Supporting Information

Fe₃O₄@WO₃-E-SMTU-Ni^{II}: as an environmentally-friendly,

recoverable, durable and noble-free nanostructured catalyst for C-C

bond formation reaction in green media

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General

All chemical reagents and solvents were purchased from Merck Chemical Companies and were used as received without further purification. The purity determinations of the products were accomplished by TLC on silica gel polygram STL G/UV 254 plates. The melting points of the products were determined with an Electrothermal Type 9100 melting point apparatus. The NMR spectra were obtained in Brucker Avance 300, 400 and 500 MHz instruments in CDCl₃ and DMSO-*d*₆. Mass spectra were recorded with a CH7A Varianmat Bremem instrument at 70 eV electron impact ionization, in m/z (rel %). The surface charge of the catalyst was determined using CAD Zeta-potential instrument, zeta compact model (France). The model Gram negative and Gram positive bacteria are *Escherichia coli* (ATCC 25922) and *Staphylococcus aureus* (ATCC 25923) strains, respectively. All yields refer to isolated products after purification by flash chromatography with silica gel.

Characterization of Fe₃O₄@WO₃-E-SMTU-Ni^{II}

The antibacterial test

The antibacterial activity of $Fe_3O_4@WO_3$ -E-SMTU-Ni^{II} was studied against *Escherichia. coli (E. coli)* and *Staphylococcus aureus (S. aureus)* as Gram negative and Gram positive bacteria, respectively.

The disk diffusion and broth microdilution methods were performed, and the minimum inhibitory concentration (MIC) and minimum bactericidal concentration (MBC) were determined. The bacteria samples were prepared in nutrient broth at 37 °C overnight to reach a cell count of about 10⁸ CFU/mL.

The MIC and MBC of Fe₃O₄@WO₃-E-SMTU-Ni^{II} for both *E. coli* and *S. aureus* bacteria were determined *via* a broth microdilution method. Different concentrations (1, 10, 25, 50 and 100 μ g/mL) of the nanostructured catalyst were prepared, mixed with the bacteria samples and incubated at 37 °C. The optical density of the solutions was read at zero and after 24 h so the MIC and MBC were expressed (Table S1). As it can be seen the MIC and MBC values are lower for *S. aureus* which revealed that Fe₃O₄@WO₃-E-SMTU-Ni^{II} had better antibacterial effects on *S. aureus* compared to *E. coli*.

Table S1. The MIC and MBC values of the $Fe_3O_4@WO_3$ -E-SMTU-Ni^{II} for *S. aureus* and *E. coli* bacteria.

S. aureus		E. coli	
MIC	MBC	MIC	MBC
(µg/mL)	(µg/mL)	(µg/mL)	(µg/mL)
10	50	25	100

The antibacterial activity of Fe₃O₄@WO₃-E-SMTU-Ni^{II} was also measured by disk diffusion method in agar medium. Due to better effect of Fe₃O₄@WO₃-E-SMTU-Ni^{II} on *S. aureus*, the disk diffusion method was carried out for *S. aureus*. The bacteria with a concentration of 10^8 CFU/mL were cultured on nutrient agar plates. The catalyst with 10μ g/mL concentration was poured on the 6-mm-diameter pieces placed on the agar surface. After incubation for 24 h at 37 °C, the diameter of the inhibition zone (DIZ) was measured in millimeter. As shown in Fig. S1, the DIZ is about 10

mm which is comparable to DIZ of antibiotic (as a control) and confirmed the considerable antibacterial effect of $Fe_3O_4@WO_3$ -E-SMTU-Ni^{II}. Meanwhile, the absence of DIZ for WO₃ means that it does not have an antibacterial effect in pure form.



Fig. S1. The disk diffusion plate of Fe₃O₄@WO₃-E-SMTU-Ni^{II} and WO₃ against the *S. aureus* bacteria.

