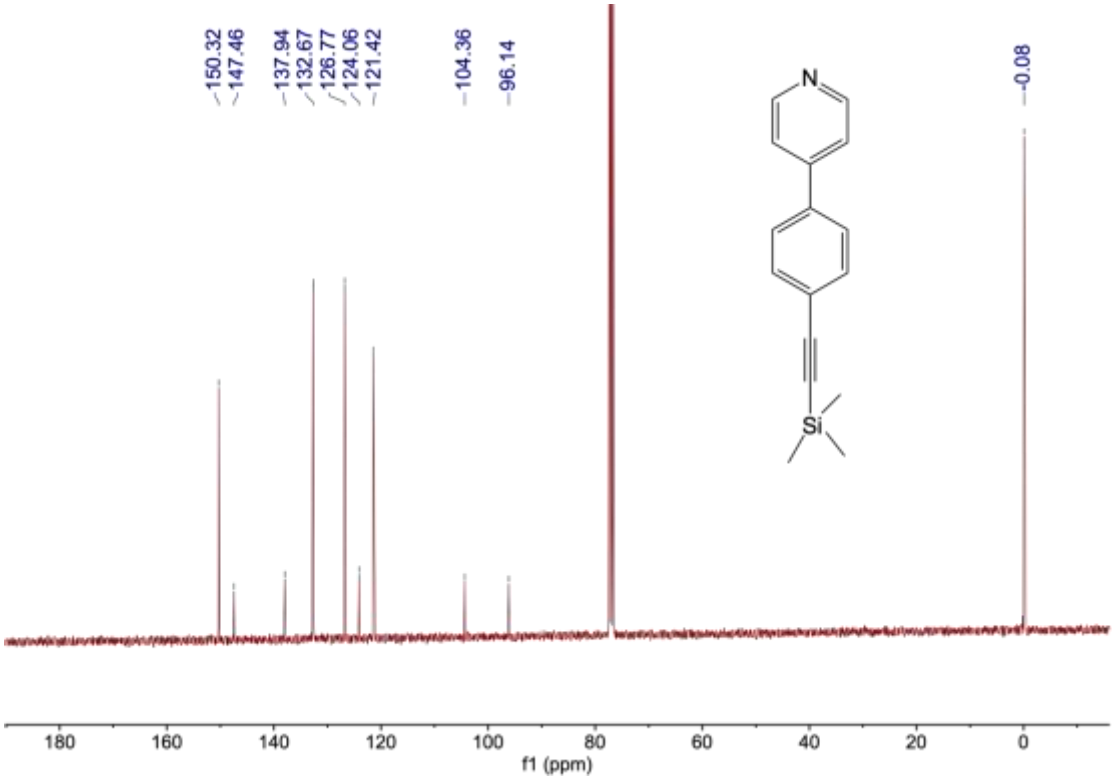


Figure S24. The ^{13}C-NMR spectrum of compound **3**.

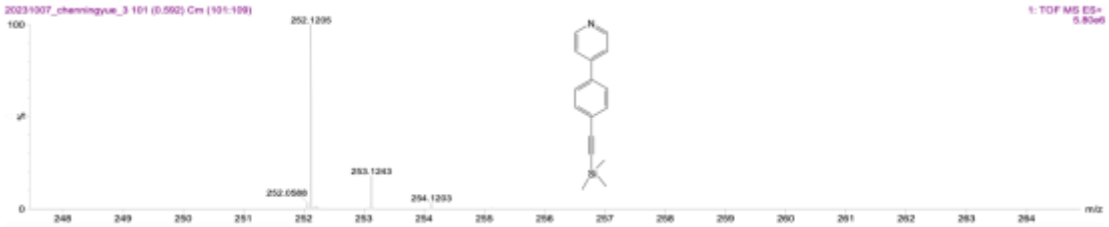
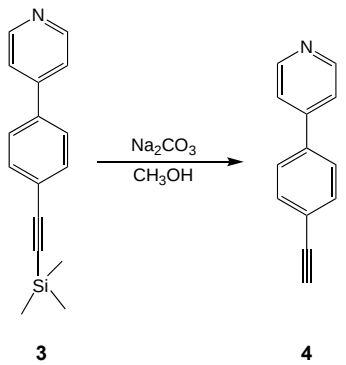


Figure S25. The HRMS spectrum of compound **3**.

Compound 4



We synthesized compound **4** according to a procedure reported in the literature[4]. A mixture of **3** (1.15 g, 4.6 mmol), potassium carbonate (1.9 g, 13.8 mmol), CH_3OH (30 mL) was stirred for 4 h, and the reaction mixture was extracted with DCM, washed with water and brine, and the combined organic layers were dried with $MgSO_4$. After removing the solvent under reduced pressure, compound **4** was obtained as pale-yellow solid without further purification. Yield: 99%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 (d, *J* = 4.3 Hz, 2H), 7.64 – 7.58 (m, 4H), 7.50 (d, *J* = 5.0 Hz, 2H), 3.18 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.26, 147.50, 138.37, 132.86, 126.92, 123.04, 121.50, 83.01, 78.76. TOF-MS m/z calc for $C_{13}H_{10}N$ $[M+H]^+$ 180.0813, found 180.0814.

