Supporting Information for:

The Effect of the Triazole Ring in Hybrid Electron Donor-Acceptor Systems towards Light Harvesting in NiO-based Devices

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EXPERIMENTAL SECTION

Synthesis

Porphyrin 3. Equimolar amounts of porphyrin **1** (100 mg, 0.116 mmol) and 4-ethynylbenzaldehyde (16 mg, 0.116 mmol) were dissolved in a 1:1 mixture of THF/CH_3CN (10 mL) under N_2 atmosphere. In the next step, CuI (22 mg, 0.116 mmol) and DIPEA (20 µL, 0.124 mmol) were added and the reaction mixture was stirred at room temperature for 12 h. Upon reaction completion, the volatiles were removed under reduced pressure and the crude solid, was purified by column chromatography (silica gel, CH_2Cl_2/EtOH, 99:1) yielding 84 mg of **1** (0.086 mmol, yield: 73%).

^{1}H NMR (500 MHz, $CDCl_3$): δ = 10.03 (s, 1H), 8.88 (d, J = 4.6 Hz, 2H), 8.82 (m, 4H), 8.79 (d, J = 4.6 Hz, 2H), 8.61 (s, 1H), 8.42 (m, 4H), 8.33 (d, J = 7.9 Hz, 2H), 8.17 (m, 4H), 8.01 (d, J = 8.2 Hz, 2H) 7.29 (s, 4H), 4.08 (s, 3H), 2.58 (s, 6H), 2.64 (s, 6H), 1.85 (s, 12H) ppm.

HRMS (MALDI-TOF): calc. for $C_{61}H_{48}N_7O_3Zn$ [M + H]$^+$: 990.3032; found 990.3040.

C_{60}*tr*ZnPCOOH. Porphyrin **3** (50 mg, 0.050 mmol) was dissolved in a THF/MeOH mixture (28 mL) with 5:2 ratio and then 3 mL of a 10% KOH aqueous solution were added. The reaction mixture was heated at 40 ^{o}C for 6 h. Upon reaction completion, we added 20 mL of 1 M citric acid aqueous solution and 20 mL of a MeOH/$CHCl_3$ (1:4 ratio). The mixture was washed with H_2O (3 x 20 mL) and the organic phase was evaporated under reduced pressure. The crude product was subsequently used as a starting material for the synthesis of **C_{60}*tr*ZnPCOOH**. In a round bottom flask porphyrin, 2-methyl glycine (sarcosine, 110 mg, 1.24 mmol) and C_{60} (43 mg, 0.060 mmol) were dissolved in dry toluene (45 mL). The reaction mixture was refluxed overnight. The purification of **C_{60}*tr*ZnPCOOH** was accomplished through silica gel column chromatography. Firstly, we used toluene as eluent to remove the excess of unreacted C_{60} and then a mixture of CH_2Cl_2/MeOH in 97:3 ratio. **C_{60}*tr*ZnPCOOH** was produced in a 46% yield (40 mg, 0.023 mmol).

^{1}H NMR (500 MHz, THF-*d_8*): δ = 11.66 (s, 1H), 9.15 (s, 1H), 8.86 (d, *J* = 4.6 Hz, 2H), 8.78 (d, *J* = 4.5 Hz, 2H), 8.70 (m, 4H), 8.40 (m, 4H), 8.31 (m, 4H), 8.19 (m, 2H), 8.00 (sb, 2H), 7.30 (s, 4H) 5.09 (s, 1H), 5.05 (d, *J* = 9.0 Hz, 1H), 4.3 (d, *J* = 8.9 Hz, 1H), 2.87 (s, 3H), 2.60 (s, 6H), 1.85 (s, 12H) ppm.

^{13}C NMR (125 MHz, THF-*d_8*): δ = 167.70, 157.70, 155.22, 154.73, 154.66, 150.57, 150.42, 150.23, 148.70, 148.52, 147.81, 147.64, 147.31, 147.08, 146.77, 146.61, 146.43, 146.37, 146.16, 146.02, 145.84, 145.65, 145.26, 145.12, 144.96, 144.91, 144.44, 144.03, 143.67, 143.49, 143.20, 143.04, 143.01, 142.91, 142.72, 142.63, 142.55, 142.49, 142.36, 142.20, 142.08, 140.66, 140.60, 140.42, 140.35, 140.05, 139.65, 137.98, 137.90, 137.63, 137.55, 137.19, 136.66, 136.47, 136.15, 135.07, 132.36, 132.24, 130.97, 130.74, 128.34, 128.31, 126.57, 119.76, 119.52, 119.27, 119.22, 118.39, 83.98, 78.32, 70.49, 70.13, 39.77, 21.85, 21.39 ppm.

HRMS (MALDI-TOF): calc. for $C_{122}H_{51}N_8O_2Zn$ [M + H]$^+$: 1723.3348; found 1723.3351.

<u>Porphyrin 7</u>. Porphyrin **5** (70 mg, 0.083 mmol) and ester **6** (6.6 mg, 0.041 mmol) were dissolved in a 1:1 mixture of THF/CH_3CN (8 mL) under N_2 atmosphere. In the next step, CuI (15.8 mg, 0.083 mmol) and DIPEA (11 µL, 0.083 mmol) were added and the reaction mixture was stirred at room temperature for 12 h. Upon reaction completion, the volatiles were removed under reduced pressure and the crude solid, was subsequently was used for another click reaction. Namely, between the newly formed clicked porphyrin derivative and aldehyde **2** (5.3 mg, 0.041 mmol) were added in a Schlenk tube and dissolved in a 1:1 mixture of THF/CH_3CN (8 mL) under N_2 atmosphere. Afterwards, CuI (15.8 mg, 0.083 mmol) and DIPEA (11 µL, 0.083 mmol) were added and the reaction mixture was stirred at room temperature for 12 h. Then, the volatiles were removed and the crude solid was purified by column chromatography (silica gel, CH_2Cl_2/EtOH, 99:1) yielding 40 mg of **7** (0.035 mmol, yield: 42%).

^{1}H NMR (500 MHz, $CDCl_3$): δ = 10.07 (s, 1H), 8.90 (d, J = 4.6 Hz, 4H), 8.83 (d, J = 4.6 Hz, 4H), 8.61 (s, 1H), 8.57 (s, 1H), 8.43 (m, 4H), 8.19 (m, 8H), 8.08 (d, J = 8.1 Hz, 2H), 8.03 (d, J = 8.0 Hz, 2H), 7.30 (s, 4H), 3.97 (s, 3H), 2.64 (s, 6H), 1.85 (s, 12H) ppm.

HRMS (MALDI-TOF): calc. for Chemical Formula: $C_{69}H_{53}N_{10}O_3Zn$ [M + H]$^+$: 1133.3515; found 1133.3519.

C_{60}*tr*ZnP*tr*COOH. Porphyrin **7** (35 mg, 0.030 mmol) was dissolved in a THF/MeOH mixture (21 mL) with 5:2 ratio and then 2 mL of a 10% KOH aqueous solution were added. The reaction mixture was heated at 40^{o}C for 6 h. Upon reaction completion, we added 15 mL of 1 M citric acid aqueous solution and 15 mL of a MeOH/$CHCl_3$ mixture (1:4 ratio). The mixture was washed with H_2O (3 x 15 mL) and the organic phase was evaporated under reduced pressure. The crude product was subsequently used as a starting material for the synthesis of **C_{60}*tr*ZnP*tr*COOH**. In a round bottom flask we added the crude porphyrin, 2-methyl glycine (sarcosine, 75 mg, 0.84 mmol) and C_{60} (29 mg, 0.040 mmol) and dissolved them in dry toluene (35 mL). The reaction mixture was refluxed overnight. The purification of **C_{60}*tr*ZnP*tr*COOH** was accomplished through silica gel column chromatography. Firstly, we used toluene as eluent to remove the excess of unreacted C_{60} and then a mixture of CH_2Cl_2/MeOH in a 97:3 ratio, providing **C_{60}*tr*ZnP*tr*COOH** in a 40% yield (22 mg, 0.012 mmol).

^{1}H NMR (300 MHz, THF-d_8): δ = 11.42 (s, 1H), 9.23 (s, 1H), 9.16 (s, 1H), 8.86 (m, 4H), 8.71 (m, 4H), 8.37 (m, 8H), 8.18 (s, 6H), 8.04 (m, 2H), 7.30 (s, 4H), 5.11 (s, 1H), 5.06 (s, 1H), 4.34 (d, J = 9.4, 1H), 2.88 (s, 3H), 2.60 (s, 6H), 1.85 (s, 12H) ppm.

^{13}C NMR (75 MHz, THF-d_8): δ = 167.30, 157.95, 155.48, 154.98, 150.77, 150.64, 148.68, 148.19, 148.06, 147.89, 147.57, 147.31, 146.99, 146.86, 146.67, 146.59, 146.26, 146.01, 145.50, 145.36, 145.21, 144.74, 144.58, 143.82, 143.44, 143.30, 143.14, 142.94, 142.80, 142.59, 142.44, 142.31, 140.89, 140.65, 140.53, 140.27, 139.82, 138.20, 138.10, 137.86, 137.67, 137.41, 136.90, 136.71, 136.35, 136.10, 132.57, 132.42, 131.33, 131.17, 130.83, 128.55, 126.73, 126.11, 120.20, 119.73, 119.41, 118.64, 84.15, 78.55, 70.66, 70.36, 39.94, 22.03, 21.57 ppm.

HRMS (MALDI-TOF): calc. for $C_{130}H_{55}N_{11}O_2Zn$ [M + H]$^+$: 1866.3832; found 1866.3836.

Porphyrin 10. Dippyrromethane **8** (1 g, 6.8 mmol) and mesityl-aldehyde **9** (1 mL, 6.8 mmol) were dissolved in EtOH (200 mL) under argon atmosphere. After 10 min of constant stirring, 50 mL of a HCl/H_2O solution (in 1:50 ratio) were added to the reaction mixture and afterwards stirring continued for 16 h. Then, $CHCl_3$ (200 mL) was added and the organic phase washed with H_2O (3 x 100 mL) and with saturated aqueous solution of $NaHCO_3$ (1 x 100 mL). The organic layer was dried over anhydrous $MgSO_4$ and hereupon oxidized using p-chloranil (2.5 g, 10.2 mmol) for 1h, under reflux. Upon reaction completion, the porphyrin mixture was filtrated using a short silica gel plug. Subsequently, column chromatography (silica gel, CH_2Cl_2/Hexane, 7:3) was performed to obtain 380 mg of the desired porphyrin derivative **10** in 21% yield (0.035 mmol).

^{1}H NMR (500 MHz, $CDCl_3$): δ = 10.23 (s, 2H), 9.33 (d, J = 4.5 Hz, 4H), 8.89 (d, J = 4.6 Hz, 4H), 7.34 (s, 4H), 2.68 (s, 6H), 1.86 (s, 12H), -3.05 (s, 2H) ppm.

HRMS (MALDI-TOF): calc. for Chemical Formula: $C_{38}H_{35}N_4$ [M + H]$^+$: 547.2783; found 547.2786.

Porphyrin 11. Porphyrin **10** (50 mg, 0.092 mmol) was dissolved in $CHCl_3$ (25 mL) at 0^{o}C. Then, pyridine (100 μL) and NBS (33 mg, 0.18 mmol) were added and the reaction mixture was stirred while checking the reaction progress via TLC every few minutes. Upon reaction completion (almost 25 min), acetone (2 mL) was added and the volatiles were removed under reduced pressure. The crude solid was purified by column chromatography (silica gel, CH_2Cl_2/Hexane, 3:2) yielding 53 mg of **11** (0.075 mmol, yield: 82%).

^{1}H NMR (500 MHz, CDCl$_3$): δ = 9.55 (d, J = 4.3 Hz, 4H), 8.69 (d, J = 4.1 Hz, 4H), 7.30 (s, 4H), 2.64 (s, 6H), 1.82 (s, 12H), -2.54 (s, 2H) ppm.

HRMS (MALDI-TOF): calc. for Chemical Formula: $C_{38}H_{33}N_4Br_2$ [M + H] $^+$: 703.0994; found 703.0998.

Porphyrin 14. Porphyrin **11** (100 mg, 0.14 mmol), boronic acid **12** (12.6 mg, 0.07 mmol) and barium hydroxide (48 mg, 0.28 mmol) were dissolved in a mixture of THF/H_2O (8 mL, in 3:1 ratio) under argon atmosphere. The solution was degassed twice using the freeze-pump-thaw technic, prior to the addition of $Pd(PPh_3)_4$ (4 mg, 3.14 µmol) and the reaction was heated at 80 ^oC overnight. Then, the mixture was cooled down to room temperature and filtrated over celite. The solvents were evaporated under reduced pressure and the crude product was subsequently used for a second Suzuki reaction with boronic acid **13** (10.5 mg, 0.07 mmol). For the successful preparation of porphyrin **14** the same experimental procedure was followed using barium hydroxide (48 mg, 0.28 mmol) and a THF/H_2O solvent mixture (8 mL, in 3:1 ratio) under argon atmosphere. Prior to the addition of $Pd(PPh_3)_4$ (4 mg, 3.14 µmol) the solution was degassed using the freeze-pump-thaw technic and the reaction mixture was heated at 80 ^oC overnight. The desired compound (porphyrin **14**) was purified through silica gel chromatography using CH_2Cl_2 as eluent yielding 31% (35 mg, 0.045 mmol).

^{1}H NMR (500 MHz, CDCl$_3$): δ = 10.42 (s, 1H), 8.76 (m, 8H), 8.46 (m, 4H), 8.36 (m, 4H), 7.32 (s, 4H), 4.14 (s, 3H), 2.66 (s, 6H), 1.87 (s, 12H), -2.60 (s, 2H) ppm.

HRMS (MALDI-TOF): calc. for Chemical Formula: $C_{69}H_{52}N_{10}O_3Zn$ [M + H] $^+$: 1133.3515; found 1133.3519.

C_{60}ZnPCOOH. To a CH_2Cl_2 solution (20 mL) of **14** (50 mg, 0.064 mmol), a MeOH (3 mL) solution containing $Zn(CH_3COO)_2.2H_2O$ (219 mg, 1 mmol) was added and the reaction mixture was stirred at room temperature overnight. The volatiles were evaporated, the porphyrin was diluted in $CHCl_3$ (25 mL) and washed with H_2O (3 x 25 mL). The solvent was removed under reduced pressure and the produced porphyrin was hydrolyzed to the corresponding acid porphyrin using the below mentioned experimental procedure. In detail, the crude product was dissolved in a THF/MeOH mixture (28 mL) with 5:2 ratio and then 3 mL of a 10% KOH aqueous solution were added. The reaction mixture was heated at 40 ^oC for 6h. Upon reaction completion, we added 20 mL of 1 M citric acid aqueous solution and 20 mL of a MeOH/$CHCl_3$ mixture (1:4 ratio). The mixture was washed with H_2O (3 x 20 mL) and the organic phase was evaporated under reduced pressure. The produced porphyrin was subsequently used as a starting material for the synthesis of **C_{60}ZnPCOOH**. In a round bottom flask we added the crude porphyrin, 2-methyl glycine (sarcosine, 75 mg, 0.84 mmol) and C_{60} (29 mg, 0.040 mmol) and dissolved them in dry toluene (35 mL). The reaction mixture was refluxed overnight. The purification of **C_{60}ZnPCOOH** was accomplished through silica gel column chromatography. The first column was performed with toluene to remove the excess of unreacted C_{60} and the second one with CH_2Cl_2/MeOH in a 97:3 ratio providing **C_{60}ZnPCOOH** in a 35% yield (22 mg, 0.012 mmol).

^{1}H NMR (500 MHz, THF-*d_8*): δ = 11.64 (s, 1H), 8.69 (m, 8H), 8.39 (d, *J* = 8.0 Hz, 4H), 8.28 (d, *J* = 8.0 Hz, 4H), 7.29 (m, 4H), 5.39 (s, 1H), 5.18 (d, *J* = 8.8 Hz, 1H), 4.48 (d, *J* = 8.8 Hz, 1H), 3.13 (s, 3H), 2.60 (m, 6H), 1.84 (m, 12H) ppm.

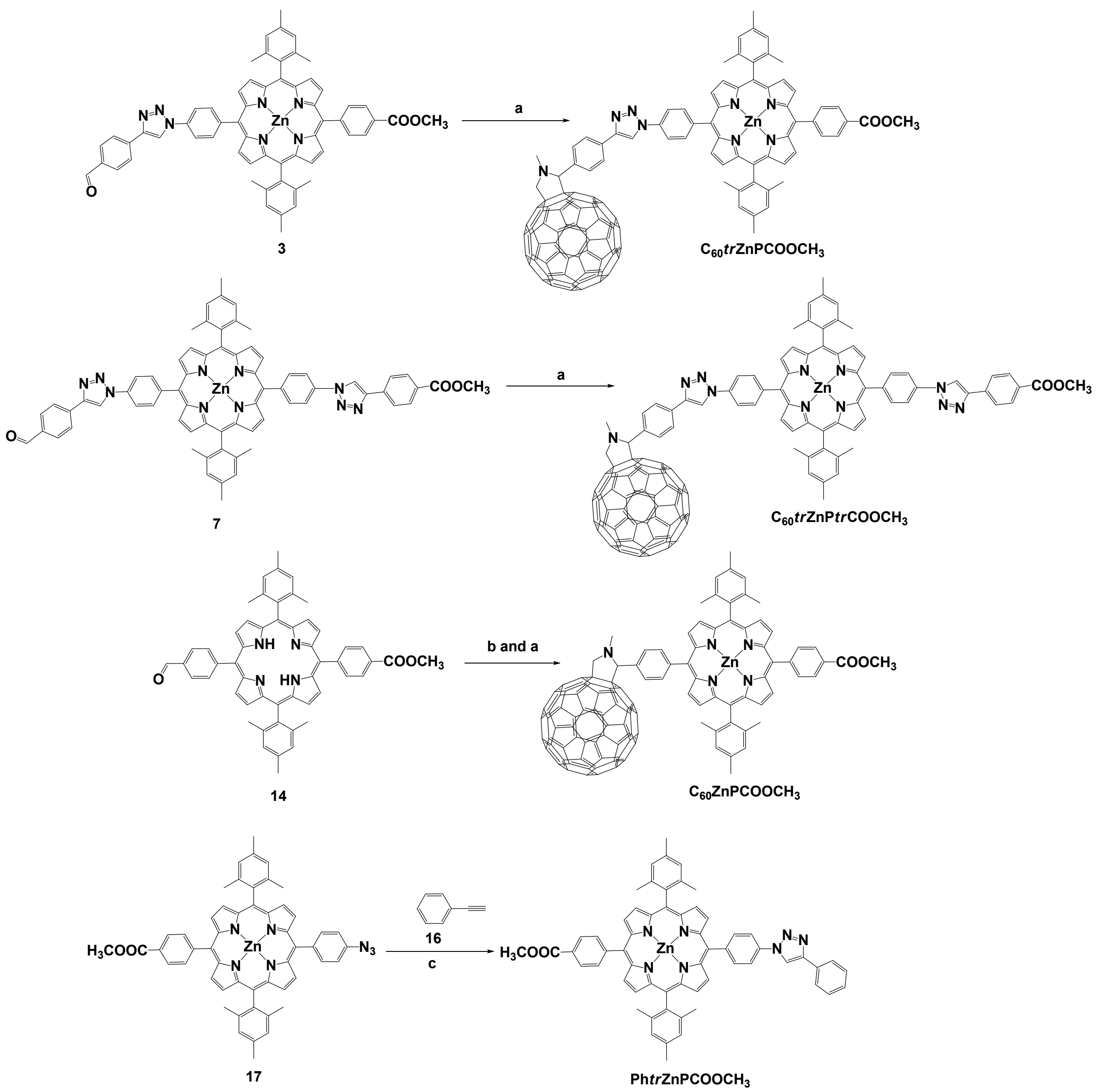
^{13}C NMR (125 MHz, THF-*d_8*): δ = 167.89, 158.00, 155.04, 150.65, 150.33, 148.94, 148.17, 147.77, 147.66, 147.07, 146.93, 146.78, 146.71, 146.48, 146.34, 146.24, 146.14, 145.67, 145.60, 145.30, 144.73, 144.04, 143.83, 143.42, 143.30, 143.01, 142.87, 142.56, 140.96, 140.85, 140.57, 140.24, 139.82, 138.09, 137.92, 137.49, 137.04, 135.94, 135.24, 132.64, 132.40, 131.00, 130.85, 130.78, 128.49, 128.44, 120.50, 119.68, 119.51, 84.17, 78.90, 70.83, 70.44, 40.17, 21.96, 21.56 ppm.