The antibacterial effect of $Fe_3O_4@WO_3$ -E-SMTU-Ni^{II} on the bacteria could be interpreted through the electrostatic interaction between $Fe_3O_4@WO_3$ -E-SMTU-Ni^{II} and the bacterial surface. The zeta potential analysis is a reliable indicator of the strength of the electrostatic interaction between the nanoparticles and the bacteria cells. ¹ The surface charge of $Fe_3O_4@WO_3$ -E-SMTU-Ni^{II} determined to be negative using the zeta potential analysis. As a result, the negatively charged $Fe_3O_4@WO_3$ -E-SMTU-Ni^{II} has more efficient electrostatic interaction with positively charged residues of the membrane proteins on the *S. aureus* bacteria surface. The physicochemical changes in the bacterial cell wall can be another antibacterial approach and the intracellular activities of bacteria cells can be disrupted by the penetration of Fe_3O_4 NPs through bacterial membranes. ² White solid; Mp = 35-37 °C (Lit. 36-38 °C); ¹H NMR (400 MHz, CDCl₃) $\delta_{\rm H}$ = 7.60 (d, *J* = 16.0 Hz, 1H), 7.44-7.41 (m, 2H), 7.29-7.27 (m, 3H), 6.35 (d, *J* = 16.0 Hz, 1H), 3.71 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) $\delta_{\rm C}$ = 166.9, 144.4, 133.96, 129.8, 128.4, 127.6, 117.4, 51.2; MS, *m/z* (%): 162 [M⁺].



Figure S2-A: ¹H NMR spectrum (400 MHz, CDCl₃) of (*E*)-Methyl cinnamate.



Figure S2-B: ¹³C NMR spectrum (100 MHz, CDCl₃) of (*E*)-Methyl cinnamate.

Figure S2-C: Mass spectrum of (*E*)-Methyl cinnamate.



(E)-Methyl 3-(4-nitrophenyl) acrylate ⁴

Pale yellow solid; Mp = 160-162 °C (Lit. 160-162 °C); ¹H NMR (300 MHz, CDCl₃) $\delta_{\rm H}$ = 8.25 (d, J = 8.8 Hz, 2H), 7.71 (s, J = 16.1 Hz, 1H), 7.68 (d, J = 8.7 Hz, 2H), 6.57 (d, J = 16.1 Hz, 1H), 3.84 (s, 3H); ¹³C NMR (75 MHz, CDCl₃) $\delta_{\rm C}$ = 166.6, 148.7, 142.1, 140.7, 128.8, 124.4, 122.3, 52.3; MS, m/z (%): 207 [M⁺].



Figure S3-A: ¹H NMR spectrum (300 MHz, CDCl₃) of (*E*)-Methyl 3-(4-nitrophenyl) acrylate.



Figure S3-B: ¹³C NMR spectrum (75 MHz, CDCl₃) of (*E*)-Methyl 3-(4-nitrophenyl) acrylate.



Figure S3-C: Mass spectrum of (*E*)-Methyl 3-(4-nitrophenyl) acrylate.

(E)-Methyl 3-(4-cyanophenyl) acrylate ³

Pale yellow solid; Mp = 120-125 °C (Lit. 122-126 °C); ¹H NMR (300 MHz, CDCl₃) $\delta_{\rm H}$ = 7.67 (d, J = 8.4, 2H), 7.66 (d, J = 16.1, 1H), 7.60 (d, J = 8.3, 2H), 6.51 (d, J = 16.0, 1H), 3.82 (s, 3H); ¹³C NMR (75 MHz, CDCl₃) $\delta_{\rm C}$ = 166.6, 142.5, 138.8, 132.7, 128.5, 121.5, 118.4, 113.6, 52.0; MS, m/z (%): 187 [M⁺].



Figure S4-A: ¹H NMR spectrum (300 MHz, CDCl₃) of (*E*)-Methyl 3-(4-cyanophenyl) acrylate.



Figure S4-B: ¹³C NMR spectrum (75 MHz, CDCl₃) of (*E*)-Methyl 3-(4-cyanophenyl) acrylate.



Figure S4-C: Mass spectrum of (*E*)-Methyl 3-(4-cyanophenyl) acrylate.

(E)-Methyl 3-(4-chlorophenyl) acrylate ⁵

White solid; Mp = 73-74 °C (Lit. 73-75 °C); ¹H NMR (300 MHz, CDCl₃) $\delta_{\rm H}$ = 7.63 (d, *J* = 16.0, 1H), 7.44 (d, *J* = 8.5, 2H), 7.35 (d, *J* = 8.6, 2H), 6.40 (d, *J* = 16.0, 1H), 3.80 (s, 3H); ¹³C NMR (75 MHz, CDCl₃) $\delta_{\rm C}$ = 167.2, 143.4, 136.3, 133.0, 129.3, 129.3, 118.5, 51.8; MS, *m/z* (%): 196 [M⁺].



Figure S5-A: ¹H NMR spectrum (300 MHz, CDCl₃) of (*E*)-Methyl 3-(4-chlorophenyl) acrylate.



Figure S5-B: ¹³C NMR spectrum (75 MHz, CDCl₃) of (*E*)-Methyl 3-(4-chlorophenyl) acrylate.