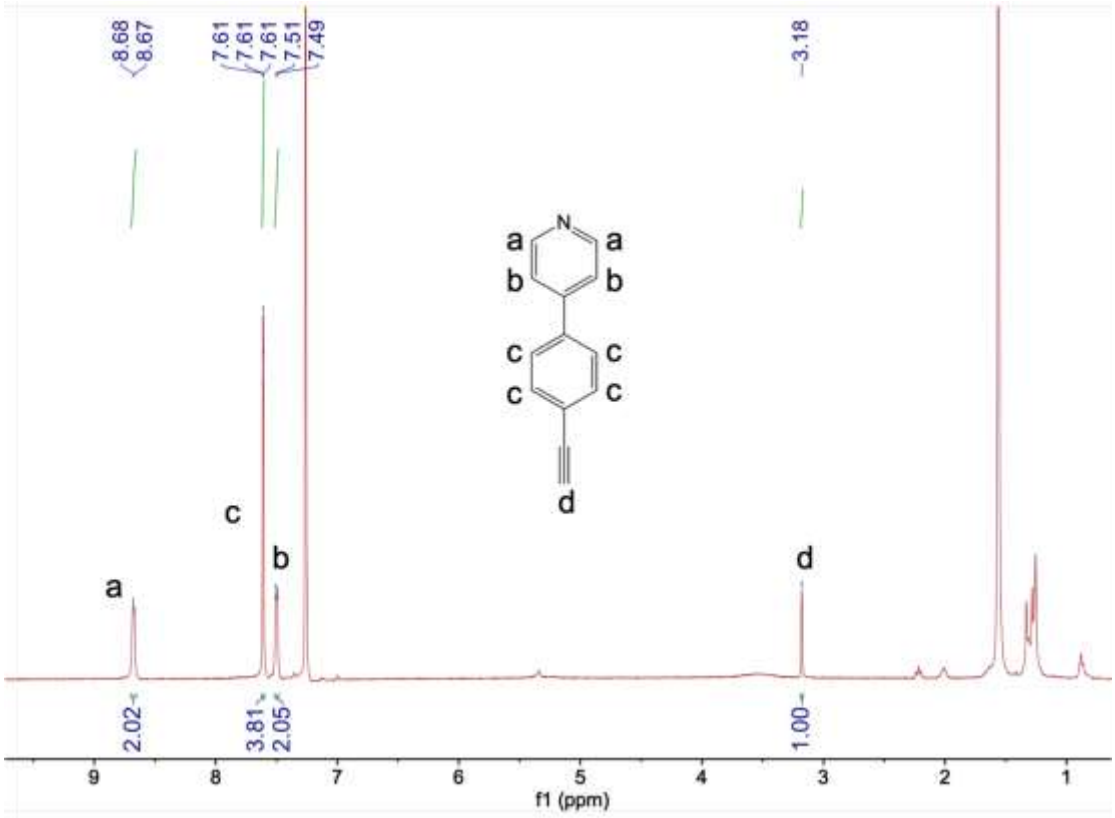


Figure S26. The ^{1}H-NMR spectrum of compound **4**.