HRMS (MALDI-TOF): calc. for $C_{114}H_{46}N_5O_2Zn$ [M + H]$^+$: 1579.2865; found 1866.2870.

Ph*tr*ZnPCOOH. Equimolar amounts of porphyrin **15** (30 mg, 0.035 mmol) and derivative **16** (3.6 mg, 0.035 mmol) were dissolved in a 1:1 mixture of THF/CH_3CN (4 mL) under N_2 atmosphere. Afterwards, CuI (6.7 mg, 0.035 mmol) and DIPEA (7 µL, 0.04 mmol) were added and the reaction mixture was stirred at room temperature for 12 hours. Then, the volatiles were removed under reduced pressure and the crude solid, was purified by column chromatography (silica gel, CH_2Cl_2/EtOH, 98:2) yielding 29 mg of **Ph*tr*ZnPCOOH** (0.031 mmol, yield: 89%).

^{1}H NMR (500 MHz, DMSO-*d*$_6$): δ = 13.19 (s, 1H), 9.65 (s, 1H), 8.82 (m, 2H), 8.73 (m, 2H), 8.60 (m, 2H), 8.41 (m, 8H), 8.08 (d, J = 7.4 Hz, 2H), 7.57 (m, 2H), 7.44 (m, 1H), 7.31 (s, 4H), 2.57 (s, 6H), 2.46 (s, 6H), 1.79 (s, 12H) ppm.

HRMS (MALDI-TOF): calc. for $C_{59}H_{45}N_7O_2Zn$ [M]$^+$: 947.2926; found 947.2932.



Scheme S1. Synthesis of the methyl ester derivatives (**C_{60}*tr*ZnPCOOCH$_3$**, **C_{60}*tr*ZnP*tr*COOCH$_3$**, **C_{60}ZnPCOOCH$_3$** and **Ph*tr*ZnPCOOCH$_3$**). Reagents and conditions: a) Toluene, C_{60}, sarcosine, reflux overnight; b) $Zn(CH_3COO)_2.2H_2O$, MeOH, CH_2Cl_2; c) CuI, DIPEA, THF/CH_3CN, RT, 12 h.

C_{60}*tr*ZnPCOOCH$_3$. In a round bottom flask we added porphyrin **3** (25 mg, 0.025 mmol), 2-methyl glycine (sarcosine, 44 mg, 0.50 mmol) and C_{60} (24 mg, 0.033 mmol) in dry toluene (25 mL). The reaction mixture was refluxed overnight and afterwards we performed the purification of the crude **C_{60}*tr*ZnPCOOCH$_3$** compound through silica gel column chromatography. The first column was performed with toluene as eluent to remove the excess of unreacted C_{60} and the second one with CH_2Cl_2/MeOH in a 99:1 ratio providing **C_{60}*tr*ZnPCOOCH$_3$** in a 79% yield (34 mg, 0.0020 mmol).

^{1}H NMR (500 MHz, CDCl$_3$): δ = 8.90 (d, *J* = 4.5 Hz, 2H), 8.83 (m, 6H), 8.55 (s, 1H), 8.41 (d, *J* = 8 Hz, 2H), 8.36 (d, *J* = 8 Hz, 2H), 8.32 (d, *J* = 8 Hz, 2H), 8.16 (d, *J* = 8 Hz, 2H), 7.89 (sb, 2H), 7.29 (s, 4H), 4.87 (s, 1H), 4.84 (d, *J* = 9 Hz, 1H), 4.14 (d, *J* = 9 Hz, 1H), 4.08 (s, 3H), 2.82 (s, 3H), 2.64 (s, 6H), 1.85 (s, 12H) ppm.

HRMS (MALDI-TOF): calc. for $C_{123}H_{53}N_8O_2Zn$ [M + H]$^+$: 1737.3505; found 1737.3511.

C_{60}*tr*ZnP*tr*COOCH$_3$. First, we added porphyrin **7** (30 mg, 0.026 mmol), sarcosine (47 mg, 0.53 mmol) and C_{60} (24 mg, 0.034 mmol) in a round bottom flask. Then we dissolved all compounds in dry toluene (30 mL). The reaction mixture was refluxed overnight. Upon reaction completion, the purification of the crude **C_{60}*tr*ZnP*tr*COOCH$_3$** was accomplished, using silica gel column chromatography. The first column was performed with toluene as eluent to remove the excess of unreacted C_{60} and the second one with CH_2Cl_2/MeOH in a 99:1 ratio providing **C_{60}*tr*ZnP*tr*COOCH$_3$** in a 75% yield (36 mg, 0.0019 mmol).

^{1}H NMR (300 MHz, CDCl$_3$): δ = 8.85 (m, 8H), 8.55 (m, 2H), 8.39 (m, 4H), 8.10 (m, 10H), 7.86 (m, 2H), 7.27 (s, 4H), 4.82 (m, 2H), 4.12 (d, *J* = 8.7 Hz, 1H), 3.93 (s, 3H), 2.79 (s, 3H), 2.61 (s, 6H), 1.83 (s, 12H) ppm.

HRMS (MALDI-TOF): calc. for $C_{131}H_{58}N_{11}O_2Zn$ [M + H]$^+$: 1880.3988; found 1880.3981.

C_{60}ZnPCOOCH$_3$. To a CH_2Cl_2 solution (25 mL) of **14** (30 mg, 0.038 mmol), a MeOH (2 mL) solution containing $Zn(CH_3COO)_2.2H_2O$ (110 mg, 0.5 mmol) was added and the reaction mixture was stirred at room temperature overnight. The volatiles were evaporated, the porphyrin was diluted in 15 mL of $CHCl_3$ and extracted with H_2O (3 x 10 mL). The solvent was removed under reduced pressure and the produced porphyrin was subsequently used in a Prato reaction. In detail, in a round bottom flask we added the crude porphyrin, 2-methyl glycine (sarcosine, 67 mg, 0.76 mmol) and C_{60} (36 mg, 0.050 mmol) and dissolved them in dry toluene (30 mL). The reaction mixture was refluxed overnight. The purification of **C_{60}ZnPCOOCH$_3$** was accomplished through silica gel column chromatography. The first column was performed with toluene to remove the excess of unreacted C_{60} and the second one with CH_2Cl_2/MeOH in a 99:1 ratio providing **C_{60}ZnPCOOCH$_3$** in a 73% yield (44 mg, 0.028 mmol).

^{1}H NMR (500 MHz, CDCl$_3$): δ = 8.77 (m, 8H), 8.31 (m, 6H), 7.71 (m, 2H), 7.24 (s, 4H), 5.30 (s, 1H), 4.93 (m, 1H), 4.25 (m, 1H), 3.87 (s, 3H), 3.07 (s, 3H), 2.59 (s, 6H), 1.80 (m, 12H) ppm.

HRMS (MALDI-TOF): calc. for $C_{115}H_{48}N_5O_2Zn$ [M + H]$^+$: 1594.3021; found 1594.3015.

Ph*tr*ZnPCOOCH$_3$. Equimolar amounts of porphyrin **17** (50 mg, 0.058 mmol) and phenylacetylene (6 mg, 0.058 mmol) were dissolved in a 1:1 mixture of THF/CH_3CN (10 mL) under N_2 atmosphere. Then, we added the copper catalyst (CuI, 11 mg, 0.58 mmol) and DIPEA (10 µL, 0.62 mmol). The reaction mixture was stirred at room temperature for 12 h. Next, the solvents were removed under reduced pressure and the crude solid was consequently purified by column chromatography (silica gel, CH_2Cl_2) yielding 45 mg of **Ph*tr*ZnPCOOCH$_3$** (0.047 mmol, yield: 81%).

^{1}H NMR (300 MHz, CDCl$_3$): δ = 8.78 (m, 8H), 8.52 (s, 1H), 8.42 (m, 4H), 8.32 (m, 2H), 8.21 (d, *J* = 8.2 Hz, 2H), 8.05 (d, *J* = 7.2 Hz, 2H), 7.55 (m, 2H), 7.45 (m, 1H), 7.29 (s, 4H), 4.12 (s, 3H), 2.64 (s, 6H), 1.86 (s, 12H) ppm.

HRMS (MALDI-TOF): calc. for $C_{60}H_{47}N_7O_2Zn$ [M]$^+$: 961.3083; found 961.3090.

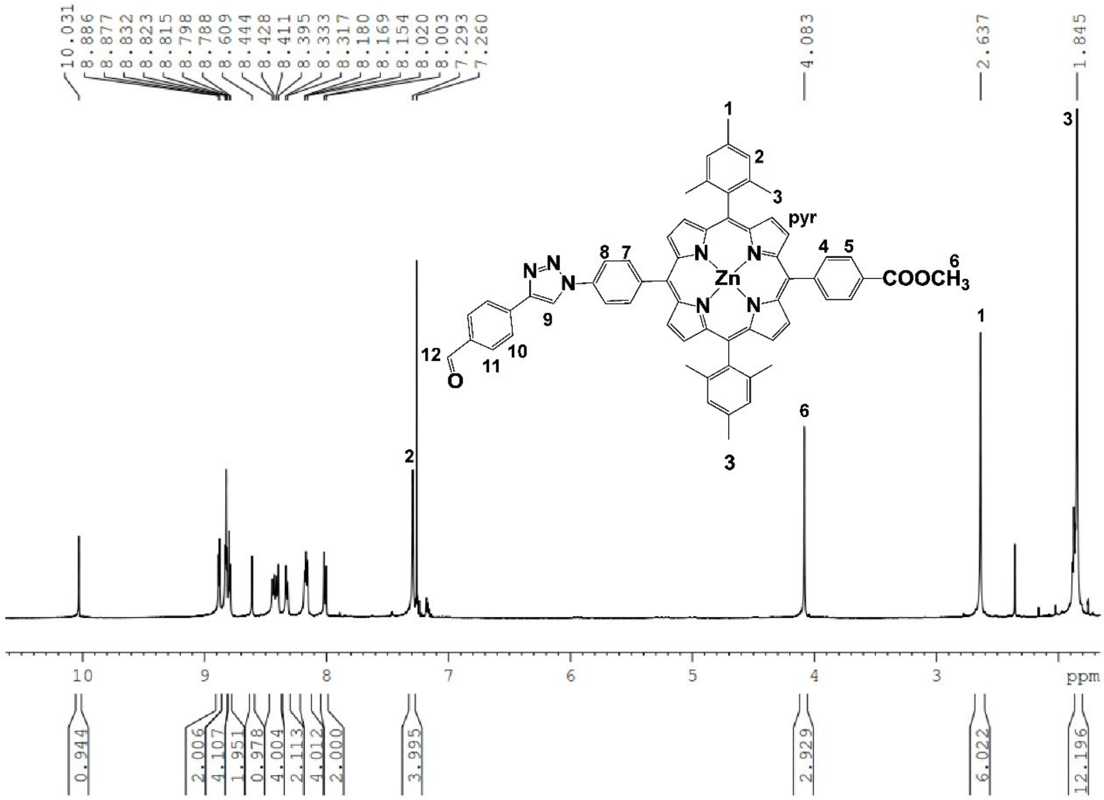


Figure S1. ^{1}H NMR spectrum of **3** (500MHz, $CDCl_3$).

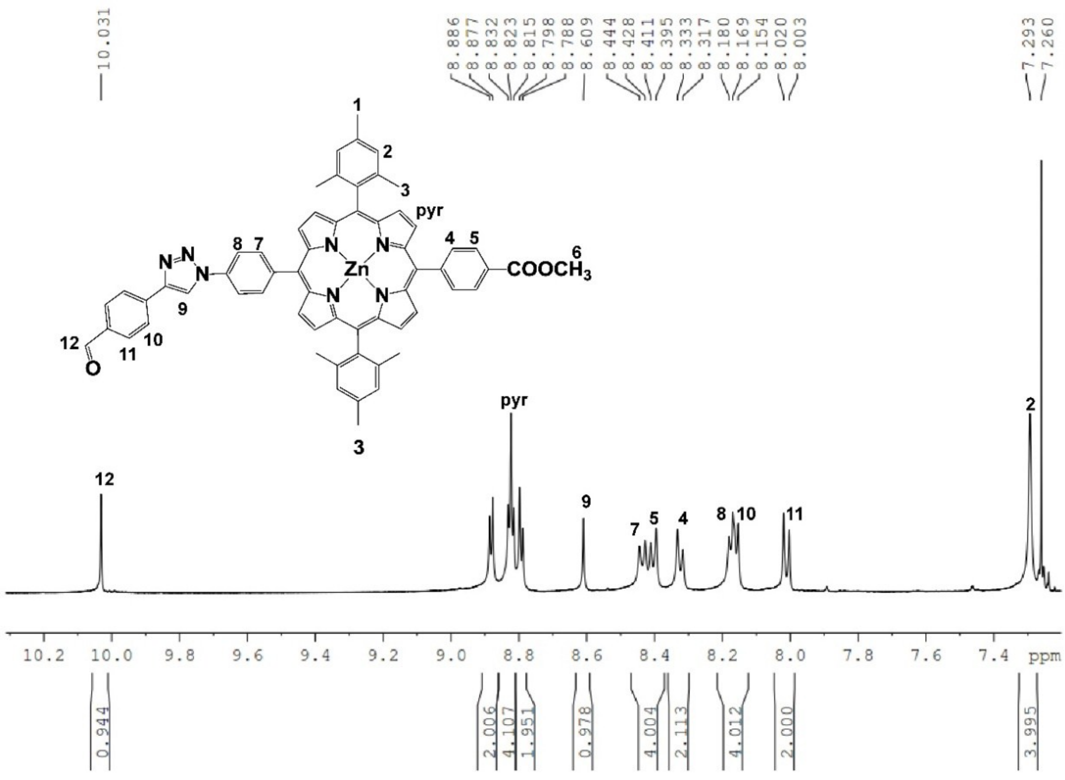


Figure S2. Aromatic region of ^{1}H NMR of **3** (500MHz, $CDCl_3$).

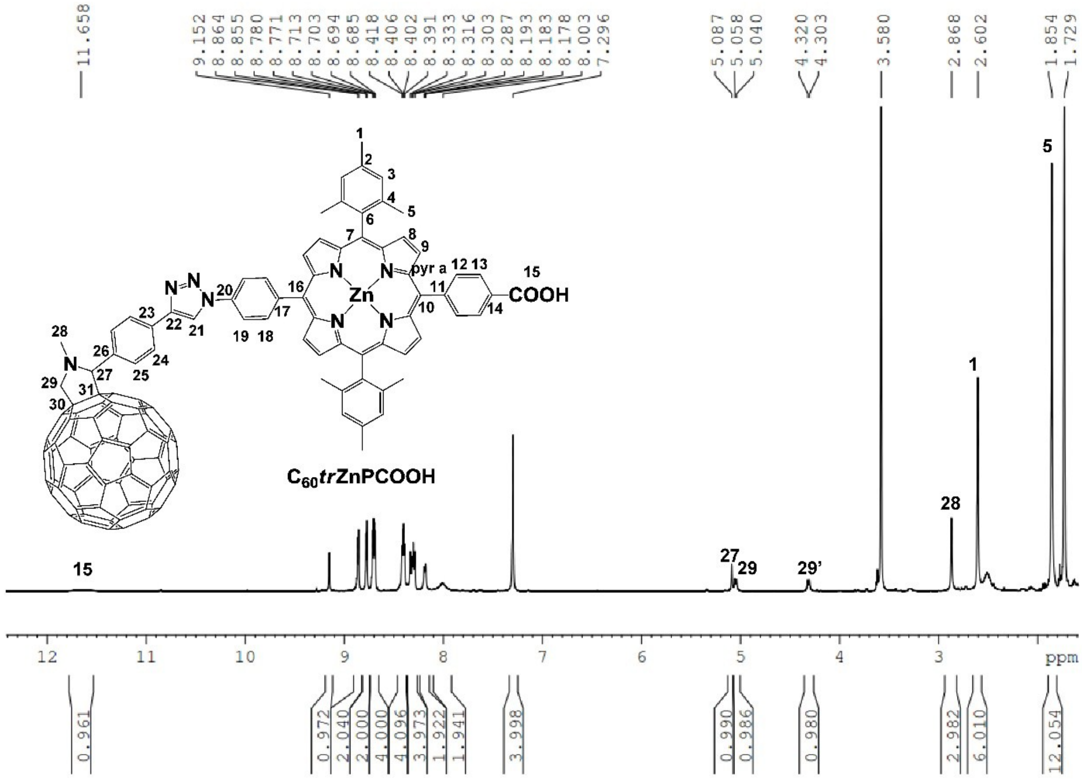


Figure S3. ^{1}H NMR spectrum of **C_{60}*tr*ZnPCOOH** (500MHz, THF-d_8).