Figure S5-C: Mass spectrum of (*E*)-Methyl 3-(4-chlorophenyl) acrylate.

(E)-Methyl 3-(4-methoxyphenyl) acrylate ⁴

Yellow solid; Mp = 88-91 °C (Lit. 88-89 °C); ¹H NMR (300 MHz, CDCl₃) δ_H = 7.67 (d, *J* = 16.3 Hz, 1H), 7.59-7.54 (m, 2H), 6.94-6.92 (m, 2H), 6.36 (d, *J* = 16.3 Hz, 1H), 3.80 (s, 3H), 3.76 (s, 3H); MS, *m/z* (%): 192 [M⁺].



Figure S6-A: ¹H NMR spectrum (300 MHz, CDCl₃) of (*E*)-Methyl 3-(4-methoxyphenyl)



Figure S6-C: Mass spectrum of (*E*)-Methyl 3-(4-methoxyphenyl) acrylate.

(E)-Methyl -3-(4-aminophenyl) acrylate ⁶

Pale yellow solid; Mp = 110-112 °C (Lit. 110-112 °C); ¹H NMR (300 MHz, CDCl₃) $\delta_{\rm H}$ = 7.60 (d, J = 15.9 Hz, 1H), 7.34 (d, J = 8.7 Hz, 2H), 6.64 (d, J = 8.6 Hz, 2H), 6.24 (d, J = 15.9 Hz, 1H), 3.96 (br, 2H), 3.78 (s, 3H); ¹³C NMR (75 MHz, CDCl₃) $\delta_{\rm C}$ = 168.1, 148.8, 145.1, 129.9, 124.6, 114.8, 113.2, 51.40.



Figure S7-A: ¹H NMR spectrum (300 MHz, CDCl₃) of (*E*)-Methyl -3-(4-aminophenyl) acrylate.



Figure S7-B: ¹³C NMR spectrum (75 MHz, CDCl₃) of (*E*)-Methyl -3-(4-aminophenyl) acrylate.

(E)-Methyl -3-(3-aminophenyl) acrylate 7



Pale yellow solid; Mp= 79-82 °C (Lit. 80-82 °C)

(E)-Methyl -3-(2-aminophenyl) acrylate ⁸

Pale yellow solid; Mp= 64-66 °C (Lit. 64-66 °C); ¹H NMR (CDCl₃, 400 MHz) $\delta_{\rm H}$ = 7.83 (d, *J* = 16.0 Hz, 1H), 7.38 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.17 (td, *J* = 7.7, 1.4 Hz, 1H), 6.77 (td, *J* = 7.6, 0.4 Hz, 1H), 6.70 (dd, *J* = 8.0, 0.8 Hz, 1H), 6.36 (d, *J* = 15.6 Hz, 1H), 3.98 (br, 2H), 3.80 (s, 3H); ¹³C NMR (CDCl₃, 100 MHz) $\delta_{\rm C}$ = 167.6, 145.6, 140.2, 131.2, 127.8, 119.5, 118.6, 117.1, 116.6, 51.4.



Figure S8-A: ¹H NMR spectrum (400 MHz, CDCl₃) of (*E*)-Methyl -3-(2-aminophenyl) acrylate.



Figure S8-B: ¹³C NMR spectrum (100 MHz, CDCl₃) of (*E*)-Methyl -3-(2-aminophenyl) acrylate.

(E)-Methyl 3-(p-tolyl) acrylate ⁴

White solid; Mp = 55-57 °C (Lit. 56-57 °C); ¹H NMR (400 MHz, CDCl₃) $\delta_{\rm H}$ = 7.69 (d, *J* = 16.0 Hz, 1H), 7.44-7.42 (m, 2H), 7.21-7.19 (m, 2H), 6.42 (d, *J* = 16.0 Hz, 1H), 3.81(s, 3H), 2.39 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) $\delta_{\rm C}$ = 167.6, 144.9., 140.7, 131.7, 129.6, 128.0, 116.7, 51.6, 21.5; MS, *m/z* (%): 176 [M⁺].



Figure S9-A: ¹H NMR spectrum (400 MHz, CDCl₃) of (*E*)-Methyl 3-(*p*-tolyl) acrylate.



Figure S9-B: ¹³C NMR spectrum (100 MHz, CDCl₃) of (*E*)-Methyl 3-(*p*-tolyl) acrylate.



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Figure S9-C: Mass spectrum of (E)-Methyl 3-(p-tolyl) acrylate.
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(E)-Methyl 3-(thiophen-2-yl) acrylate 9

White solid; Mp= 43-46 °C (Lit. 44-46 °C).