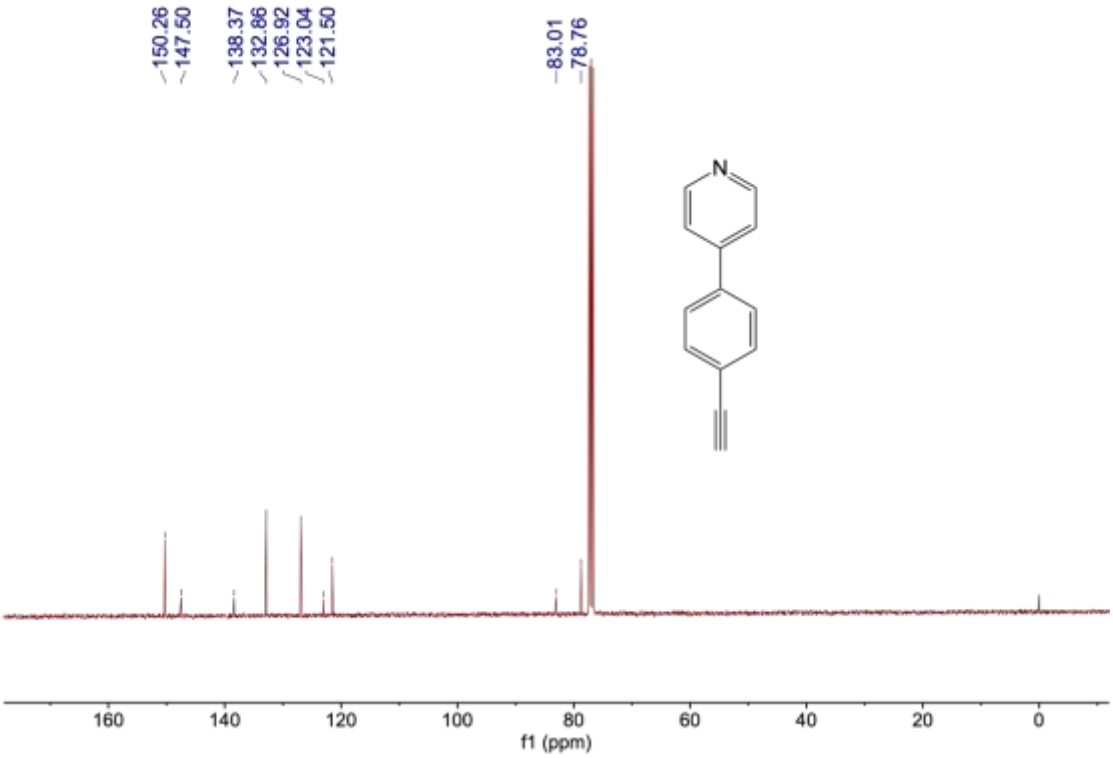


Figure S27. The ^{13}C-NMR spectrum of compound **4**.

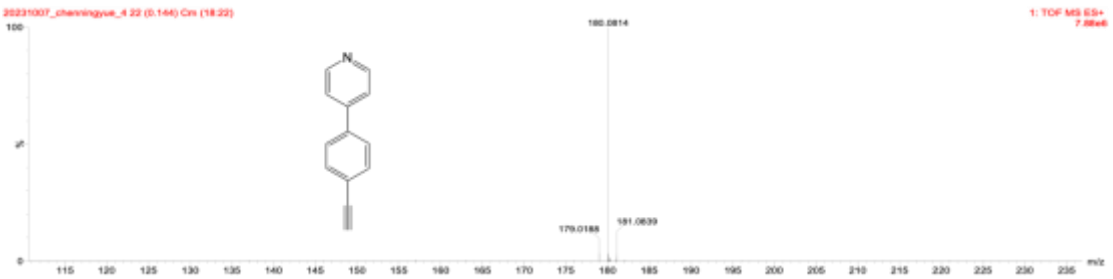
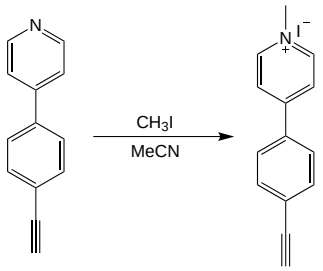


Figure S28. The HRMS spectrum of compound **4**.

I+MPP-CC



4

We synthesized I+MPP-CC according to a procedure reported in the literature[5]. To the corresponding solution of **4** (5.0 mmol, 1.0 equiv.) in acetonitrile (5 mL) was added iodoalkane (10 mmol, 2.0 equiv.) in a two-necked flask under nitrogen. The reaction mixture was refluxed overnight. Then it was cooled to room temperature, and the solvent was removed under reduced pressure to obtain the crude product, which was recrystallized in MeCN/EtOAc co-solvent to afford a pure product. ^{1}H NMR (400 MHz, DMSO) δ 9.01 (d, *J* = 6.6 Hz, 2H), 8.51 (d, *J* = 6.8 Hz, 2H), 8.12 – 8.05 (m, 2H), 7.76 – 7.70 (m, 2H), 4.50 (s, 1H), 4.32 (s, 3H). ^{13}C NMR (101 MHz, DMSO) δ 153.68, 146.18, 134.21, 133.27, 128.82, 125.75, 124.70, 84.54, 83.09, 47.65. TOF-MS m/z calc for $C_{14}H_{13}NI$ $[M+H]^+$ 322.0093, found 322.0101.