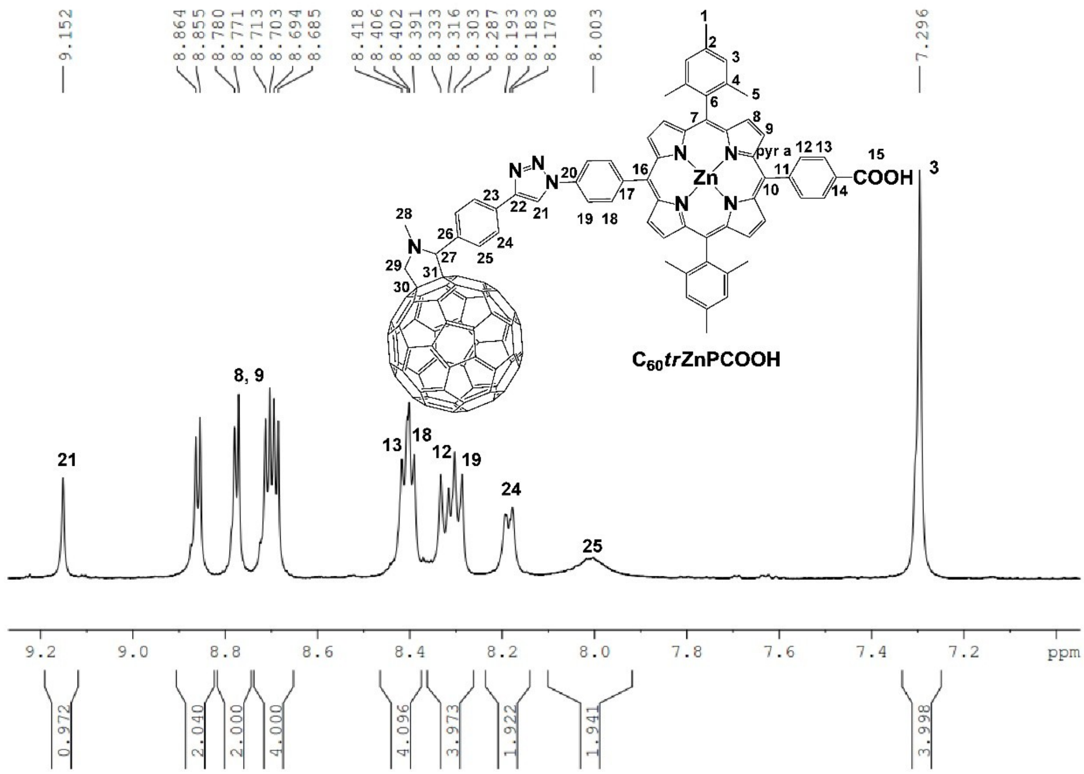


Figure S4. Aromatic region of ^{1}H NMR of **C_{60}*tr*ZnPCOOH** (500MHz, THF-d_8).

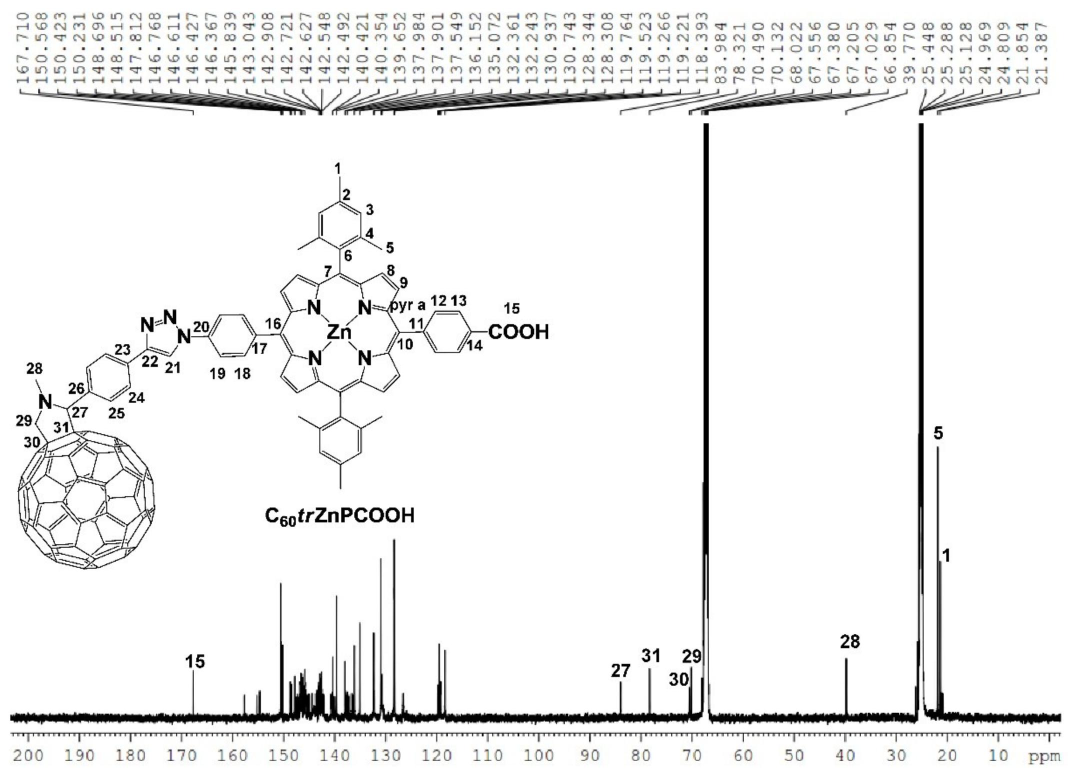


Figure S5. Full ^{13}C NMR spectrum of **C_{60}*tr*ZnPCOOH** (75MHz, THF-d_8).

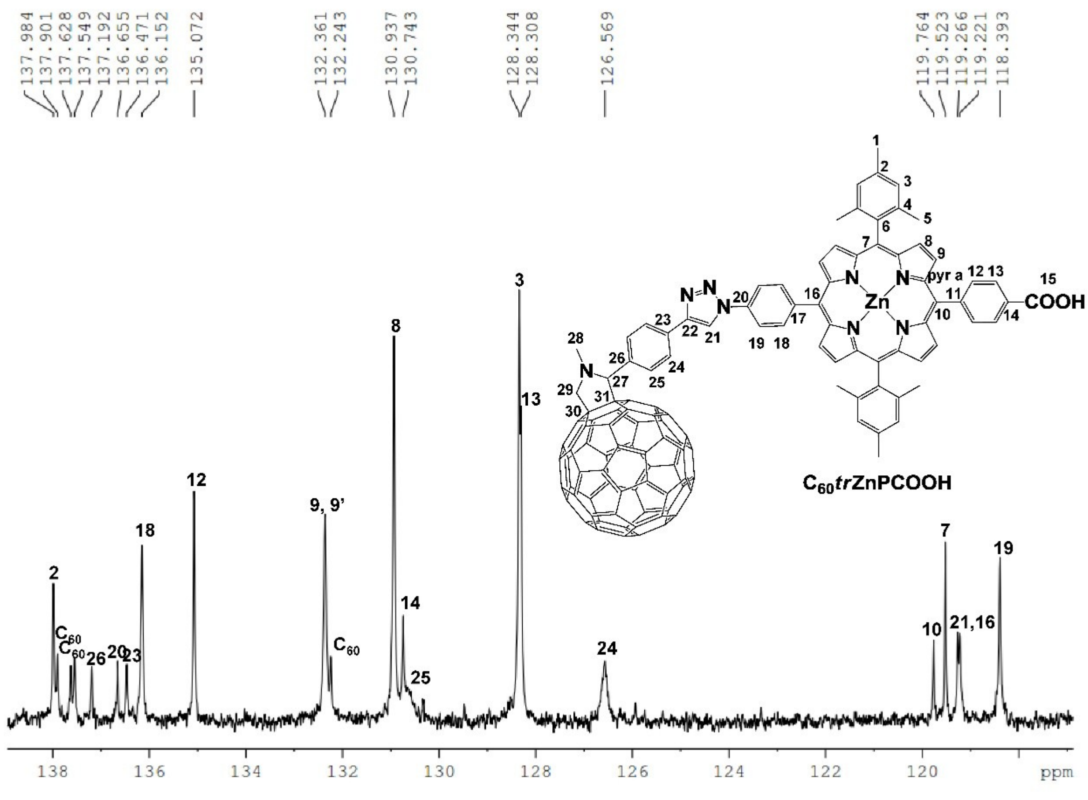


Figure S6. Zoom on the ^{13}C NMR spectrum of **C_{60}*tr*ZnPCOOH** (75MHz, THF-d_8).

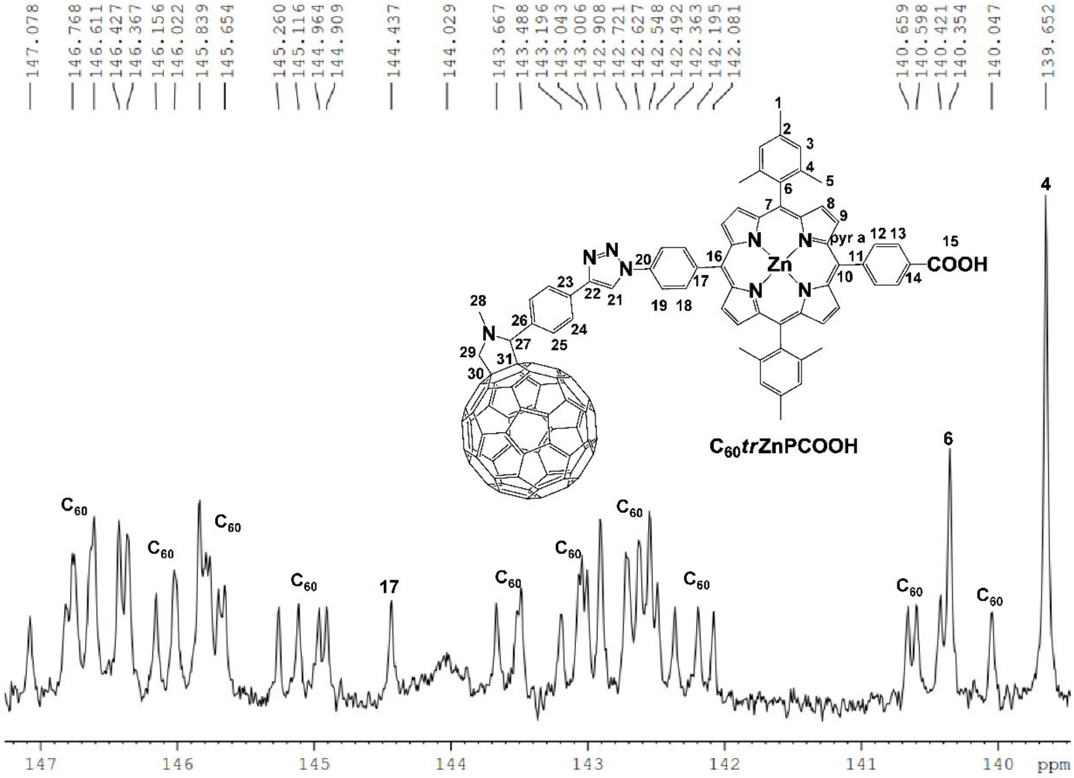


Figure S7. Zoom on the ^{13}C NMR spectrum of **C_{60}*tr*ZnPCOOH** (75MHz, THF-d_8).

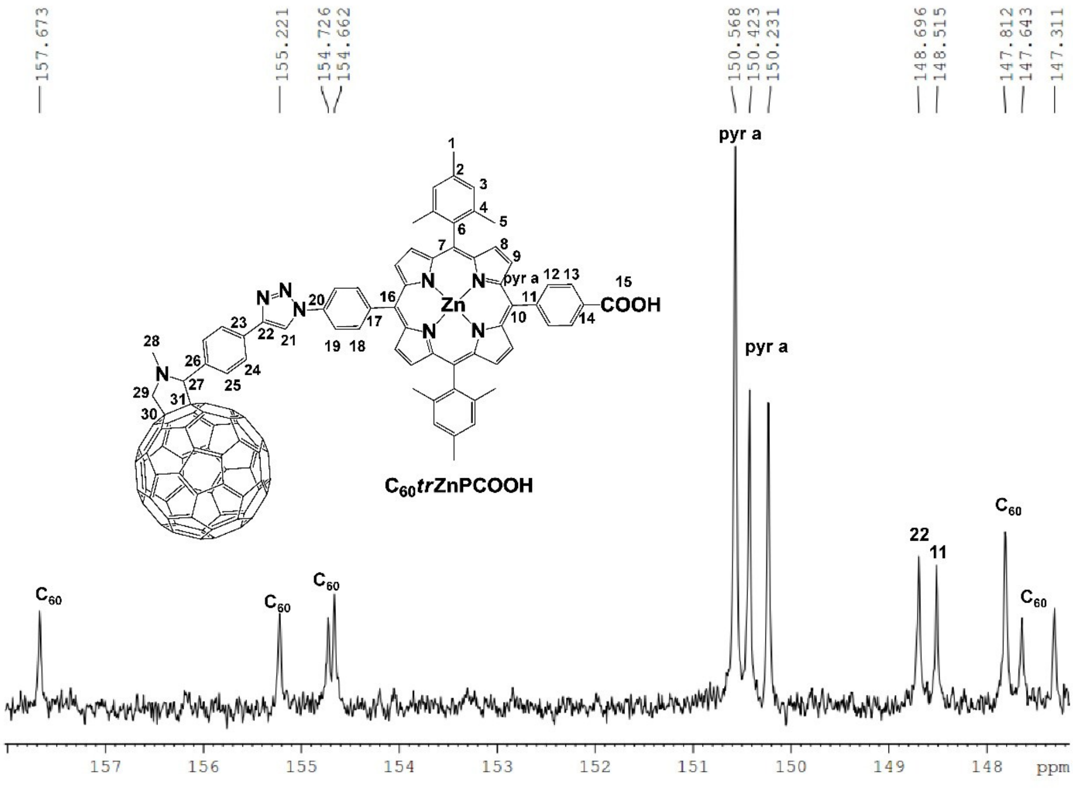


Figure S8. Zoom on the ^{13}C NMR spectrum of **C_{60}*tr*ZnPCOOH** (75MHz, THF-d_8).

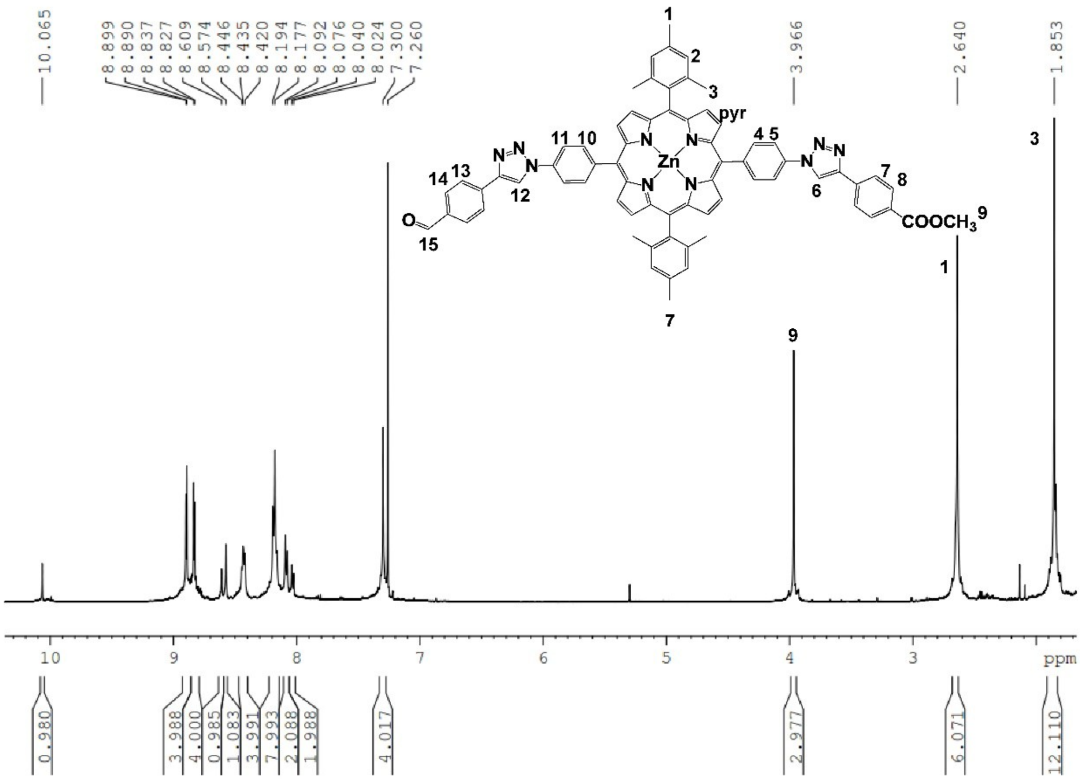


Figure S9. ^{1}H NMR spectrum of **7** (500MHz, $CDCl_3$).

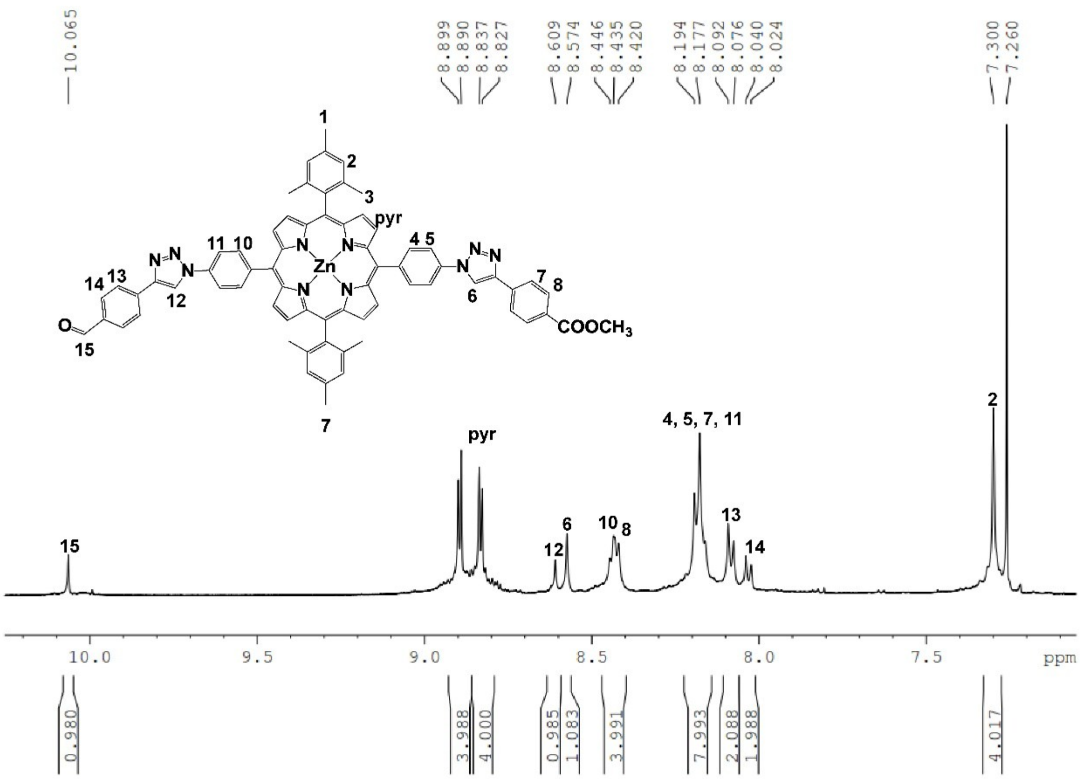


Figure S10. Aromatic region of ^{1}H NMR of **7** (500MHz, $CDCl_3$).