(E)-Methyl-3-(4-formylphenyl) acrylate ⁴

Yellow solid; Mp = 82-84 °C (Lit. 82-84 °C); ¹H NMR (400 MHz, CDCl₃) $\delta_{\rm H}$ = 10.02 (s, 1H), 7.90 (d, *J* = 8Hz, 2H), 7.71 (d, *J* = 16Hz, 1H), 7.67 (d, *J* = 8Hz, 2H), 6.55 (d, *J* = 16Hz, 1H), 3.82 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) $\delta_{\rm C}$ = 191.5, 166.8, 143.7, 140.0, 137.2, 130.2, 128.5, 120.9, 52.0.







Figure S10-B: ¹³C NMR spectrum (100 MHz, CDCl₃) of (*E*)-Methyl-3-(4-formylphenyl)

(E)-Methyl 3-(3-formylphenyl) acrylate 10

White solid; Mp = 54-56 °C (Lit. 54-56 °C); ¹H NMR (300 MHz; CDCl₃) $\delta_{\rm H}$ = 10.05 (s, 1H), 7.9-7.2 (m, 5H), 6.5 (d, *J* = 15Hz, 1H), 3.8 (s, 3H); ¹³C NMR (75 MHz, CDCl₃) $\delta_{\rm C}$ =191.65, 166.95, 143.13, 136.9, 135.39, 133.57, 131.11, 129.6, 128.8, 119.7, 51.9.



Figure S11-A: ¹H NMR spectrum (300 MHz, CDCl₃) of (*E*)-Methyl-3-(3-formylphenyl)



Figure S11-B: ¹³C NMR spectrum (75 MHz, CDCl₃) of (*E*)-Methyl-3-(3-formylphenyl) acrylate.

Oil; ¹H NMR (400 MHz, CDCl₃) $\delta_{\rm H} = 7.60$ (d, J = 16.4 Hz, 1H), 7.45 -7.43 (m, 2H), 7.31 -7.28 (m, 3H), 6.36 (d, J = 16.0 Hz,1H), 4.13 (t, J = 6.8 Hz, 2H), 1.62 -1.59 (m, 2H), 1.36 -1.34 (m, 2H), 0.88 (t, J = 7.6 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) $\delta_{\rm C} = 166.8$, 144.4, 134.4, 130.1, 128.8, 128.0, 118.2, 64.3, 30.8, 19.2, 13.7.



Figure S12-A: ¹H NMR spectrum (400 MHz, CDCl₃) of (*E*)-Butyl cinnamate.



Figure S12-B: ¹³C NMR spectrum (100 MHz, CDCl₃) of (*E*)-Butyl cinnamate.

(E)-Butyl 3-(4-nitrophenyl) acrylate ¹²

Yellow solid; Mp = 67-69 °C (Lit. 59-69 °C); ¹H NMR (400 MHz, CDCl₃) $\delta_{\rm H}$ = 8.20 (d, J = 8.0 Hz, 2H), 7.68-7.63 (m, 3H), 6.53 (d, J = 16.0 Hz, 1H), 4.24-4.17 (m, 2H), 1.69-1.63 (m, 2H), 1.44-1.35 (m, 2H), 0.92 (t, J = 7.2 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) $\delta_{\rm C}$ = 166.0, 148.3, 141.5, 140.5, 128.6, 124.0, 122.5, 64.7, 30.6, 19.1, 13.6.



Figure S13-A: ¹H NMR spectrum (400 MHz, CDCl₃) of (*E*)-Butyl 3-(4-nitrophenyl) acrylate.



Figure S13-B: ¹³C NMR spectrum (100 MHz, CDCl₃) of (*E*)-Butyl 3-(4-nitrophenyl) acrylate.

(E)-Butyl-3-(4-cyanophenyl) acrylate ¹³

Yellow solid; 43-46 °C (Lit. 43-46 °C); ¹ H NMR (400 MHz, CDCl₃) $\delta_{\rm H}$ = 7.68-7.59 (m, 5H) 6.49 (d, *J* = 16 Hz, 1H), 4.22 (t, *J* = 6.7 Hz, 2H), 1.69(quint, *J* = 7.6 Hz, 2H), 1.44 (sext, *J* = 7.6 Hz, 2H), 0.96 (t, *J* = 7.6 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) $\delta_{\rm C}$ = 166.3, 142.2, 138.9, 132.8, 128.5, 122.0, 118.5, 113.5, 65.0, 30.8, 19.3, 13.8.