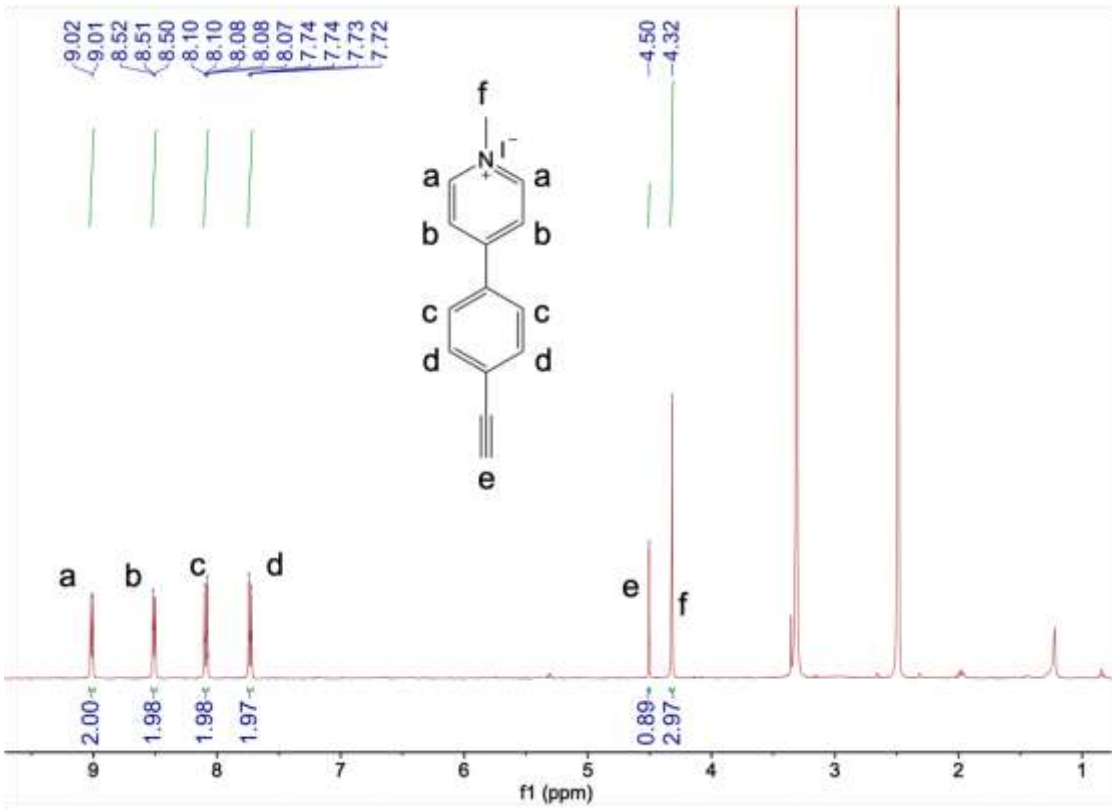


Figure S29. The ^{1}H-NMR spectrum of I+MPP-CC.

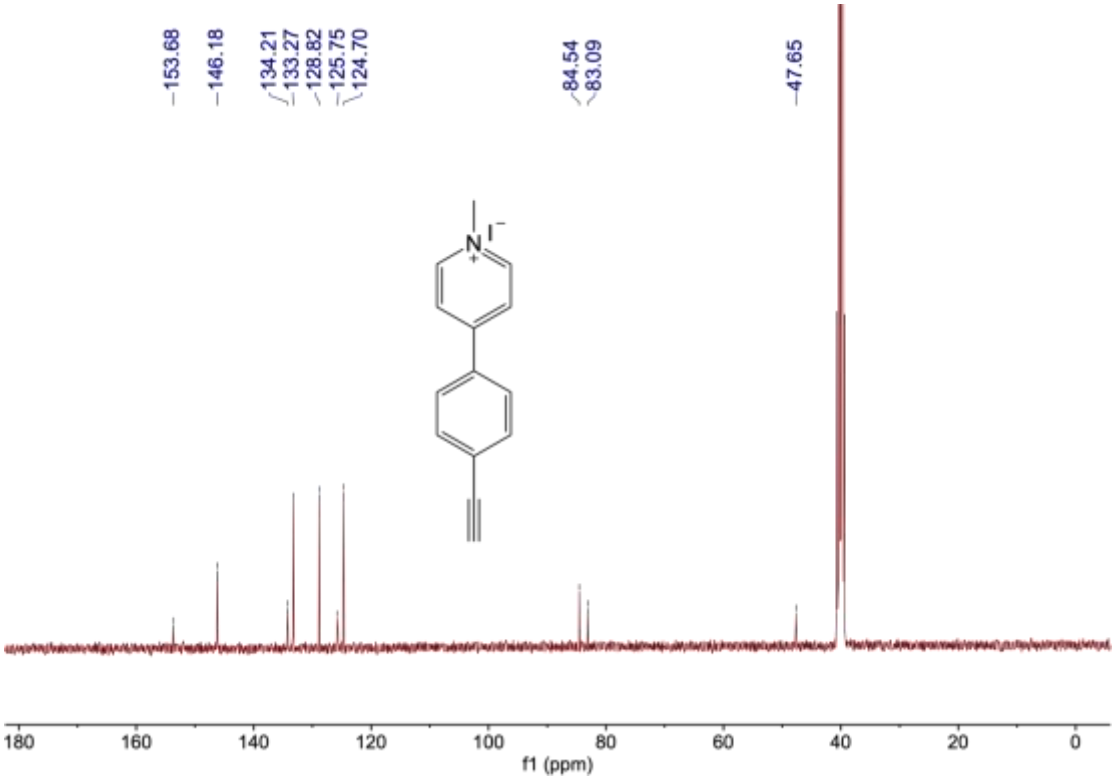


Figure S30. The ^{13}C-NMR spectrum of I+MPP-CC.

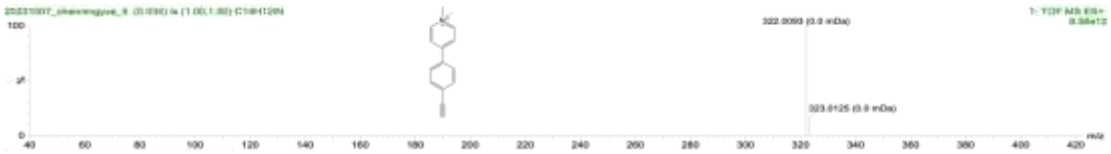


Figure S31. The HRMS spectrum of I+MPP-CC.