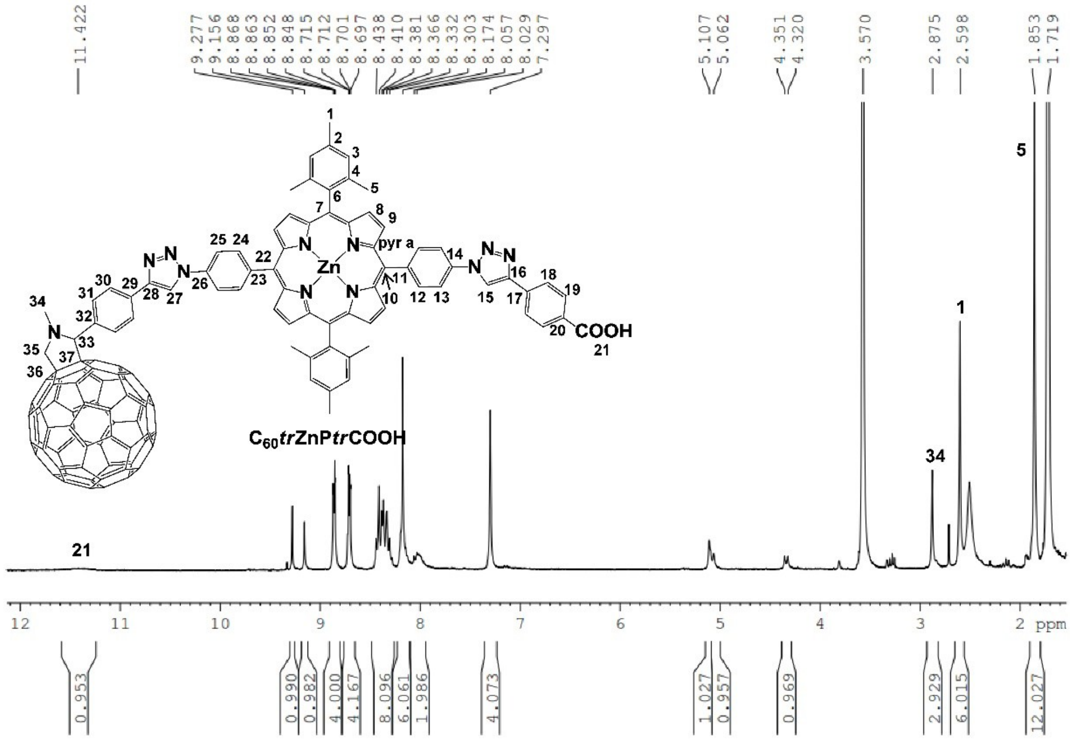


Figure S11. ^{1}H NMR spectrum of **C$_{60}$*tr*ZnP*tr*COOH** (500MHz, THF-d_8).

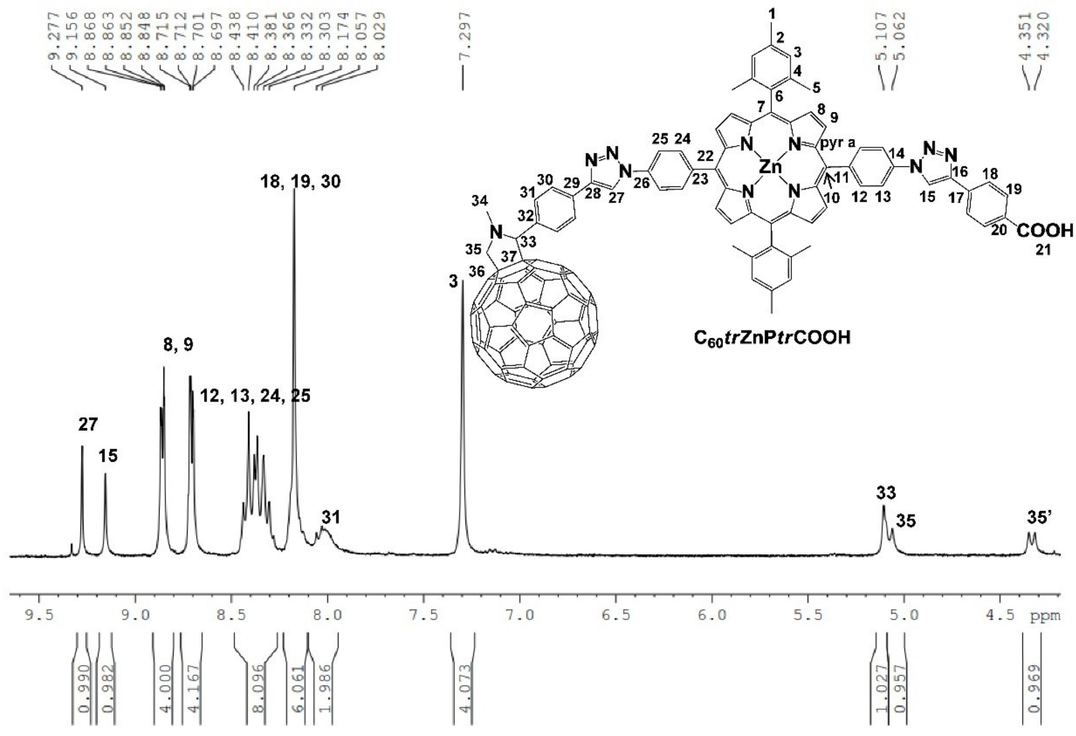


Figure S12. ^{1}H NMR spectrum of **C$_{60}$*tr*ZnP*tr*COOH** (500MHz, THF-d_8).

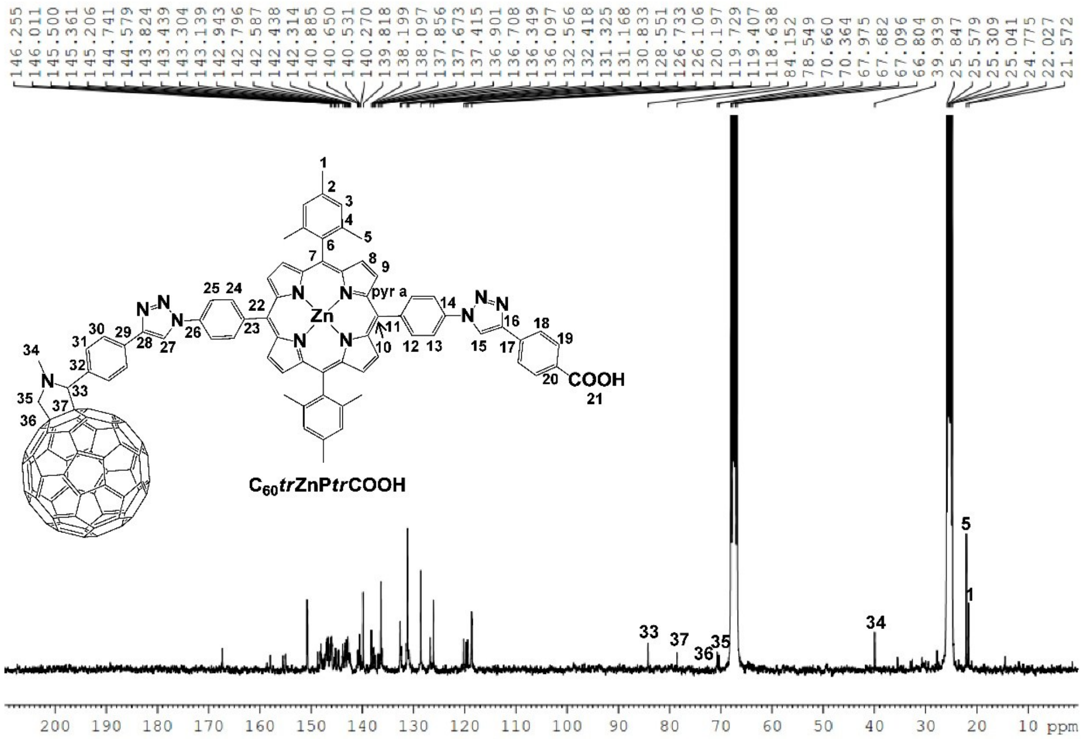


Figure S13. Full ^{13}C NMR spectrum of **C$_{60}$*tr*ZnP*tr*COOH** (500MHz, THF-d_8).

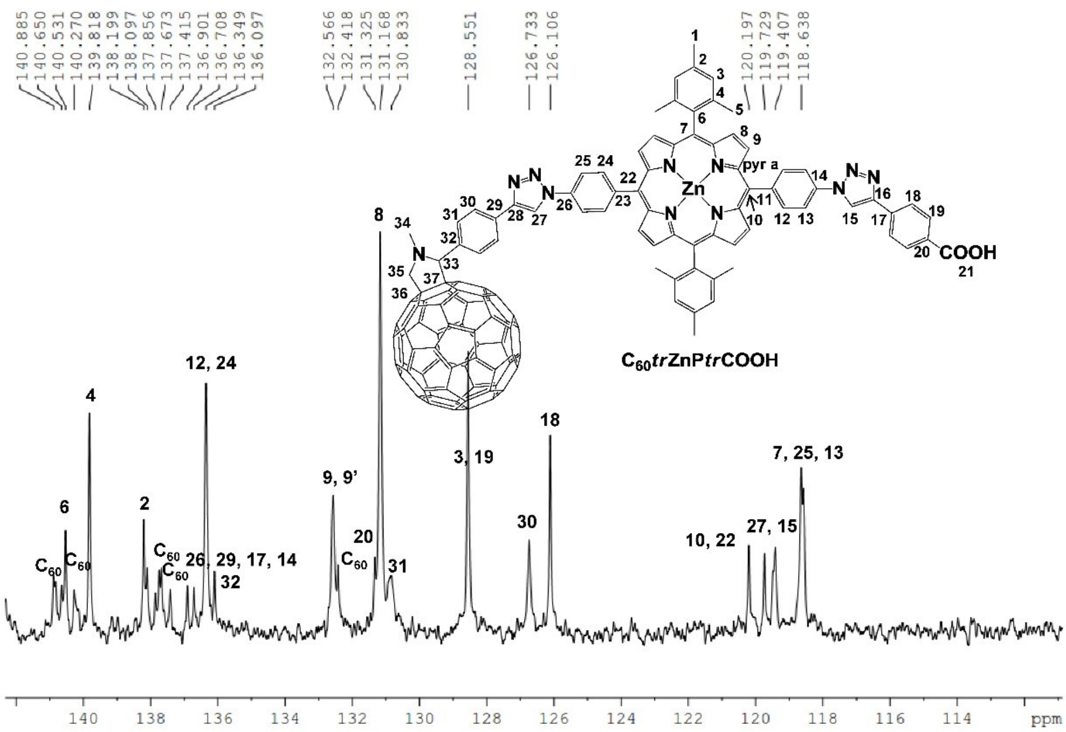


Figure S14. Zoom on the ^{13}C NMR spectrum of **C$_{60}$*tr*ZnP*tr*COOH** (75MHz, THF-d_8).

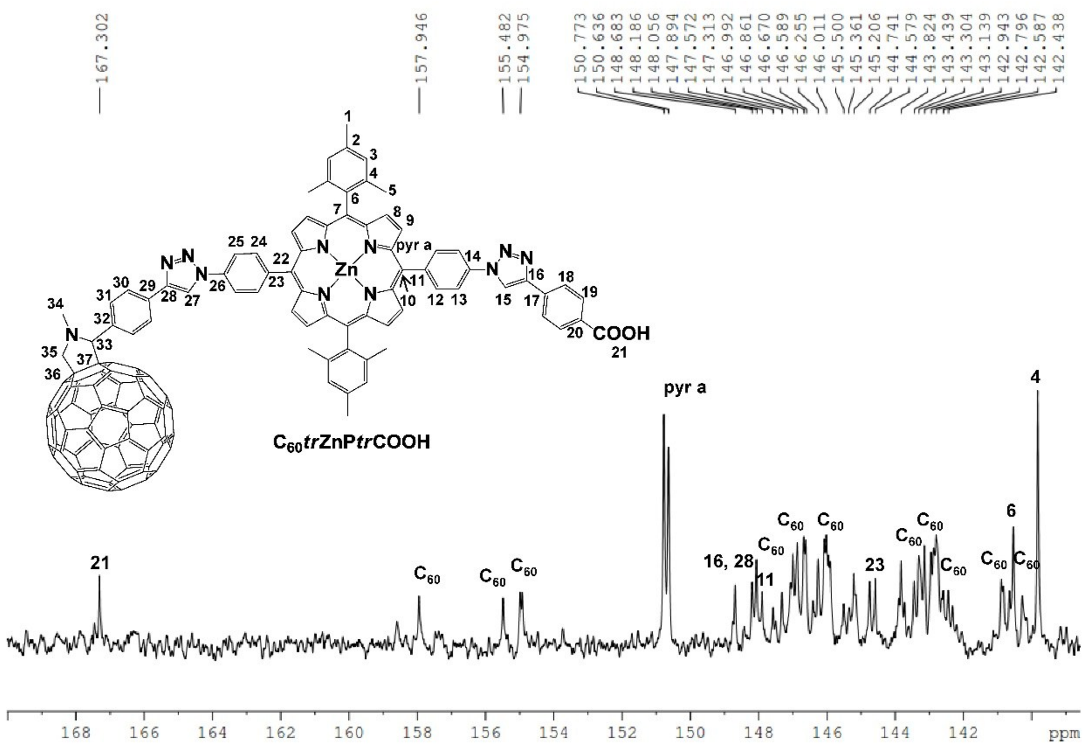


Figure S15. Zoom on the ^{13}C NMR spectrum of **C_{60}*tr*ZnP*tr*COOH** (75MHz, THF-d_8).

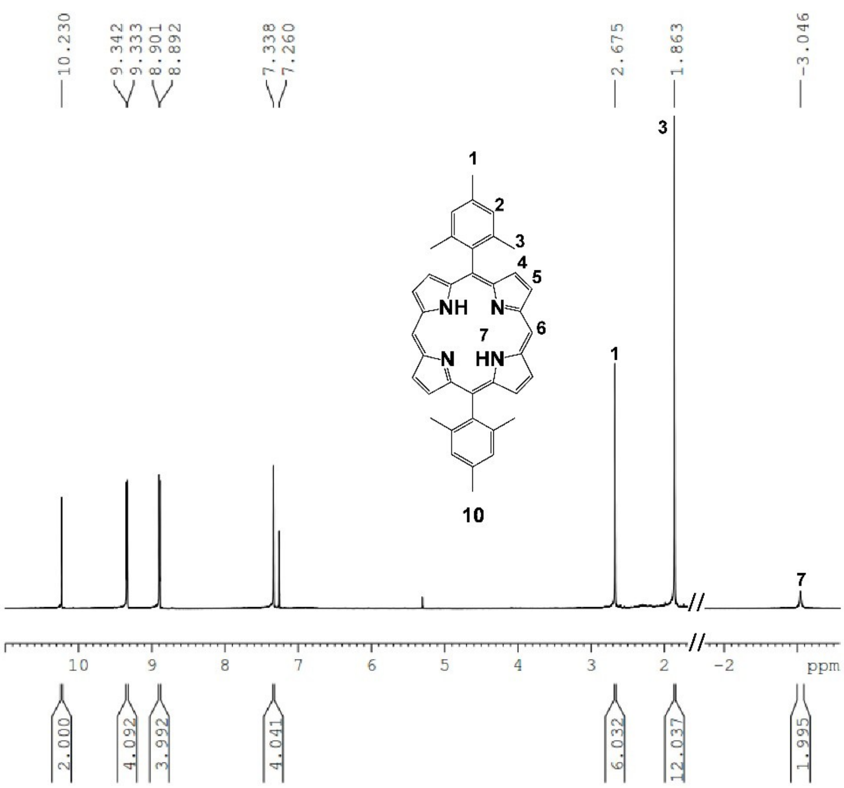


Figure S16. ^1H NMR spectrum of **10** (500MHz, $CDCl_3$).

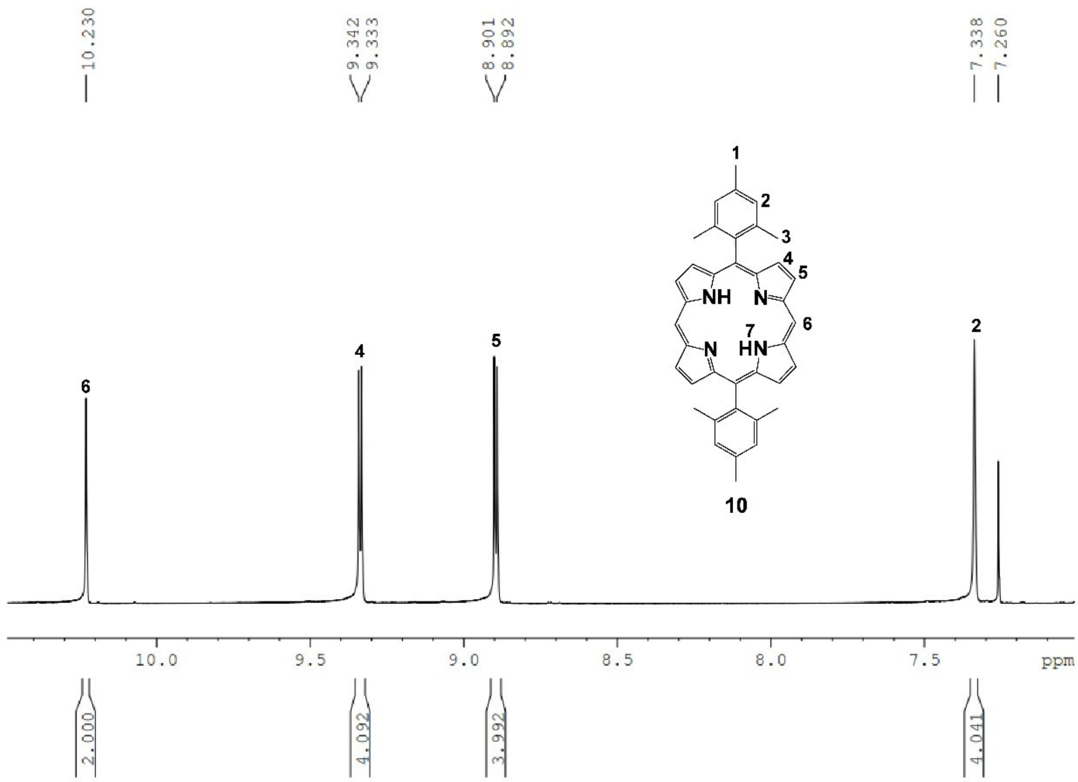


Figure S17. Aromatic region of ^{1}H NMR of **10** (500MHz, $CDCl_3$).