Figure S14-A: ¹H NMR spectrum (400 MHz, CDCl₃) of (*E*)-Butyl-3-(4-cyanophenyl) acrylate.



Figure S14-B: ¹³C NMR spectrum (100 MHz, CDCl₃) of (*E*)-Butyl-3-(4-cyanophenyl) acrylate.

(E)-Butyl-3-(4-chlorophenyl) acrylate ¹⁴

White solid; Mp= 37-39 °C (Lit. 38-40 °C); ¹H NMR (400 MHz, CDCl₃) $\delta_{\rm H}$ = 7.62 (d, *J* = 16.0 Hz, 1H), 7.45 (d, *J* = 8.3 Hz, 2H), 7.35 (d, *J* = 8.4 Hz, 2H), 6.41 (d, *J* = 16.0 Hz, 1H), 4.21 (t, *J* = 6.7 Hz, 2H), 1.72-1.65 (m, 2H), 1.44 (dq, *J* = 14.7, 7.4 Hz, 2H), 0.96 (t, *J* = 7.4 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) $\delta_{\rm C}$ = 166.8, 143.1, 136.1, 133.0, 129.2, 129.2, 118.9, 64.6, 30.7, 19.2, 13.7.



Figure S15-A: ¹H NMR spectrum (400 MHz, CDCl₃) of (*E*)-Butyl 3-(4-chlorophenyl) acrylate.



Figure S15-B: ¹³C NMR spectrum (100 MHz, CDCl₃) of (*E*)-Butyl 3-(4-chlorophenyl) acrylate.

(E)-Butyl 3-(4-methoxyphenyl) acrylate ¹⁵

White solid; Mp = 90-92 °C (Lit. 92-93 °C); ¹H NMR (400 MHz, CDCl₃) $\delta_{\rm H}$ = 7.58 (d, *J* = 16.0 Hz, 1H), 7.39 (d, *J* = 4.2 Hz, 2H), 6.81 (d, *J* = 4.8 Hz, 2H), 6.24 (d, *J* = 16.0 Hz, 1H), 4.13 (t, *J* = 7.0 Hz, 2H), 3.72 (s, 3H), 1.62-1.60 (m, 2H), 1.40-1.35 (m, 2H), 0.91 (t, *J* = 7.0 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) $\delta_{\rm C}$ = 167.1, 161.2, 144.0, 129.5, 127.0, 115.5, 114.1, 64.0, 55.0, 30.7, 19.1, 13.6; MS, *m/z* (%): 234 [M⁺].



Figure S16-A: ¹H NMR spectrum (400 MHz, CDCl₃) of (*E*)-Butyl 3-(4-methoxyphenyl)



Figure S16-B: ¹³C NMR spectrum (100 MHz, CDCl₃) of (*E*)-Butyl 3-(4-methoxyphenyl) acrylate.



Figure S16-C: Mass spectrum of (*E*)-Butyl 3-(4-methoxyphenyl) acrylate.

(E)-Butyl-3-(4-aminophenyl) acrylate ¹⁶

Yellowish-brown solid; Mp= 84-86 °C (Lit. 85-86 °C).



(E)-Butyl-3-(2-aminophenyl) acrylate ¹⁷

Yellow solid; Mp= 69-71 °C (Lit. 70-71 °C); ¹H NMR (400 MHz, DMSO- d_6) $\delta_{\rm H}$ = 7.85 (d, J = 16.0 Hz, 1H), 7.43 (d, J = 8.0 Hz, 1H), 7.06 (t, J = 6.8 Hz, 1H), 6.68 (d, J = 8.0 Hz, 1H), 6.52 (t, J = 7.2 Hz, 1H), 6.33 (d, J = 16.0 Hz, 1H), 5.57 (s, 2H), 4.11 (t, J = 6.4 Hz, 2H), 1.62-1.57 (m, 2H), 1.39-1.33 (m, 2H), 0.90 (t, J = 7.2 Hz, 3H); ¹³C NMR (100 MHz, DMSO- d_6) $\delta_{\rm C}$ = 166.8, 148.3, 140.8, 131.3, 127.4, 117.6, 116.5, 115.2, 63.4, 30.4, 18.7, 13.6.