2 SAMs preparation

2.1 Fabrication and characterization of template-stripped bottom electrodes.

We fabricated the template-stripped bottom electrodes following the previous reports[3]. We used gold pellets (0.125” (diameter) × 0.125” (length)) with the purity of 99.999% obtained from Dimu Materials, Inc (China). Silicon (100, p-type) wafers are from KST (Japan), with a thickness of 525 ± 25 μm with one side polished. We used a thermal evaporator (Shen Yang Ke Yi, China) to deposit Au vapour on top of polished surfaces of Si/SiO2 wafers. The vacuum of deposition was about 8×10^{-5} Pa, and the evaporation rate was about 0.2 Å/s at the first 50 nm and then increased to ~1.0 Å/s for the rest 150 nm. The glass slides (1.5×1.5 cm^2) were ultrasonically cleaned with acetone and then ethanol for 20 minutes, and the slides were blown to dryness in a stream of N_2 gas. After we cleaned the glass slides with a plasma of air for 5 mins at a pressure of 100 Pa, the glass slides were glued on the Au surfaces by photo-curable optical adhesive (Norland, No. 61). A 100-Watt UV lamp was used to cure the optical adhesive for 1 hour at a distance of 60 cm from the light source. The Au surface that had been in contact with the Si/SiO_2 wafer was lifted off by a razor blade.

2.2 Fabrication of N_3-SAMs

To prepare the basic SAMs for click reaction, we formed the N_3-terminated SAMs (N_3-SAMs) by immersing freshly prepared template-stripped Au (Au^{TS}) substrates[6] into a solution of 1.0 mM $N_3(CH_2)_{11}SH$ in absolute ethanol. Following a 3-hour immersion

period, the N_3-SAMs samples were meticulously rinsed with pure ethanol and subsequently dried with nitrogen gas. After these steps, the $N_3(CH_2)_{11}SH$ molecules were primed for assembly onto the gold substrates through a thiol-Au reaction, forming N_3-SAMs.

2.3 Fabrication of clicked-SAMs

To immobilize organic functional groups including Fc, C_3-Fc and exTTF, we immersed N_3-SAMs in a DMF solution containing 1.0 mM $CuSO_4 \cdot 5H_2O$, 100.0 mM ascorbic acid (AA), and 10.0 mM functional group molecules, with a ratio of $CuSO_4 \cdot 5H_2O$/AA/functional groups 1:1:4 in volume ratio for 24h[7]. To prevent potential photooxidation of the SAMs, we stored the samples in a dark, room-temperature environment under a nitrogen atmosphere. After the reaction was completed, we sequentially rinsed the samples with ethanol and dichloromethane to remove the physisorbed functional groups yielding Fc-SAMs, Fc-C_3-SAMs and exTTF-SAMs respectively.

Meanwhile, for ion-type functional groups MPP+I, the click reaction was performed in EtOH/H_2O (3:1 in volume ratio). The N_3-SAMs was immersed in an ethanolic solution of 1.25 mM 4-(4-ethynylphenyl)-1-methylpyridin-1-ium iodide. Additionally, solution of 0.4 mM $CuSO_4 \cdot 5H_2O$ and 0.8 mM ascorbic acid in deionized water was added. Also, the samples were stored in a dark under a nitrogen atmosphere for 2.5 days at 50 °C. After the completion of the reaction, we rinsed the samples with ethanol and dichloromethane and the MPP+I-SAMs were obtained[8].

3 X-Ray Photoelectron Spectroscopy & Ultraviolet photo-electron spectroscopy

X-ray photoelectron spectroscopy (XPS) was conducted with the NCESBJ (National Centre of Electron Spectroscopy in Beijing). All measurements were performed in an ultrahigh vacuum chamber with a base pressure of 1×10^{-8} Pa. The

energy of the incident X-ray beam (1486.6 eV) was used by the Thermo Scientific K-Alpha XPS system. To probe the valence band, the photon energy at 21.22 eV was used and –10 V bias was applied to the sample to overcome the work function of the analyzer. All UPS spectra were referenced to the Fermi edge of Au.