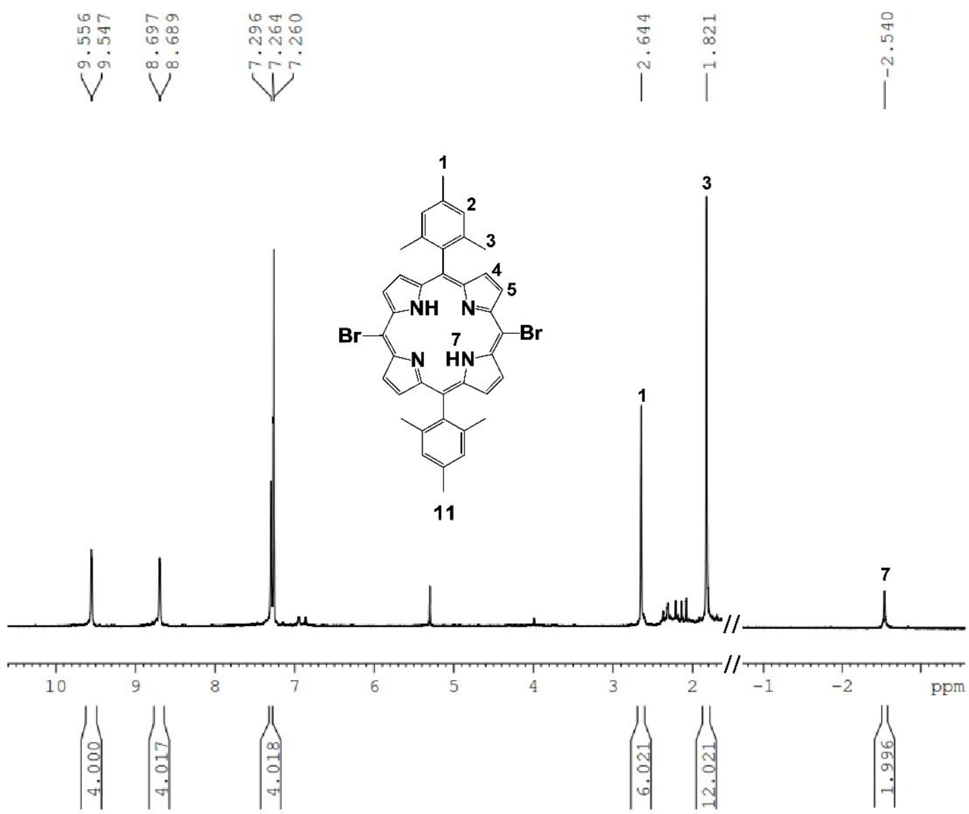


Figure S18. ^{1}H NMR spectrum of **11** (500MHz, $CDCl_3$).

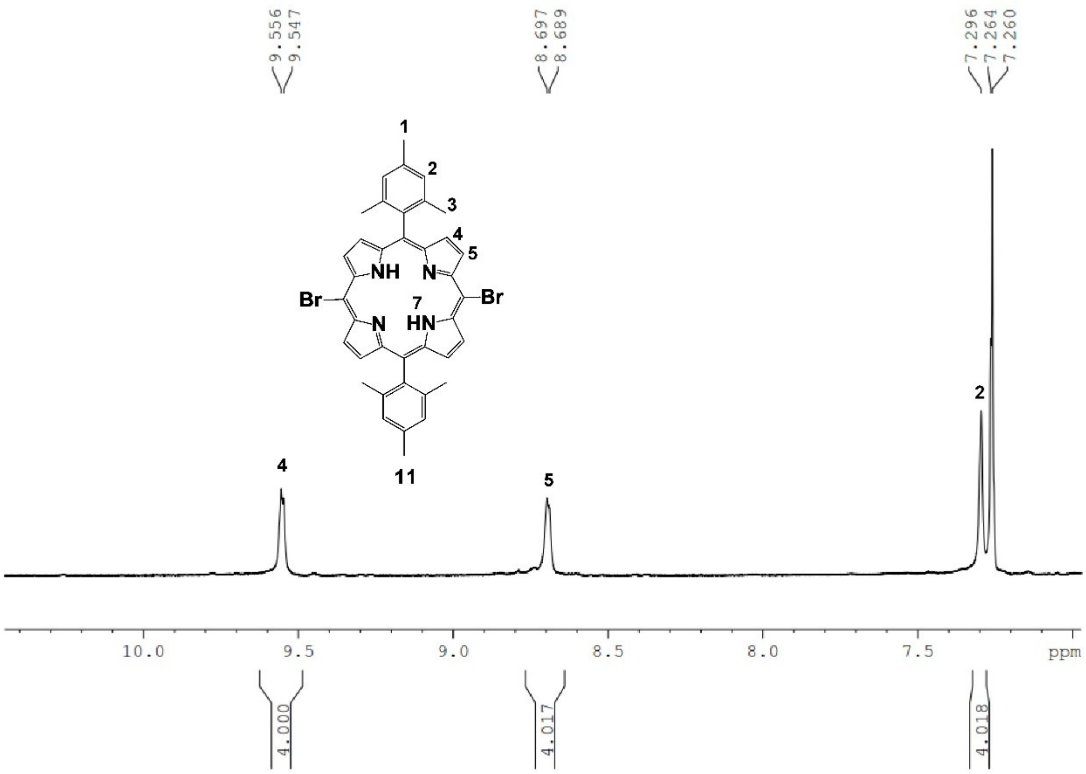


Figure S19. Aromatic region of ^{1}H NMR of **11** (500MHz, $CDCl_3$).

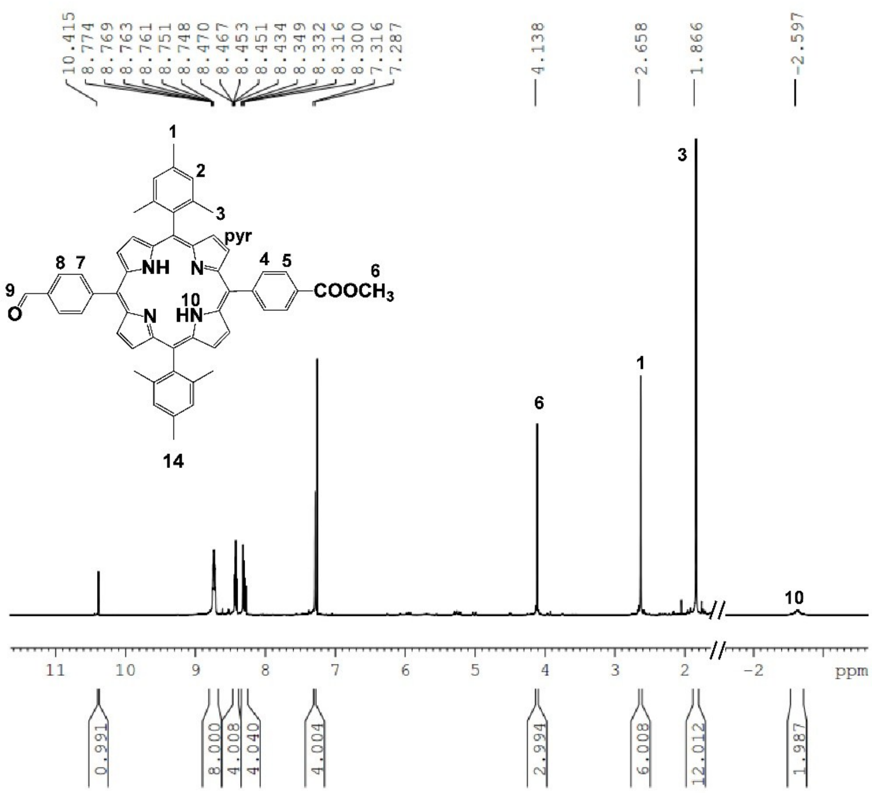


Figure S20. ^{1}H NMR spectrum of **14** (500MHz, $CDCl_3$).

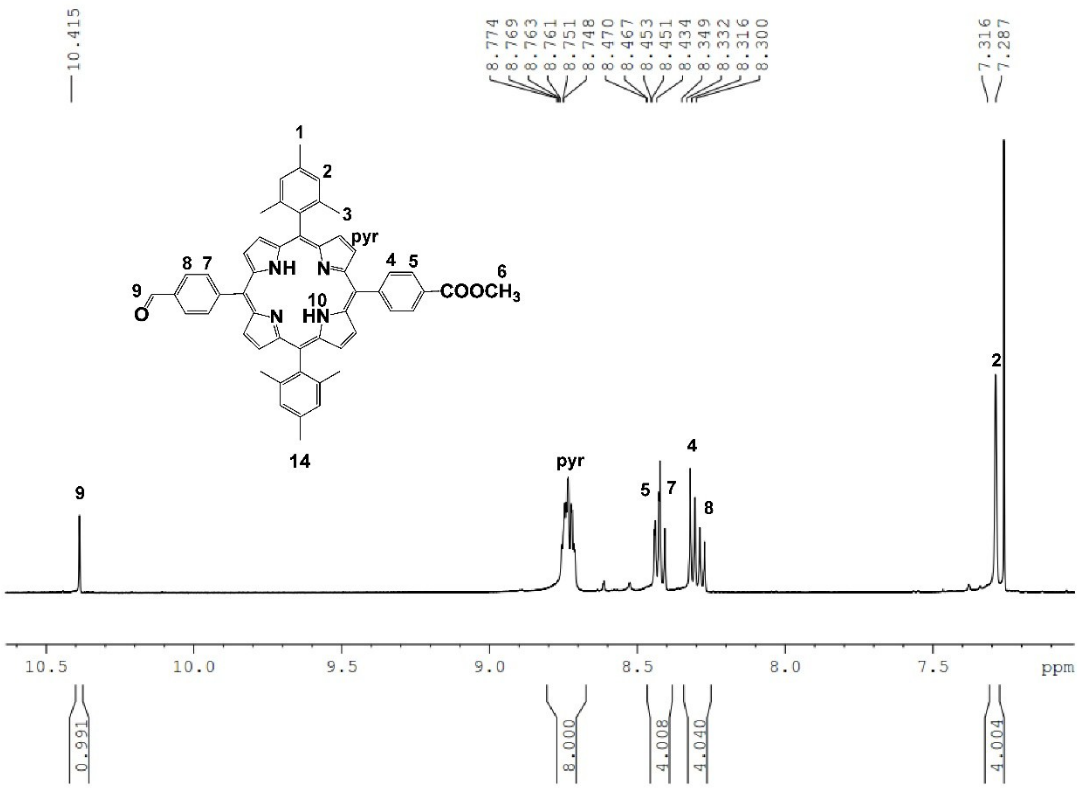


Figure S21. Aromatic region of ^{1}H NMR of **14** (500MHz, $CDCl_3$).

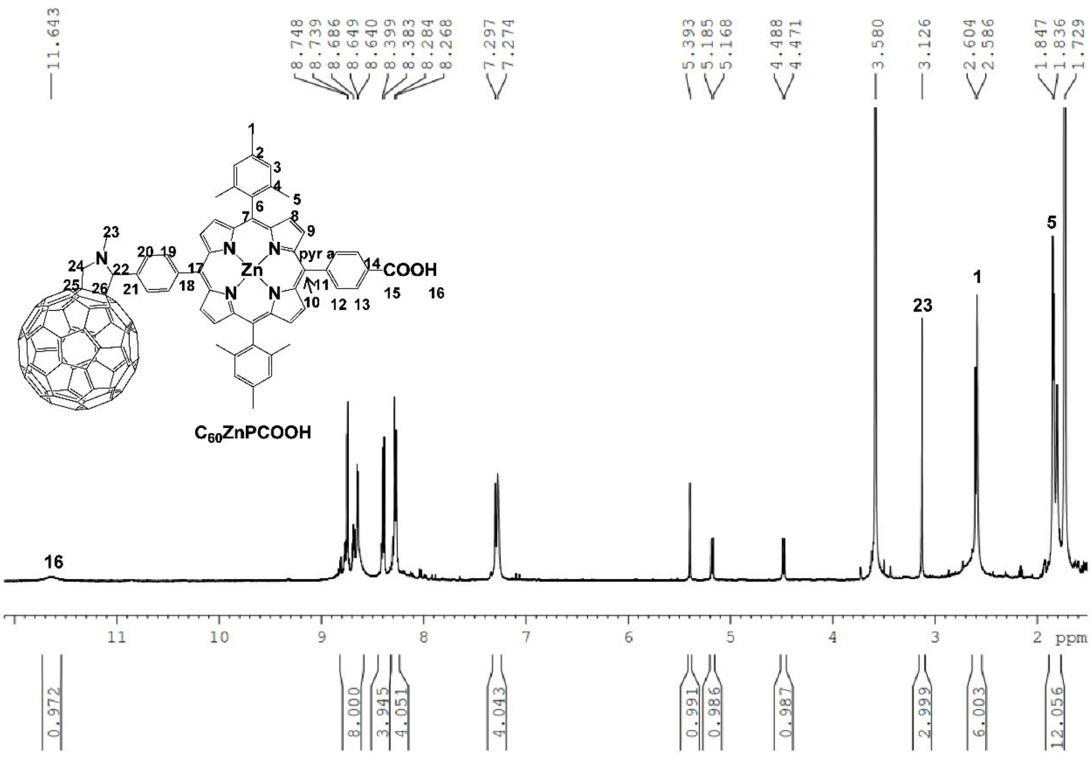


Figure S22. ^{1}H NMR of of $\mathbf{C_{60}ZnPCOOH}$ (500MHz, THF-d_8).

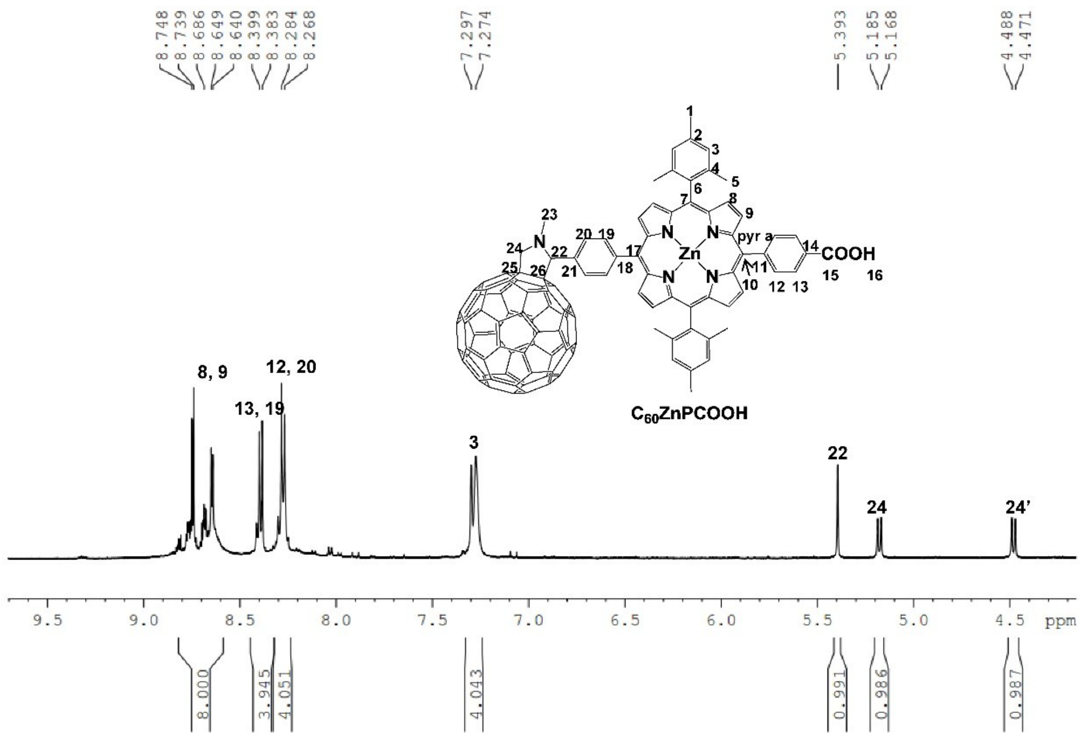


Figure S23. Zoom of ^{1}H NMR of **C_{60}ZnPCOOH** (500MHz, THF-d_8).

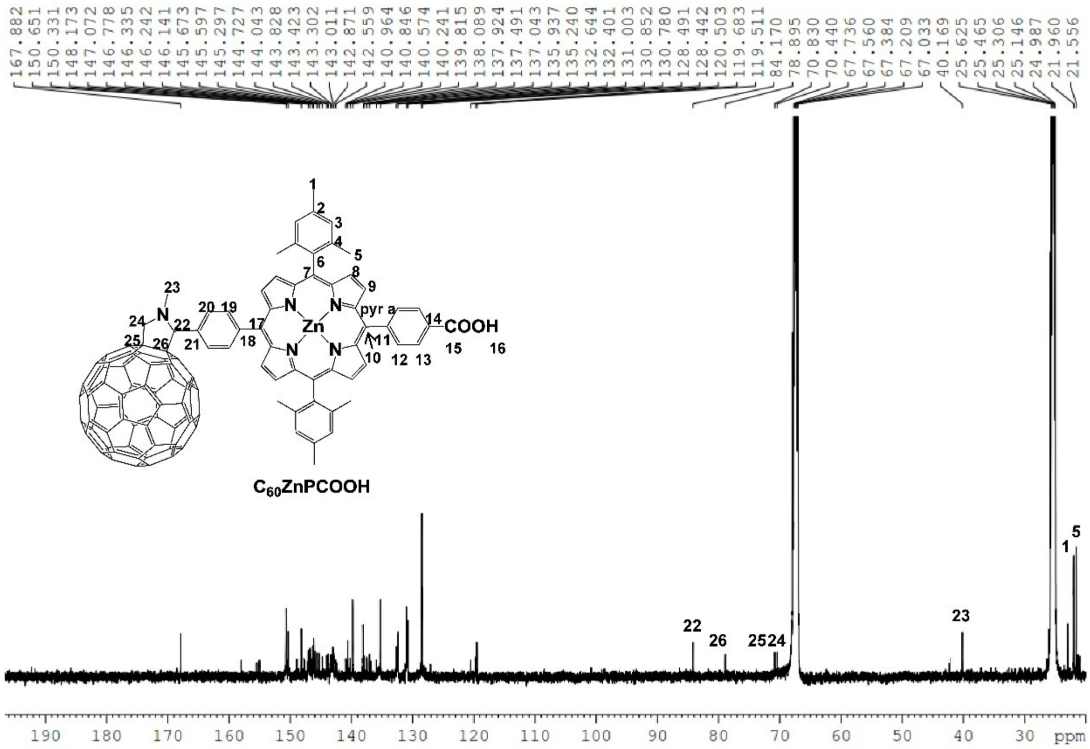


Figure S24. ^{13}C NMR spectrum of **C_{60}ZnPCOOH** (75MHz, THF-d_8).