Figure S17-A: ¹H NMR spectrum (400 MHz, DMSO-*d*₆) of (E)-Butyl-3-(2-aminophenyl)



Figure S17-B: ¹³C NMR spectrum (100 MHz, DMSO- d_6) of (*E*)-Butyl-3-(2-aminophenyl)

Oil; ¹H NMR (400 MHz, CDCl₃) $\delta_{\rm H}$ = 7.52 (d, *J* = 18.2 Hz, 1H), 7.32-7.28 (m, 2H), 7.07-7.04 (m, 2H), 6.30 (d, *J* = 16 Hz, 1H), 4.09 (t, *J* = 5.0 Hz, 2H), 2.24 (s, 3H), 1.40-1.32 (m, 2H), 1.31-1.23 (m, 2H), 0.85 (t, *J* = 7.4 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) $\delta_{\rm C}$ = 167.2, 144.5, 140.5,131.7, 129.5, 128.0, 117.1, 64.2, 30.8, 21.4, 19.2, 13.7.



Figure S18-A: ¹H NMR spectrum (400 MHz, CDCl₃) of (*E*)-Butyl 3-(*p*-tolyl) acrylate.



Figure S18-B: ¹³C NMR spectrum (100 MHz, CDCl₃) of (*E*)-Butyl 3-(*p*-tolyl) acrylate.

(E)-Butyl 3-(thiophen-2-yl) acrylate 19

Oil; ¹H NMR (300 MHz, CDCl₃) $\delta_{\rm H} = 7.78$ (d, J = 15.6 Hz, 1H), 7.36 (d, J = 4.8 Hz, 1H), 7.25 (d, J = 4.5 Hz, 1H), 7.04 (d, J = 4.8 Hz, 1H), 6.24 (d, J = 15.6 Hz, 1H), 4.20 (t, J = 6.6 Hz, 2H), 1.72-1.63 (m, 2H), 1.49-1.37 (m, 2H), 0.94 (t, J = 7.2 Hz, 3H); ¹³C NMR (75 MHz, CDCl₃) $\delta_{\rm C} = 167.0$, 139.6, 137.0, 130.8, 128.3, 128.1, 117.1, 64.4, 30.8, 19.2, 13.7.



Figure S19-A: ¹H NMR spectrum (300 MHz, CDCl₃) of (*E*)-Butyl 3-(thiophen-2-yl) acrylate.



Figure S19-B: ¹³C NMR spectrum (75 MHz, CDCl₃) of (*E*)-Butyl 3-(thiophen-2-yl) acrylate.

(E)-Butyl-3-(4-formylphenyl) acrylate ²⁰

Colorless oil; ¹H NMR (400 MHz, CDCl₃) $\delta_{\rm H}$ = 10.02 (s, 1H), 7.89 (d, *J* = 8.4 Hz, 2H), 7.71-7.66 (m, 3H), 6.54 (d, *J* = 16.0 Hz, 1H), 4.22 (t, *J* = 6.8 Hz, 2H), 1.72-1.65 (m, 2H), 1.48-1.38 (m, 2H), 0.96 (t, *J* = 7.6 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) $\delta_{\rm C}$ = 191.44, 166.42, 142.75, 140.09, 137.06, 130.12, 128.45, 121.43, 64.72, 30.67, 19.14, 13.70.



Figure S20-A: ¹H NMR spectrum (400 MHz, CDCl₃) of (*E*)-Butyl-3-(4-formylphenyl) acrylate.



Figure S20-B: ¹³C NMR spectrum (100 MHz, CDCl₃) of (*E*)-Buthyl-3-(4-formylphenyl) acrylate.

White solid; Mp = 70-71 °C (Lit. 70-71 °C); ¹H NMR (400 MHz, CDCl₃) $\delta_{\rm H}$ = 7.54 (d, *J* = 8.0 Hz, 4H), 7.39 (t, *J* = 8.0 Hz, 4H), 7.31-7.27 (m, 2H); ¹³C NMR (100 MHz, CDCl₃) $\delta_{\rm C}$ = 141.25, 128.75, 127.24, 126.17; MS, *m/z* (%): 154 [M⁺].



Figure S21-A: ¹H NMR spectrum (400 MHz, CDCl₃) of 1, 1'-Biphenyl.



Figure S21-B: ¹³C NMR spectrum (100 MHz, CDCl₃) of 1, 1'-Biphenyl.

Figure S21-C: Mass spectrum of 1, 1'-Biphenyl.



Nitro-1, 1'-biphenyl²²

White solid; Mp = 107-109 °C (Lit. 106-109 °C); ¹H NMR (400 MHz, CDCl₃) $\delta_{\rm H}$ = 8.33 (d, *J* = 8.8 Hz, 2H), 7.78-7.76 (m, 2H), 7.67-7.65 (t, 2H) 7.55-7.46 (m, 3H); ¹³C NMR (100 MHz, CDCl₃) $\delta_{\rm C}$ = 147.18, 146.65, 138.32, 128.72, 128.49, 127.35, 126.95, 123.66; MS, *m/z* (%): 199 [M⁺].