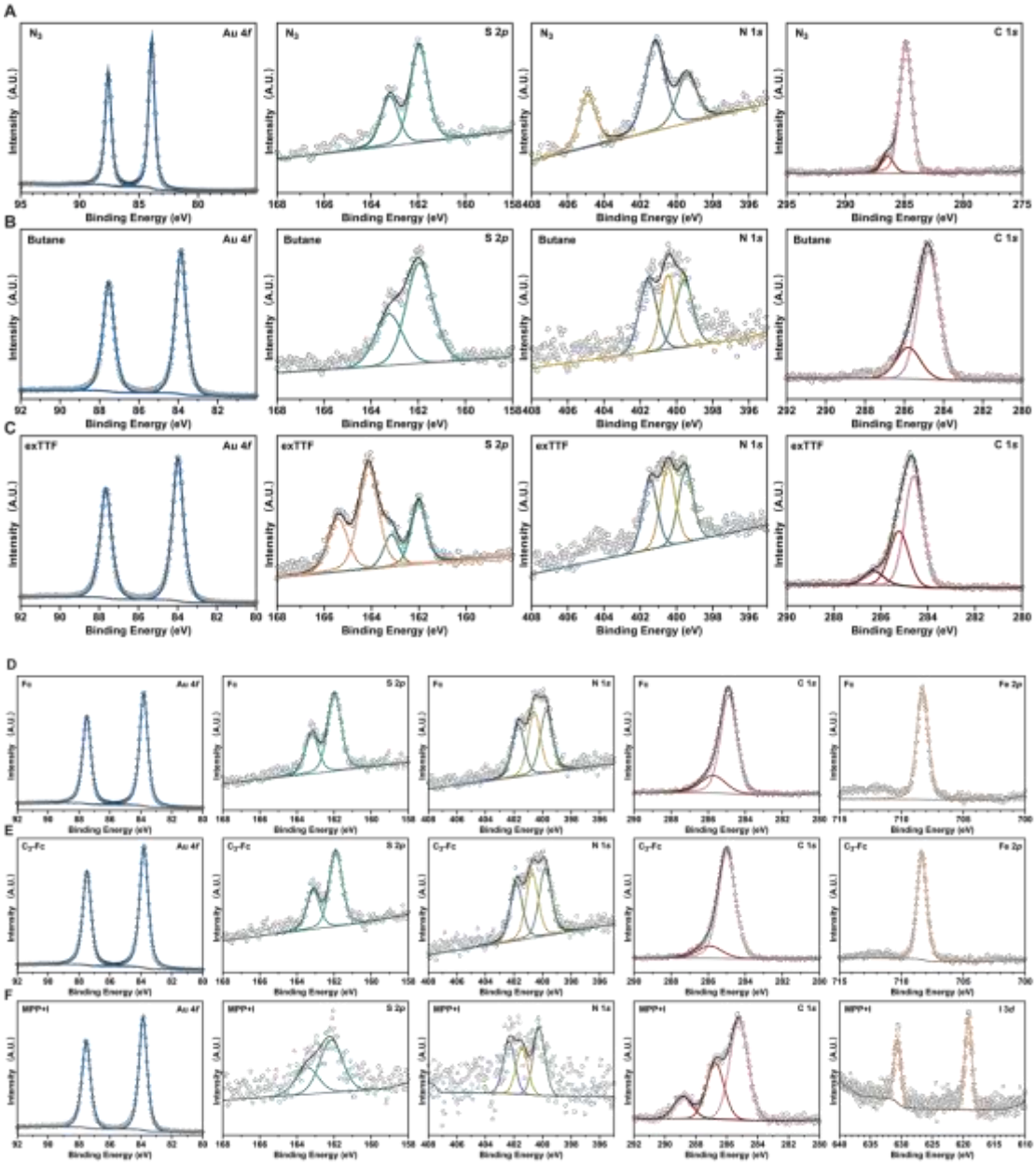


Figure S32. The XPS spectrum of all SAMs. (**A**) N_3; (**B**) Butane; (**C**) exTTF; (**D**) Fc; (**E**) C_3-Fc; (**F**) MPP-I