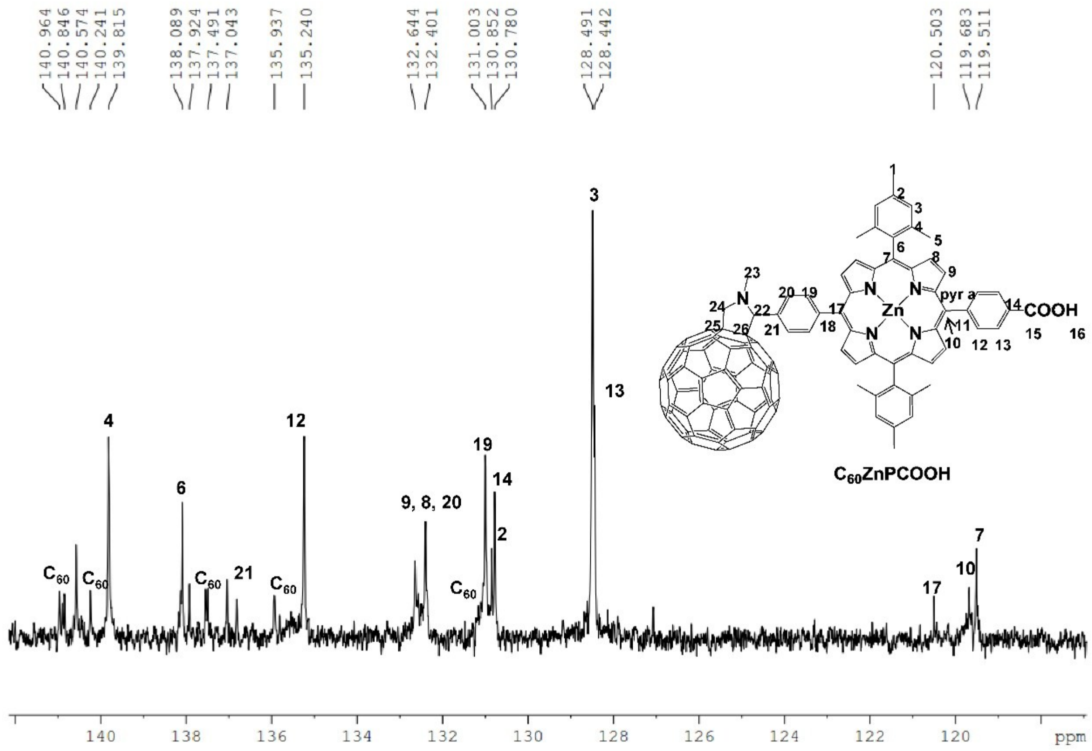


Figure S25. Zoom on the ^{13}C NMR spectrum of **C_{60}ZnPCOOH** (75MHz, THF-d_8).

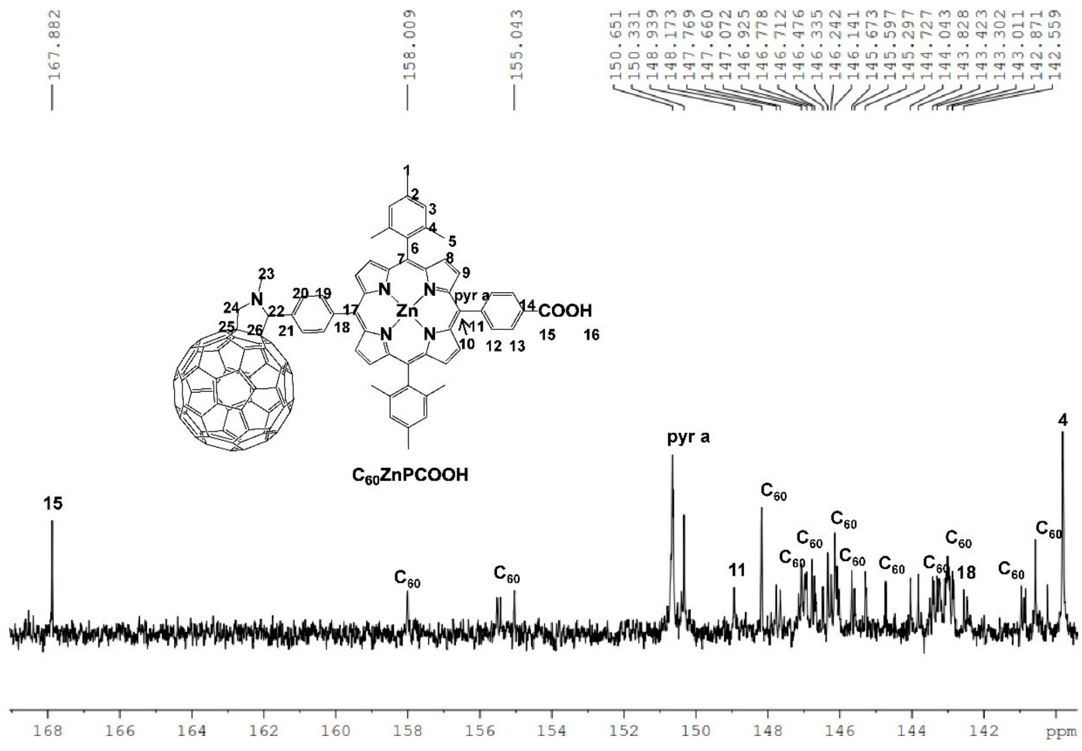


Figure S26. Zoom on the ^{13}C NMR spectrum of **C_{60}ZnPCOOH** (75MHz, THF-d_8).

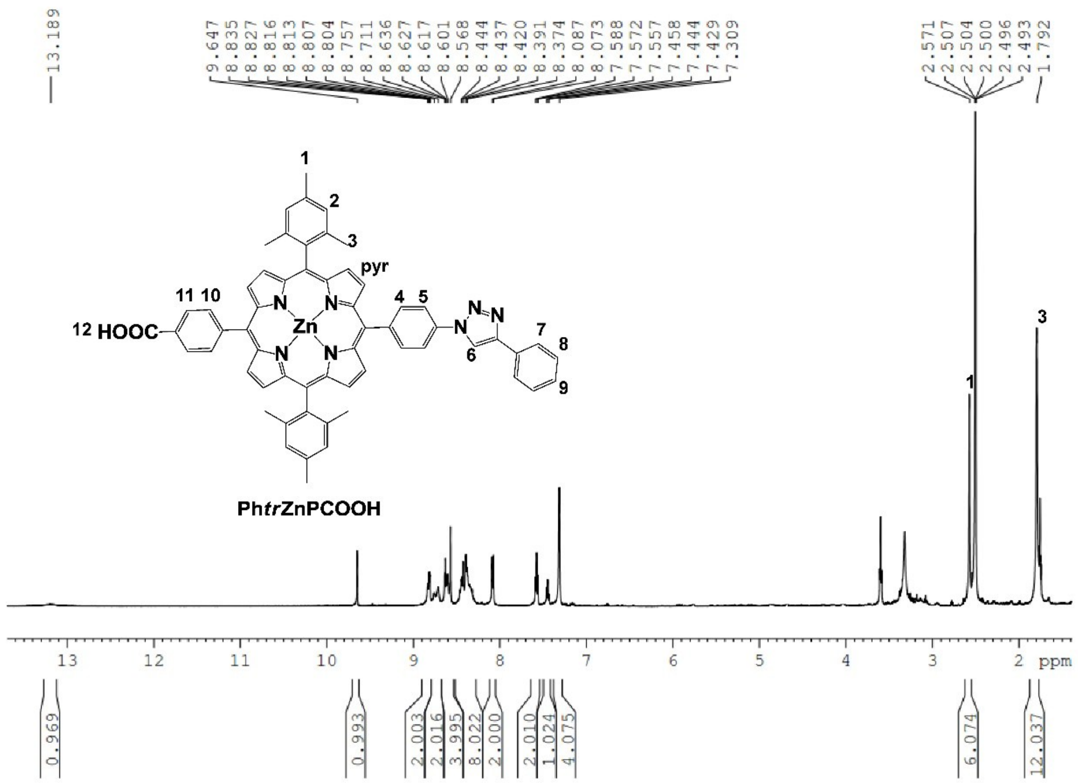


Figure S27. [1]H NMR spectrum of **Ph*tr*ZnPCOOH** (500MHz, DMSO-d_6).

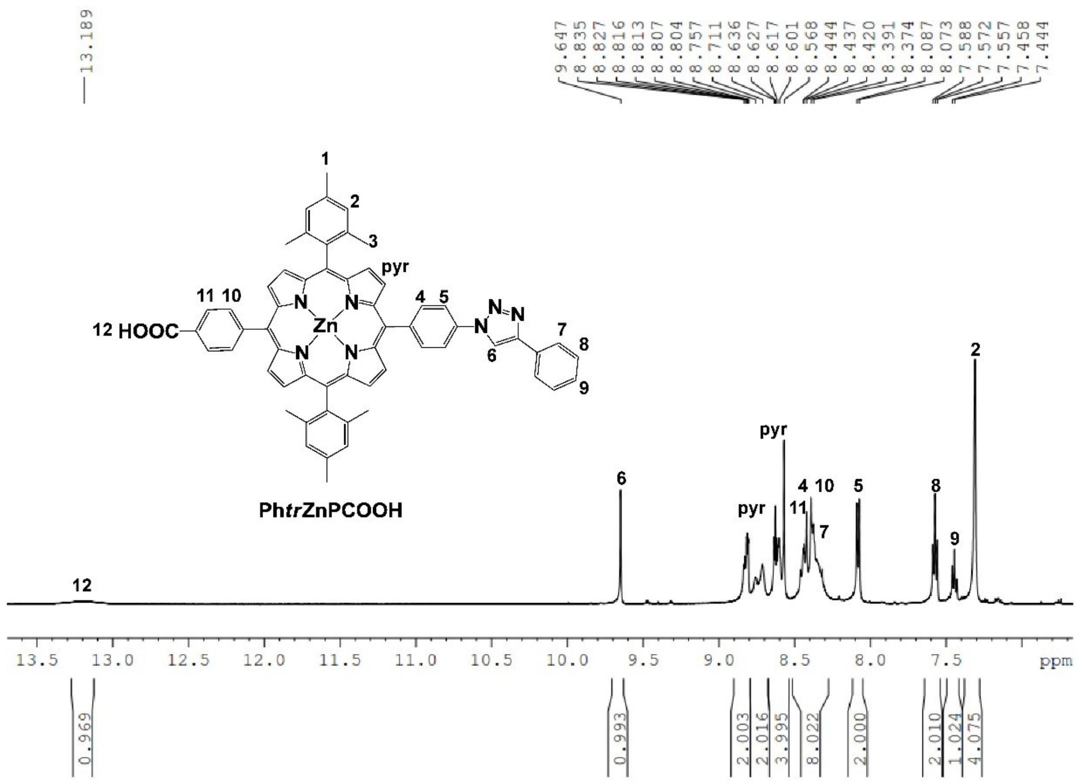


Figure S28. Aromatic region of [1]H NMR spectrum of **Ph*tr*ZnPCOOH** (500MHz, DMSO-d_6).

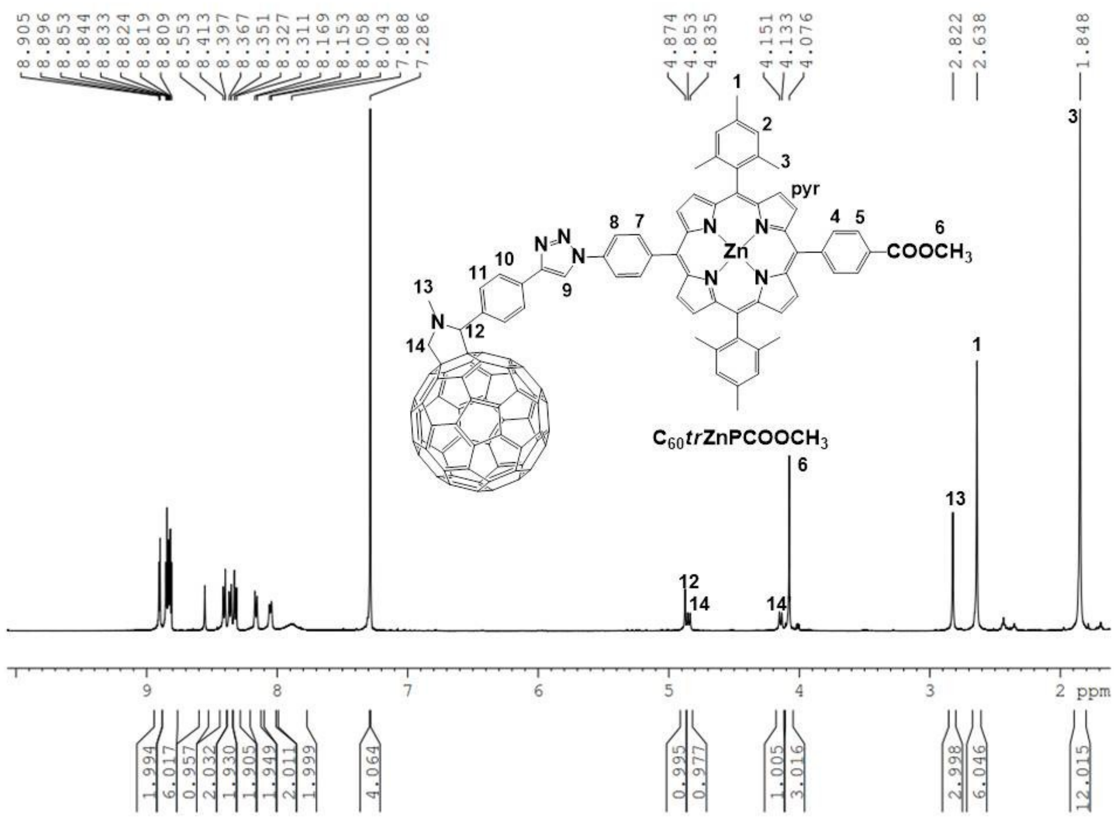


Figure S29. ^{1}H NMR spectrum of **C_{60}*tr*ZnPCOOCH$_3$** (500MHz, $CDCl_3$).

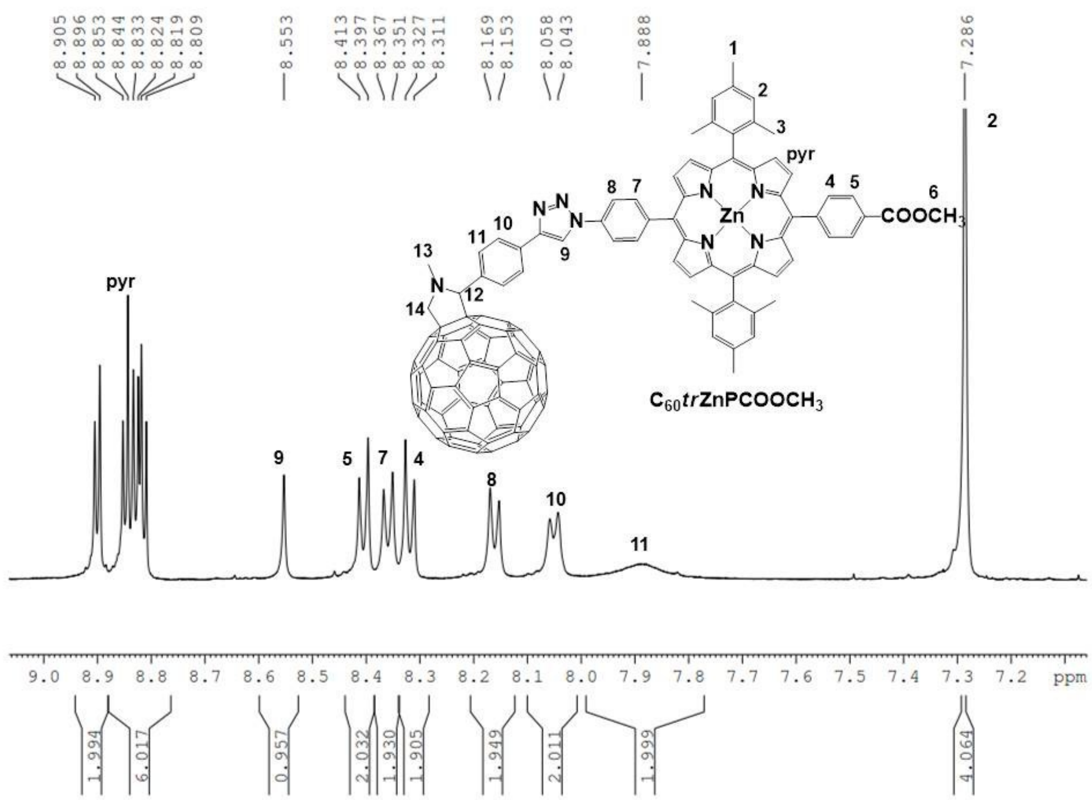


Figure S30. Aromatic region of ^{1}H NMR spectrum of **C_{60}*tr*ZnPCOOCH$_3$** (500MHz, $CDCl_3$).