Figure S22-A: ¹H NMR spectrum (400 MHz, CDCl₃) of 4-Nitro-1, 1'-biphenyl.



Figure S22-B: ¹³C NMR spectrum (100 MHz, CDCl₃) of 4-Nitro-1, 1'-biphenyl.

Figure S22-C: Mass spectrum of 4-Nitro-1, 1'-biphenyl.



4-Cyano-1, 1'-biphenyl²³

White solid; Mp = 85-87 °C (Lit. 84-86 °C); ¹H NMR (400 MHz, CDCl₃) $\delta_{\rm H}$ = 7.77-7.70 (q, 4H), 7.62 (d, *J* = 7.2 Hz, 2H), 7.54-7.46 (m, 3H); ¹³C NMR (100 MHz, CDCl₃) $\delta_{\rm C}$ = 145.68, 139.19, 132.60, 129.11, 128.66, 127.74, 127.23, 118.94, 110.93; MS, *m/z* (%): 179 [M⁺].



Figure S23-A: ¹H NMR spectrum (400 MHz, CDCl₃) of 4-Cyano-1, 1'-biphenyl.



Figure S23-B: ¹³C NMR spectrum (100 MHz, CDCl₃) of 4-Cyano-1, 1'-biphenyl.



Figure S23-C: Mass spectrum of 4-Cyano-1, 1'-biphenyl.

4-Chloro-1, 1'-biphenyl²⁴

Colorless solid; Mp = 71-73 °C (Lit. 71-73 °C); MS, *m/z* (%): 189 [M⁺].



Figure S24-C: Mass spectrum of 4-Chloro-1, 1'-biphenyl.

White solid; Mp = 87-90 °C (Lit. 89-91 °C); ¹H NMR (400 MHz, CDCl₃) $\delta_{\rm H}$ = 7.45 (t, *J* = 8.4 Hz, 4H), 7.34 (t, *J* = 7.6 Hz, 2H), 7.21 (t, *J* = 6.8 Hz, 1H), 6.89 (d, *J* = 8.8 Hz, 2H), 3.75 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) $\delta_{\rm C}$ = 159.17, 140.88, 133.82, 128.72, 128.16, 126.75, 114.23, 55.36; MS, *m/z* (%): 184 [M⁺].



Figure S25-A: ¹H NMR spectrum (400 MHz, CDCl₃) of 4-Methoxy-1, 1'-biphenyl.



Figure S25-B: ¹³C NMR spectrum (100 MHz, CDCl₃) of 4-Methoxy-1, 1'-biphenyl.



Figure S25-C: Mass spectrum of 4-Methoxy-1, 1'-biphenyl.

4-Amino-1, 1'-biphenyl²⁶

Pale yellow solid; Mp= 51-54 °C (Lit. 52-54 °C); ¹H NMR (500 MHz, CDCl₃) $\delta_{\rm H}$ = 7.53 (d, *J* = 7.52 Hz, 2H), 7.41 (m, 4H), 7.27 (t, *J* = 7.56 Hz, 1H), 6.76 (d, *J* = 8.18 Hz, 2H), 3.72 (br, 2H); ¹³C NMR (125 MHz, CDCl₃) $\delta_{\rm C}$ = 146.0, 141.3, 131.7, 128.8, 128.1, 126.5, 126.4, 115.5.



Figure S26-A: ¹H NMR spectrum (500 MHz, CDCl₃) of 4-Amino-1, 1'-biphenyl.



Figure S26-B: ¹³C NMR spectrum (125 MHz, CDCl₃) of 4-Amino-1, 1'-biphenyl.

White Solid; Mp= 27-30 °C (Lit. 28-30 °C); ¹H NMR (400 MHz, CDCl₃) $\delta_{\rm H}$ = 7.58 (d, *J* = 7.8 Hz, 2H), 7.48- 7.36 (m, 4H), 7.36 -7.23 (m, 1H), 6.78 (t, *J* = 10.2 Hz, 2H), 3.74 (s, 2H); ¹³C NMR (100 MHz, CDCl₃) $\delta_{\rm C}$ = 145.86, 141.20, 131.63, 128.66, 128.02, 126.42, 126.26, 115.40.



Figure S27-A: ¹H NMR spectrum (400 MHz, CDCl₃) of 3-Amino-1, 1'-biphenyl.