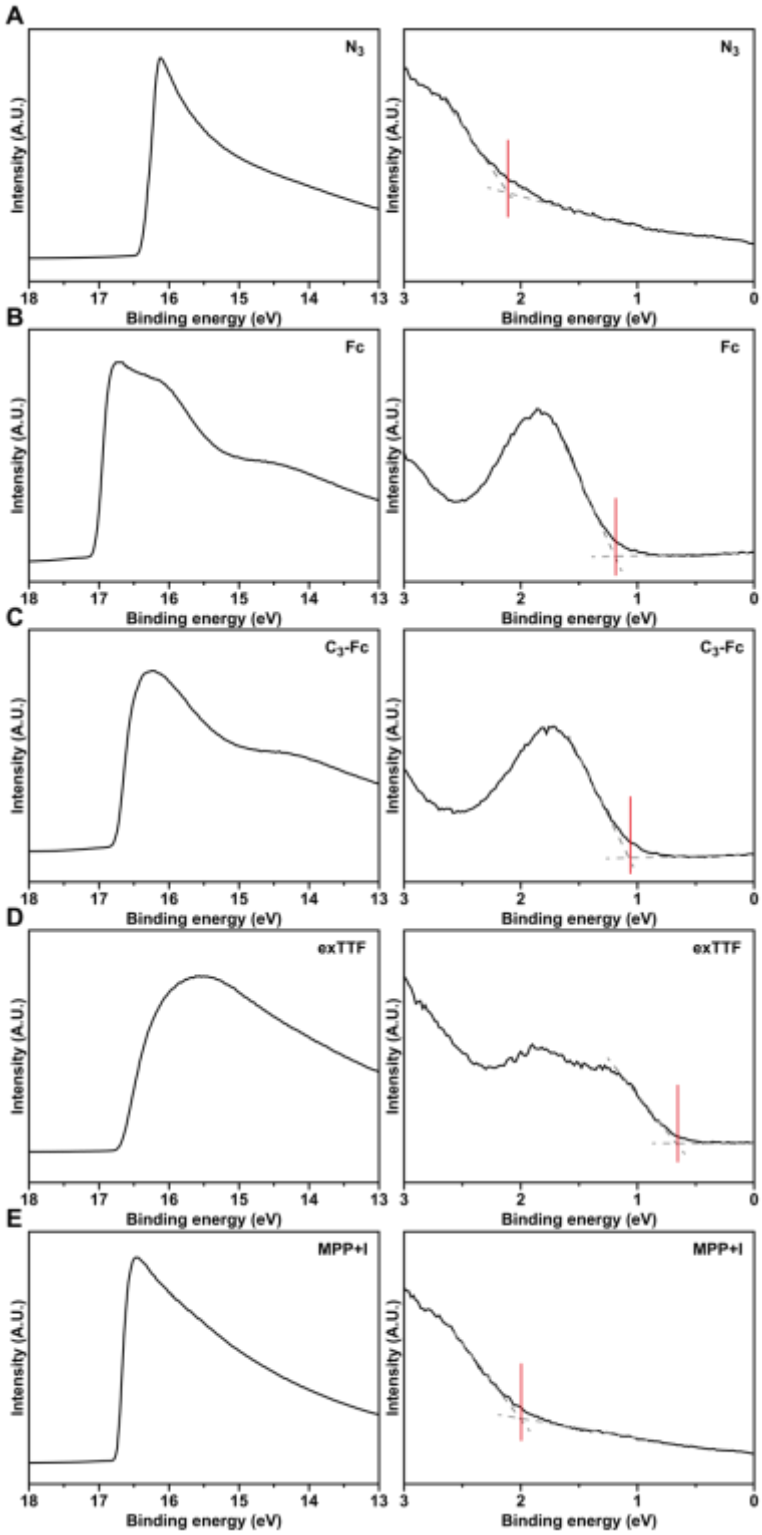


Figure S33. The UPS spectrum (Zoom-in to show work function and HOMO energy position) of all SAMs, referenced to the Fermi level of a clean polycrystalline Au surface. (**A**) N_3; (**B**) Fc; (**C**) C_3-Fc; (**D**) exTTF; (**E**) MPP-I

4 Cyclic voltammetry

The SAMs of all functional groups on Au^{TS} electrodes were electrochemically characterized by cyclic voltammetry (CV)[3]. Electrochemical measurements were performed with an AUTOLAB PGSTAT302N with NOVA 2.1 software. To perform the CV measurements, we used a custom-built electrochemical cell equipped with a platinum counter electrode, an Ag/AgCl reference electrode and the Au^{TS} film served as a working electrode. Cyclic voltammograms were recorded in an aqueous solution of 1.0 M $HClO_4$. The CVs were recorded in the range of –0.1 to +0.9 V for Fc and C3-Fc; –0.4 to +0.9 V for exTTF and –0.5 to +0.9 V for MPP+I. We measured 3 substrates for each SAMs.

We calculated the surface coverage (Γ, mol/cm^2) with equation 1, where Q_{tot} is the total charge obtained by integration of the CV, n is the number of electrons per mole of reaction, F is the Faraday constant (96485 C/mol), and A is the surface area of the electrode exposed to the electrolyte solution (0.65 cm^2). The results are shown in Table S1.