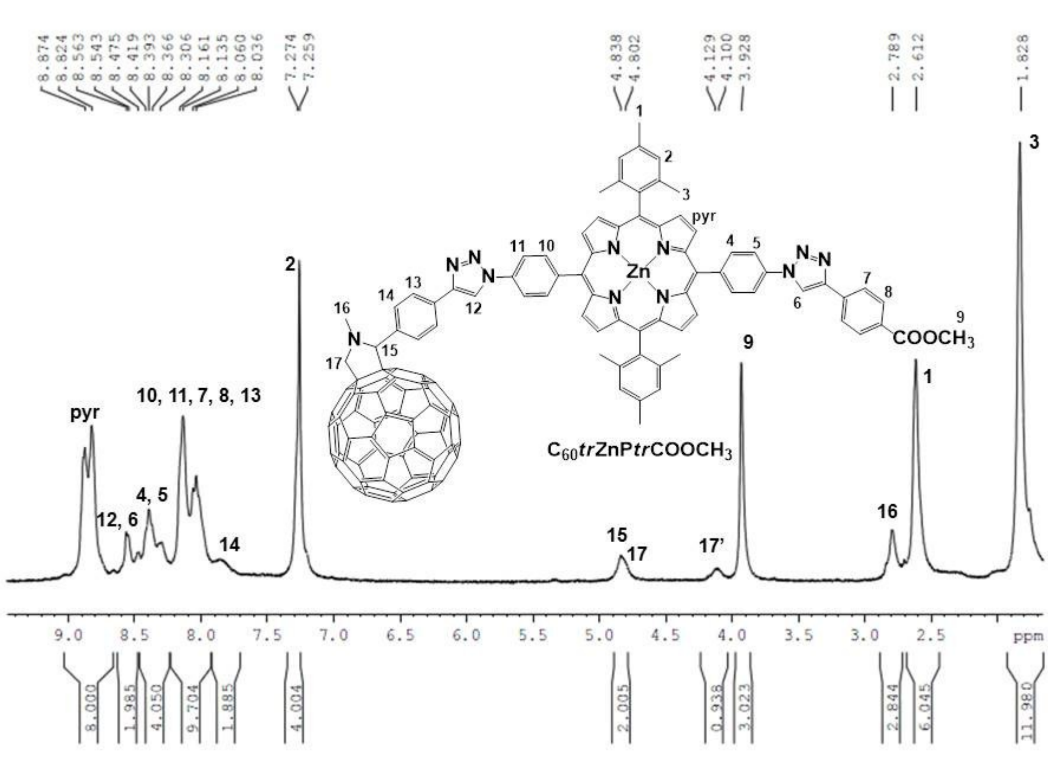


Figure S31. [1]H NMR spectrum of **C_{60}*tr*ZnP*tr*COOCH$_3$** (300MHz, $CDCl_3$).

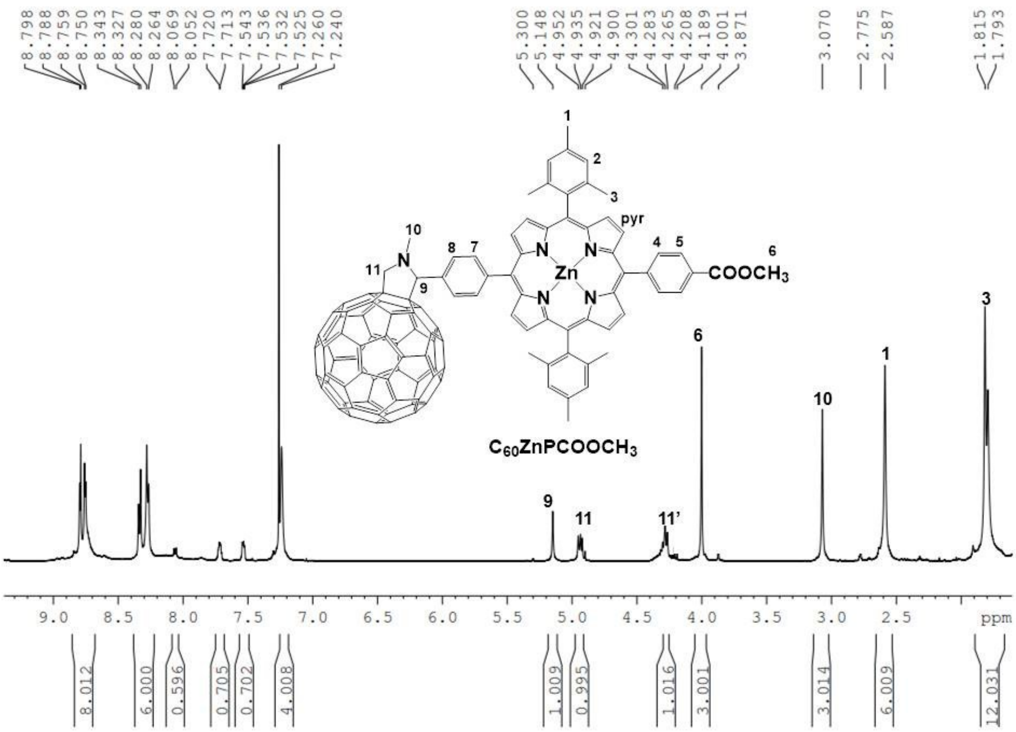


Figure S32. [1]H NMR spectrum of **C_{60}ZnPCOOCH$_3$** (500MHz, $CDCl_3$).

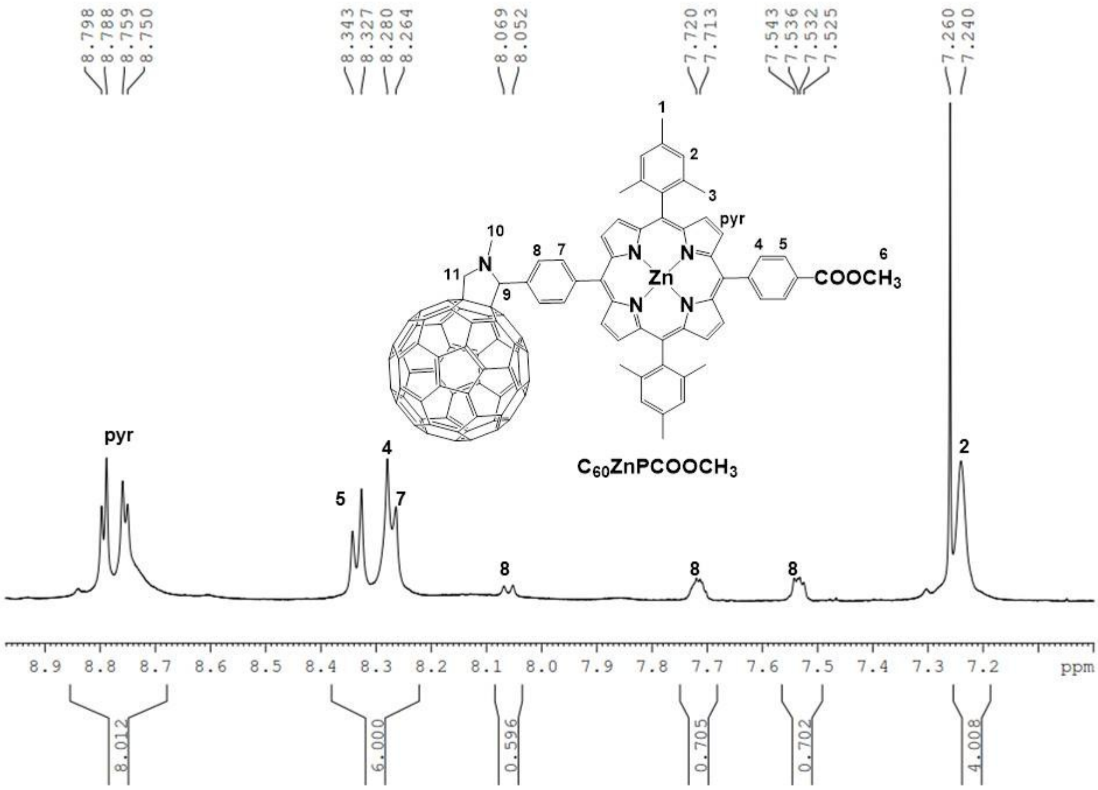


Figure S33. Aromatic region of ^{1}H NMR spectrum of **C_{60}ZnPCOOCH$_3$** (500MHz, $CDCl_3$).

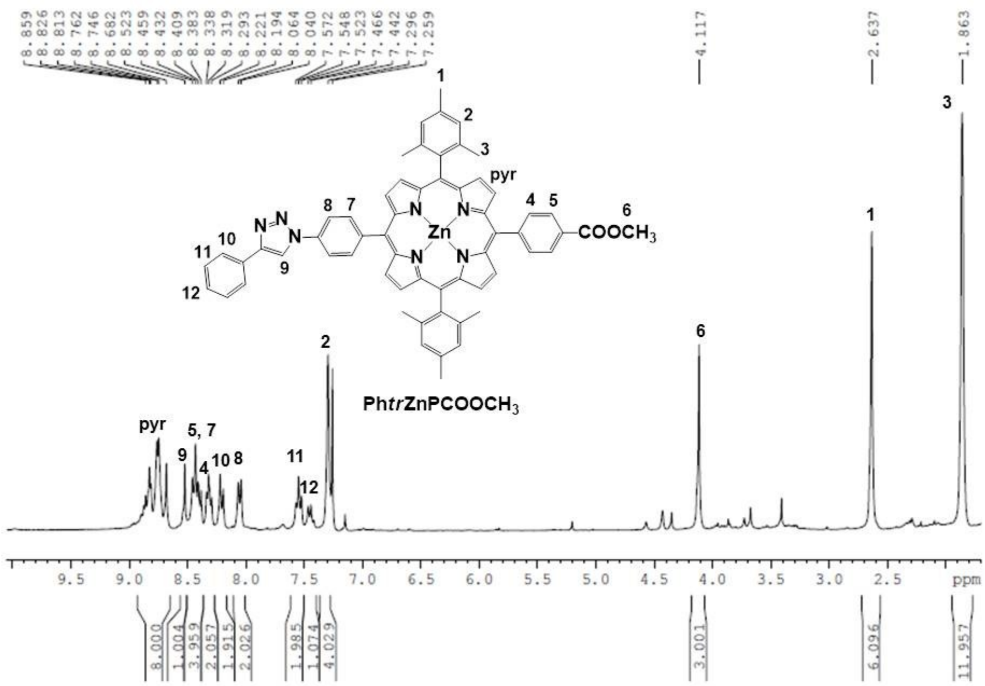


Figure S34. ^{1}H NMR spectrum of **Ph*tr*ZnPCOOCH$_3$** (500MHz, $CDCl_3$).

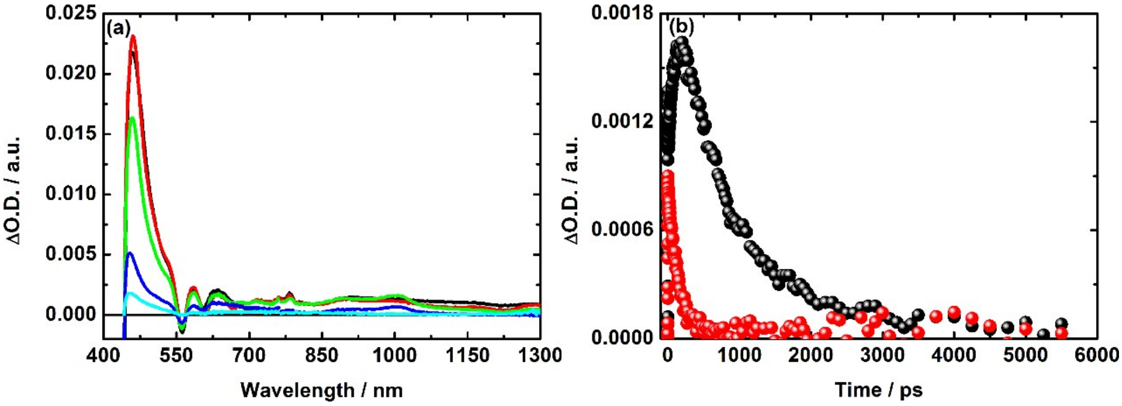


Figure S35. (a) Femtosecond transient absorption spectra of $\mathbf{C_{60}}$***tr*****ZnPCOOCH$_3$** in argon saturated benzonitrile upon photoexcitation at 430 nm; 1 ps (black), 10 ps (red), 100 ps (green), 1000 ps (blue), and 5500 ps (cyan) after excitation. (b) Corresponding time–absorption profiles at 1017 nm (black) and 1300 nm (red).

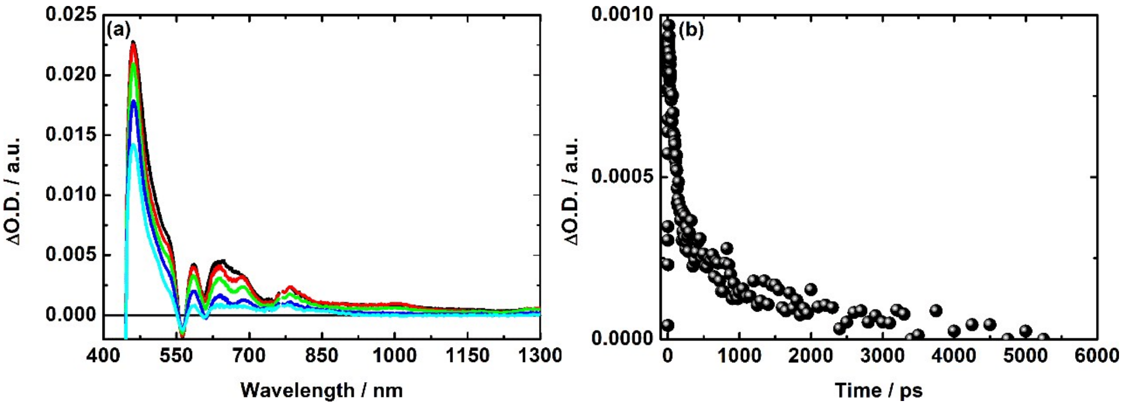


Figure S36. (a) Femtosecond transient absorption spectra of **C_{60}ZnPCOOCH$_3$** in argon saturated benzonitrile upon photoexcitation at 430 nm; 1 ps (black), 10 ps (red), 100 ps (green), 1000 ps (blue), and 5500 ps (cyan) after excitation. (b) Corresponding time–absorption profile at 1017 nm (black).

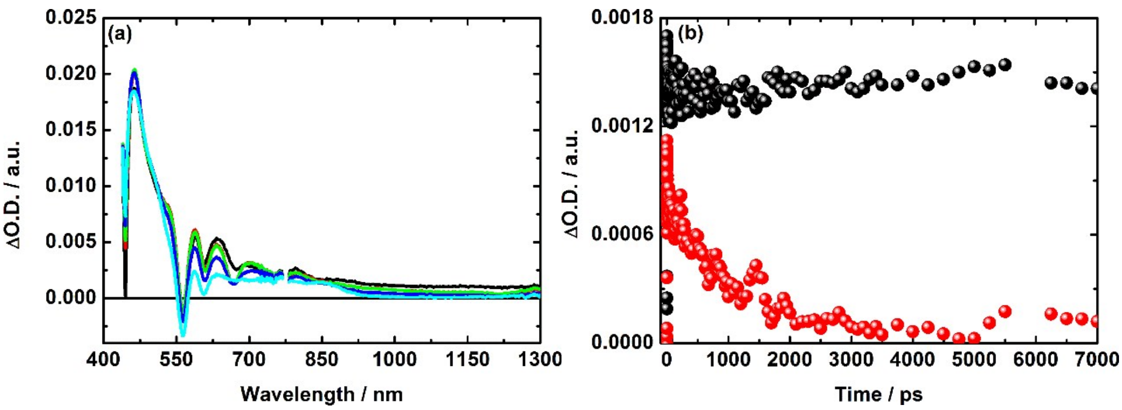


Figure S37. (a) Femtosecond transient absorption spectra of **Ph*tr*ZnPCOOH** in argon saturated benzonitrile upon photoexcitation at 430 nm; 1 ps (black), 10 ps (red), 100 ps (green), 1000 ps (blue), and 7000 ps (cyan) after excitation. (b) Corresponding time–absorption profiles at 850 nm (black) and 1300 nm (red).

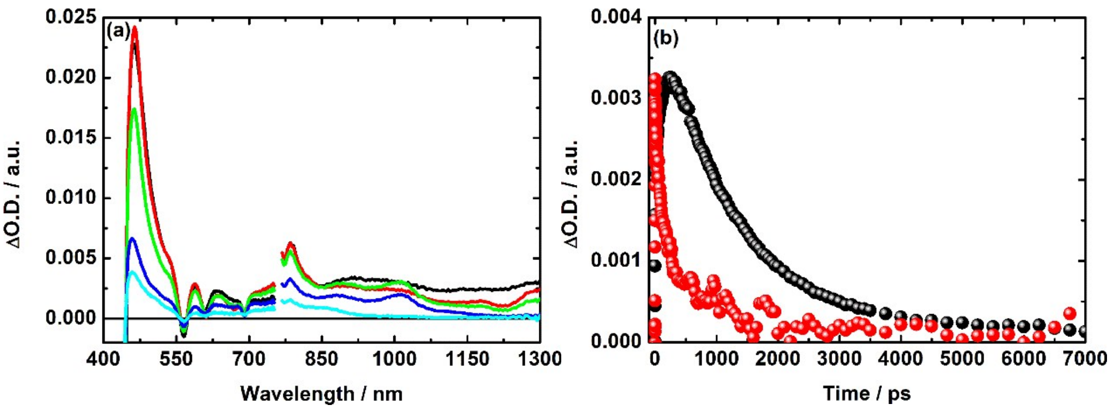


Figure S38. (a) Femtosecond transient absorption spectra of **C_{60}*tr*ZnPCOOH** in argon saturated benzonitrile upon photoexcitation at 430 nm; 1 ps (black), 10 ps (red), 100 ps (green), 1000 ps (blue), and 7000 ps (cyan) after excitation. (b) Corresponding time–absorption profiles at 1017 nm (black) and 1300 nm (red).