Figure S27-B: ¹³C NMR spectrum (100 MHz, CDCl₃) of 3-Amino-1, 1'-biphenyl.

2-Amino-1, 1'-biphenyl²⁸

White solid; Mp = 48-51 °C (Lit 48-51 °C); ¹H NMR (400 MHz, CDCl₃) $\delta_{\rm H}$ = 8.27 (d, *J* = 7.1 Hz, 1H), 7.59-7.36 (m, 4H), 7.23-7.04 (m, 2H), 6.86-6.67 (m, 2H), 4.02 (m, 2H); ¹³C NMR (100 MHz, CDCl₃) $\delta_{\rm C}$ =143.6, 139.6, 135.8, 132.8, 130.6, 129.2, 128.9, 128.6, 128.1, 127.8, 127.3, 118.8, 115.8.



Figure S28-A: ¹H NMR spectrum (400 MHz, CDCl₃) of 2-Amino-1, 1'-biphenyl.



Figure S28-B: ¹³C NMR spectrum (100 MHz, CDCl₃) of 2-Amino-1, 1'-biphenyl.

4-Methyl-1, 1'-biphenyl²⁹

White solid; Mp= 44-46 °C (Lit. 45-47 °C); ¹H NMR (CDCl₃, 400 MHz) $\delta_{\rm H}$ = 7.67-7.64 (t, 2H), 7.56 (d, *J* = 8 Hz, 2H), 7.51-7.47 (t, 2H), 7.41-7.37 (t, 1H), 7.32 (d, *J* = 7.6 Hz, 2H), 2.46 (s, 3H); ¹³C NMR (CDCl₃, 100 MHz) $\delta_{\rm C}$ = 141.7, 138.9, 137.7, 130.0, 129.3, 127.7, 127.5, 127.5, 21.6.



Figure S29-A: ¹H NMR spectrum (400 MHz, CDCl₃) of 4-Methyl-1, 1'-biphenyl.



Figure S29-B: ¹³C NMR spectrum (100 MHz, CDCl₃) of 4-Methyl-1, 1'-biphenyl.

2-([1,1'-biphenyl]-2-yl) thiophene ³⁰

White solid; Mp= 34-36 °C (Lit. 34-36 °C); ¹H NMR (300 MHz, CDCl₃) $\delta_{\rm H}$ = 7.62-7.59 (m, 2H), 7.38-7.06 (m, 6H); ¹³ C NMR (75 MHz, CDCl₃) $\delta_{\rm C}$ = 142.6, 139.6, 138.7, 136.1, 129.02, 128.9, 128.7, 127.9, 127.8, 127.7, 127.6, 127.2, 125.7.



Figure S30-A: ¹H NMR spectrum (300 MHz, CDCl₃) of 2-([1,1'-biphenyl]-2-yl) thiophene.



[1, 1'-

biphenyl]-

4-

carbaldehyde

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White to light yellow solid; Mp = 62-63 °C (Lit. 62-63 °C); ¹H NMR (400 MHz, CDCl₃) $\delta_{\rm H}$ = 9.96 (s, 1H), 7.86 (d, *J* = 8.0 Hz, 2H), 7.66 (d, *J* = 8.0 Hz, 2H), 7.55 (d, *J*= 8.4 Hz, 2H), 7.39 (t, *J* = 7.2 Hz, 2H), 7.34 (t, *J* = 7.2 Hz, 1H); MS, *m/z* (%): 182 [M⁺].



Figure S31-A: ¹H NMR spectrum (400 MHz, CDCl₃) of [1, 1'-biphenyl]-4-carbaldehyde.



Figure S31-C: Mass spectrum of [1, 1'-biphenyl]-4-carbaldehyde.

White solid; Mp= 53-54 °C (Lit. 53-54 °C); ¹H NMR (500 MHz, CDCl₃) $\delta_{\rm H}$ = 10.11 (s, 1H), 8.13 (d, *J* = 1.5 Hz, 1H), 7.89 (dd, *J* = 7.5, 1.5 Hz, 2H), 7.66 -7.62 (m, 3H), 7.52 -7.49 (m, 2H), 7.43 (t, *J* = 7.5 Hz, 1H); MS, *m/z* (%): 182 [M⁺].



Figure S32-A: ¹H NMR spectrum (500 MHz, CDCl₃) of [1,1'-biphenyl]-3-carbaldehyde.



Figure S32-C: Mass spectrum of [1,1'-biphenyl]-3-carbaldehyde.

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