$$\Gamma = Q_{tot}/nFA \quad (1)$$

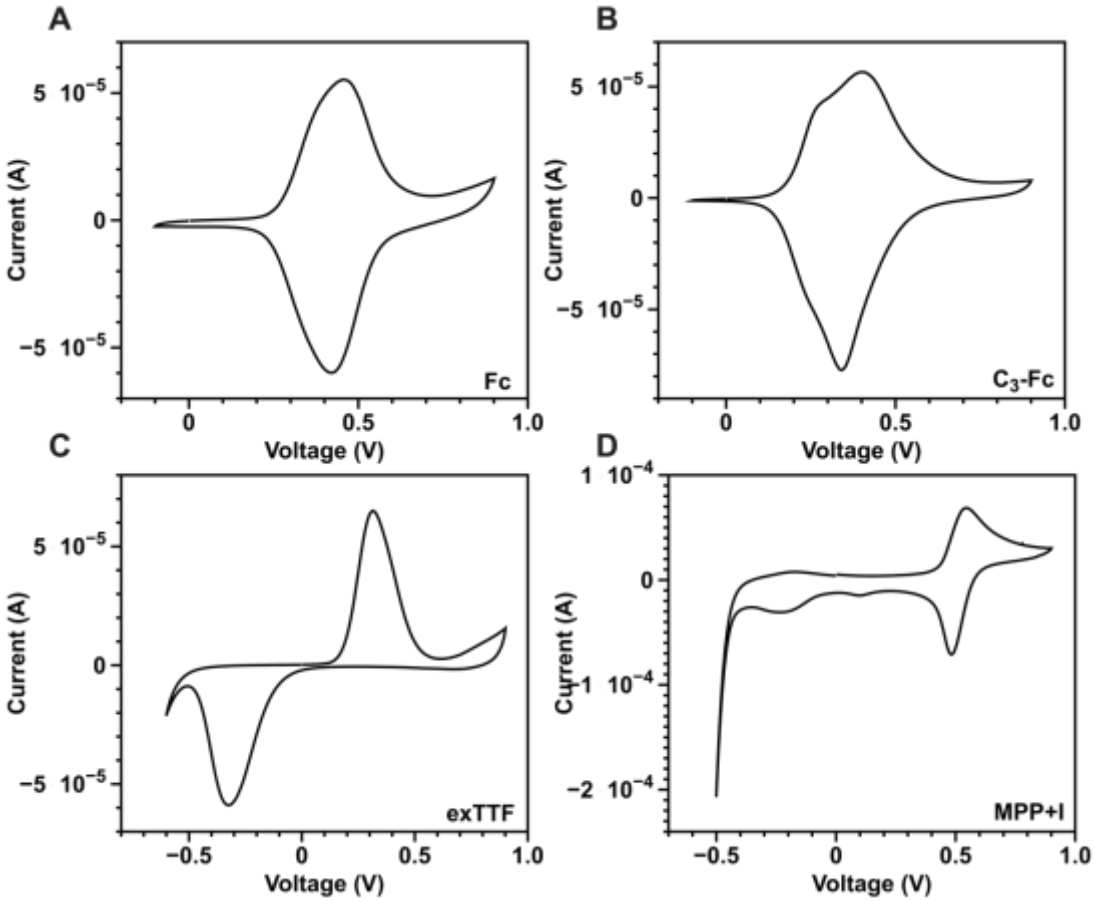


Figure S34. The CV spectrum of all SAMs. (**A**) Fc; (**B**) C_3-Fc; (**C**) exTTF; (**D**) MPP+I

5 EGaIn measurement

We used cone-shaped tips of Ga_2O_3/EGaIn as the top electrodes following by a previously described home-built system[3]. This technique makes it possible to form junctions in which the electrical characteristics are dominated by the chemical and supramolecular structure of the SAMs inside the junctions and to record data with statistically large numbers. We have shown before that the device properties are not dominated by any of the other asymmetries, nor by the Ga_2O_3 layer, present in these junctions[9].

6 Statistical analysis

For the freshly prepared SAMs, the junctions of each type of SAM were fabricated on three different Au samples using the 'EGaIn-technique'. We formed seven junctions on each substrate. For each junction, we recorded 24 scans (0 V → $+V_{max}$→ 0 V →$-V_{min}$ → 0 V) with a step size of V_{max}/20 V and a delay of 0.1 s. We collected large statistically large number of traces for each type of SAMs (see Table S2), and we calculated log|J| using previously reported methods[3].

7 Molecular structure optimization

We optimized molecular geometry and molecular orbits (MOs) using the DFT/B3LYP function with basis set 6-31G (d) as implemented in Gaussian 09[10].

Table S1. Summary properties of the SAMs

SAMs	UPS		CV			DFT	
	E_{HOMO} (eV)	WF (eV)	E_{pa} (mV)	E_{pc}(mV)	Γ（×10^{-10}mol/cm^2）	HOMO (eV)	LUMO (eV)
Fc	-5.36	4.16	458	419	3.40	-5.08	-0.04
C3-Fc	-5.51	4.46	393	332	4.43	-5.07	0.16
TTF	-5.16	4.46	315	-320	1.93	-4.54	-1.22
MPP+I	-6.45	4.46	540	483	3.09	-7.08	-5.88
N_3	-6.83	4.83	/	/	/	-6.35	-0.68

Table S2. Yields of the click reaction

SAMs	Γ (×10^{-10}mol/cm^2)	Theoretical value(×10^{-10}mol/cm^2)	Yields / %
Fc	3.40	4.50	75.5
C3-Fc	4.43	4.50	98.8
TTF	1.93	2.98	66.7
MPP+I	3.09	5.00	61.8

a

Table S3. Statistics for Au-SAMs//Ga_2O_3/EGaIn junctions.

	Number of Junctions	Number of shorts[a]	Number of traces[b]	Yields / (%)[c]
N_3	21	0	504	100
Butane	21	0	504	100
Fc	21	0	504	100
C_3-Fc	21	0	504	100
exTTF	15	0	360	100
MPP+I	20	0	408	100

[a] A junction short was defined when the value of J exceeds 10^2 A/cm^2 (the upper limit of J measurable by our instrument) while recording 20 $J(V)$ scans.

[b] The number of J(V) traces of the Au-SAMs/Ga_2O_3/EGaIn junctions.

[c] The yield is defined as the percentage number of non-shorting junctions divided by the total number of junctions.

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