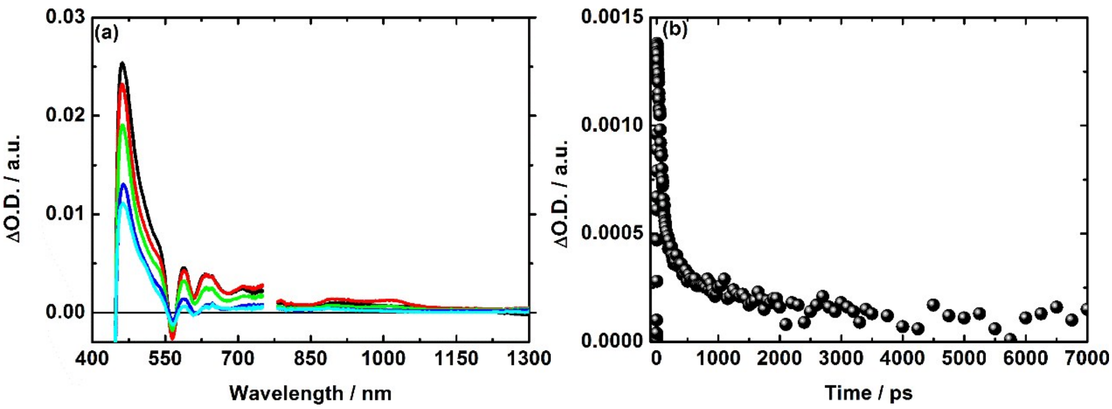


Figure S39. (a) Femtosecond transient absorption spectra of **C_{60}ZnPCOOH** in argon saturated benzonitrile upon photoexcitation at 430 nm; 1 ps (black), 10 ps (red), 100 ps (green), 1000 ps (blue), and 7000 ps (cyan) after excitation. (b) Corresponding time–absorption profiles at 1017 nm (black).

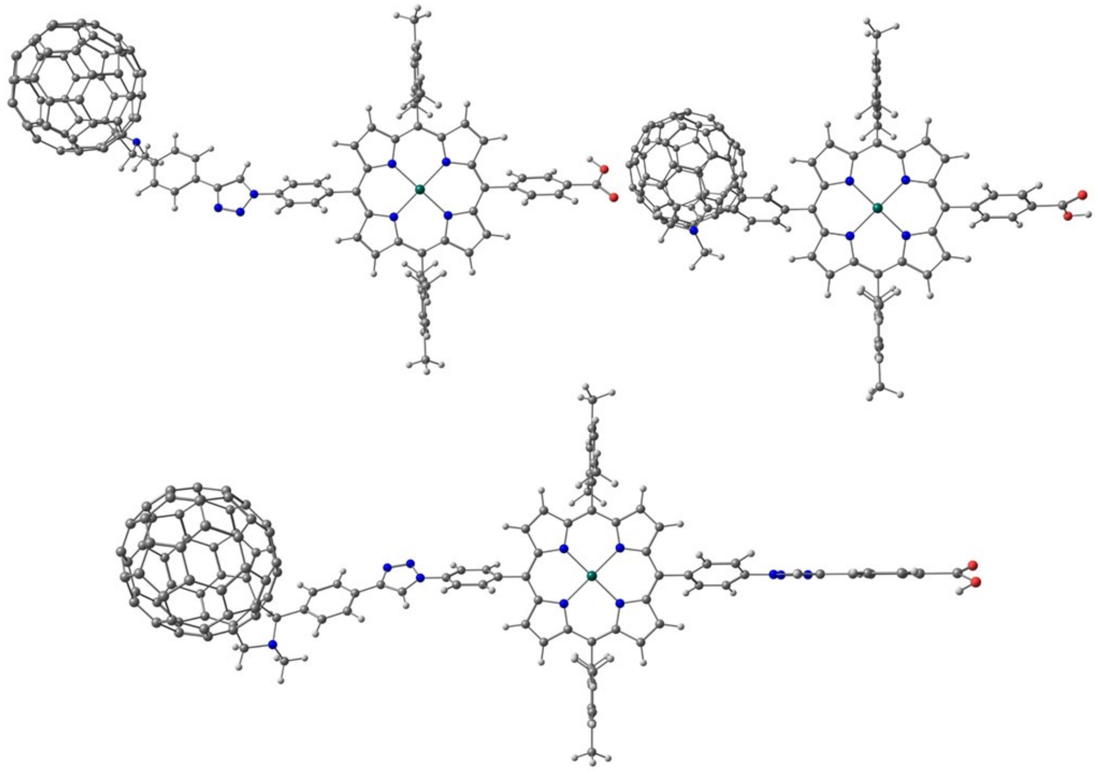


Figure S40. Gas phase geometry optimized structure of **C_{60}*tr*ZnPCOOH** (upper left part), **C_{60}*tr*ZnP*tr*COOH** (lower part) and **C_{60}ZnPCOOH** (upper right). Carbon, nitrogen, hydrogen, oxygen and zinc correspond to grey, blue, white, red and green, respectively.

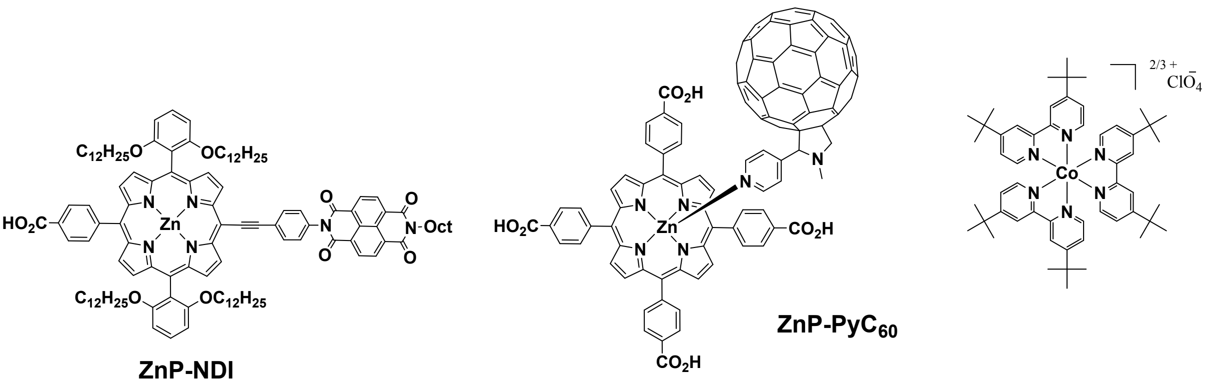


Figure S41. Structures of the dyads **ZnP-NDI**, **ZnP-PyC$_{60}$** and of the cobalt redox mediator.

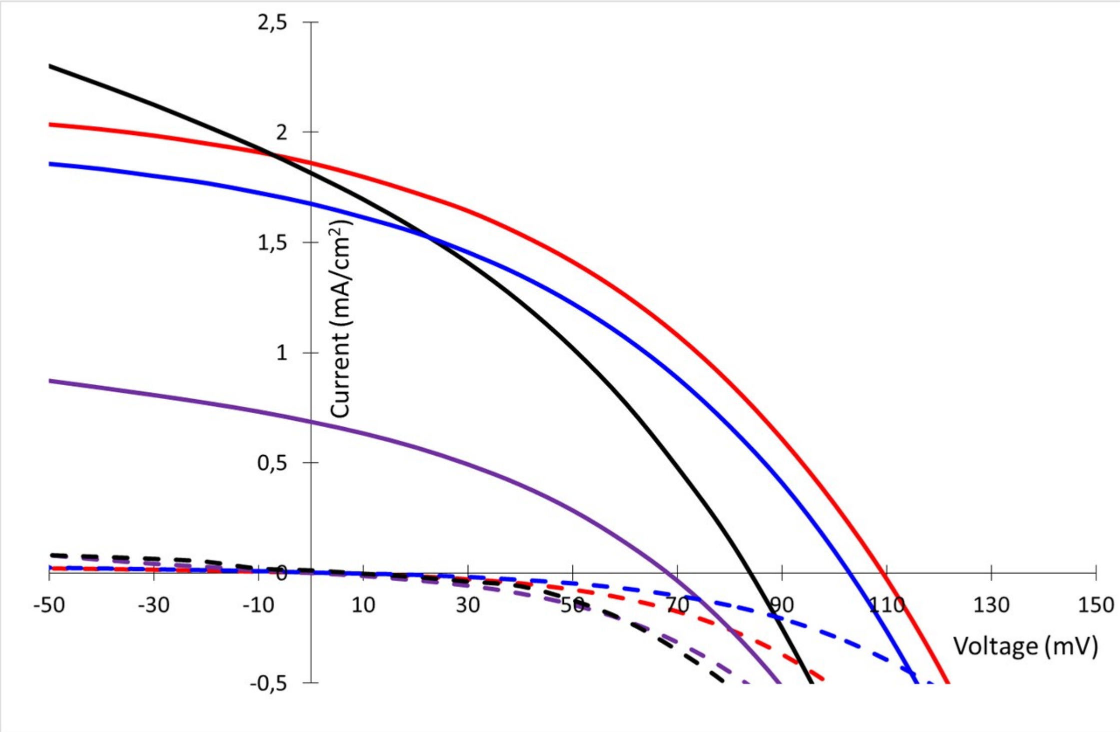


Figure S42. Current voltage characteristic of the solar cell with iodide electrolyte. Straight light = under AM1.5 and dashed line = in the dark. **C_{60}*tr*ZnPCOOH** (red), **C_{60}*tr*ZnP*tr*COOH** (black) and **C_{60}ZnPCOOH** (blue) as well as the reference compound **Ph*tr*ZnPCOOH** (purple).

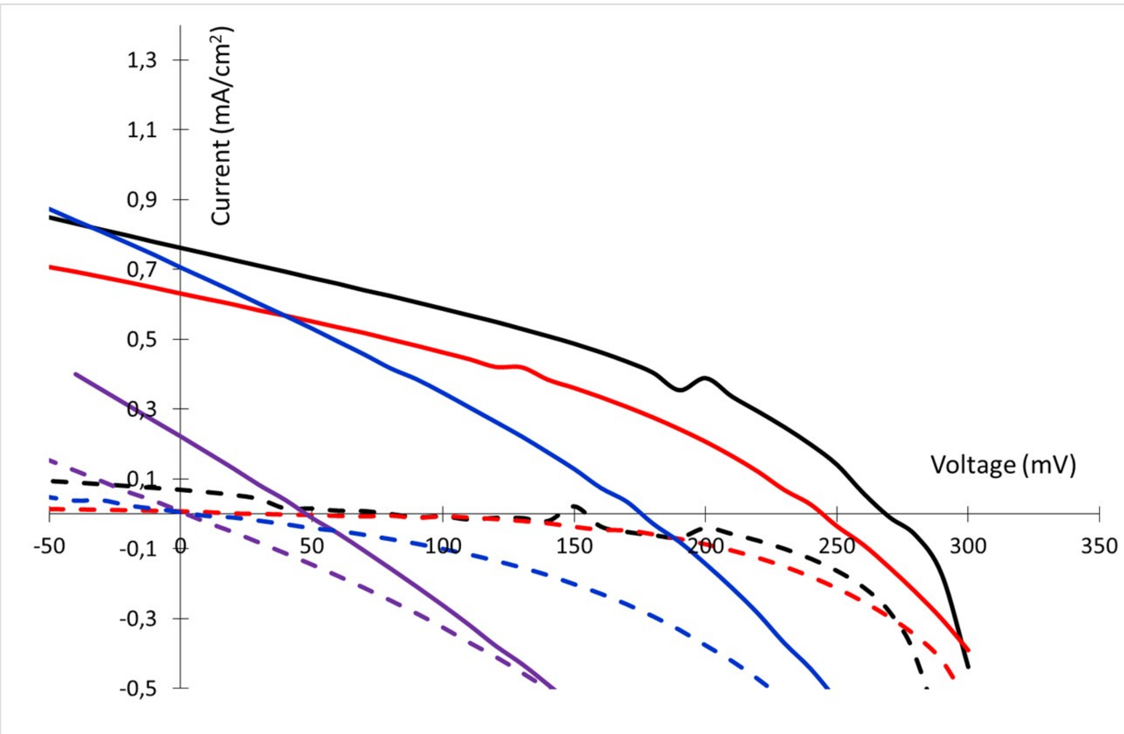


Figure S43. Current voltage characteristic of the solar cell with cobalt electrolyte. Straight light = under AM1.5 and dashed line = in the dark. **C_{60}*tr*ZnPCOOH** (red), **C_{60}*tr*ZnP*tr*COOH** (black) and **C_{60}ZnPCOOH** (blue) as well as the reference compound **Ph*tr*ZnPCOOH** (purple).

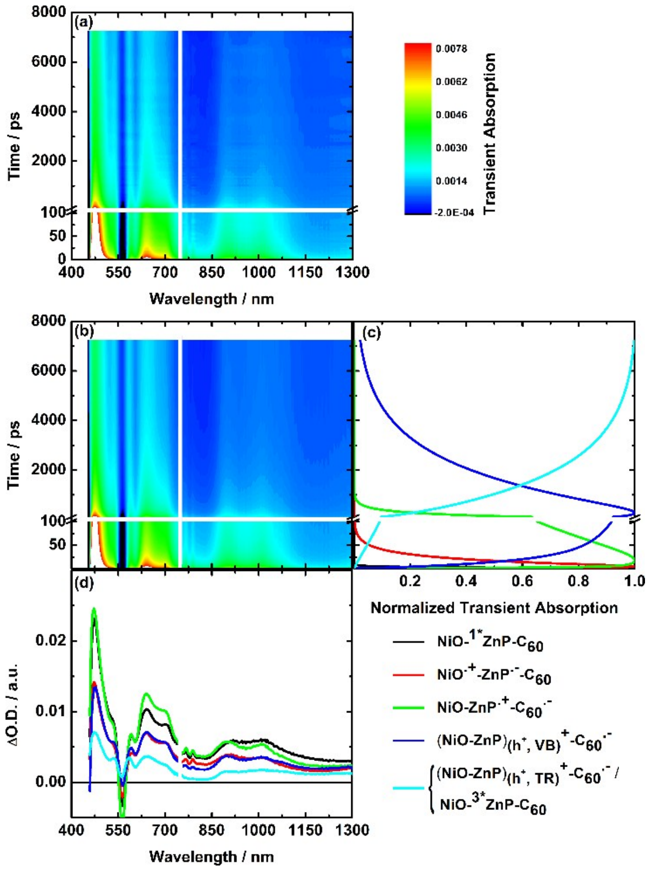


Figure S44. Transient absorption spectra obtained upon femtosecond laser flash photolysis (430 nm) of **C_{60}*tr*ZnPCOOH@NiO**. (a) Raw data measured (b) The data matrix is analyzed by SVD decomposition into five significant components that are related to each other through the kinetic scheme based on Figure 7 with optimized rate constants presented in Table 2. The fitting result is displayed in the middle 2D graph (b), and the time and spectral components are shown in the right (c) and bottom (d) panels, respectively.

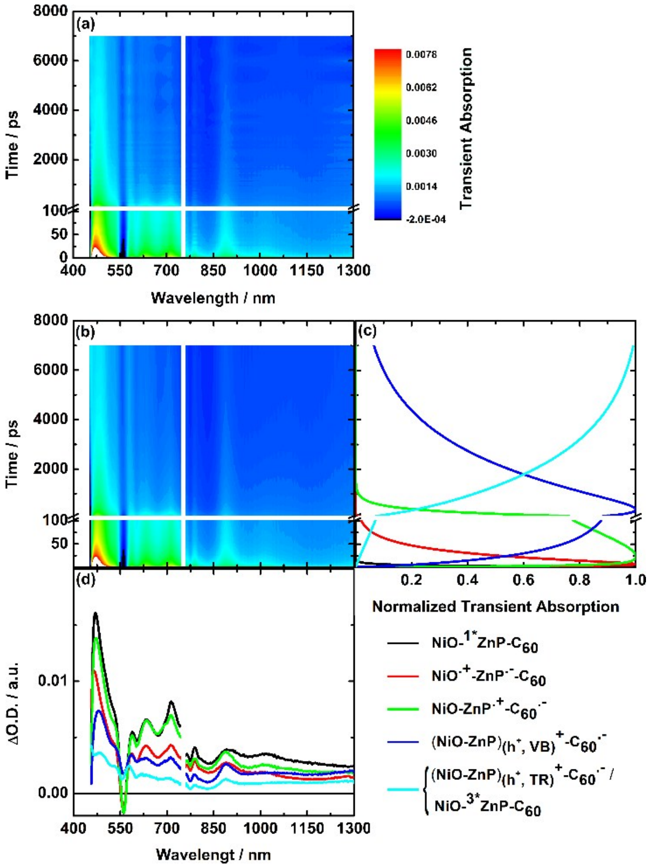


Figure S45. Transient absorption spectra obtained upon femtosecond laser flash photolysis (430 nm) of **C_{60}ZnPCOOH@NiO**. (a) Raw data measured (b) The data matrix is analyzed by SVD decomposition into five significant components that are related to each other through the kinetic scheme based on Figure7 with optimized rate constants presented in Table 2. The fitting result is displayed in the middle 2D graph (b), and the time and spectral components are shown in the right (c) and bottom (d) panels, respectively.

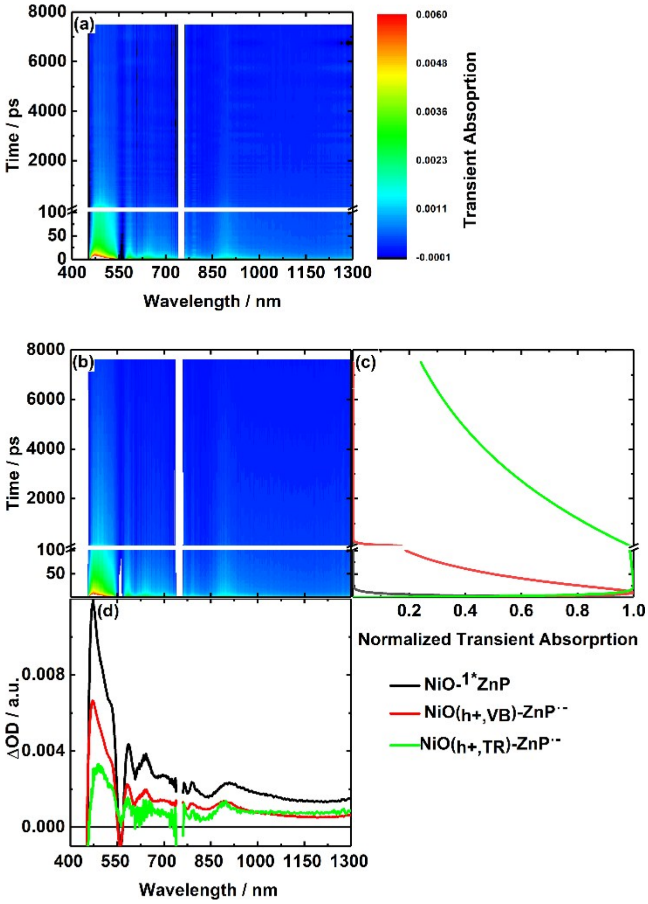


Figure S46. Transient absorption spectra obtained upon femtosecond laser flash photolysis (430 nm) of **Ph*tr*ZnPCOOH@NiO**. (a) Raw data measured (b) The data matrix is analyzed by SVD decomposition into three significant components. The fitting result is displayed in the middle 2D graph (b), and the time and spectral components are shown in the right (c) and bottom (d) panels, respectively.

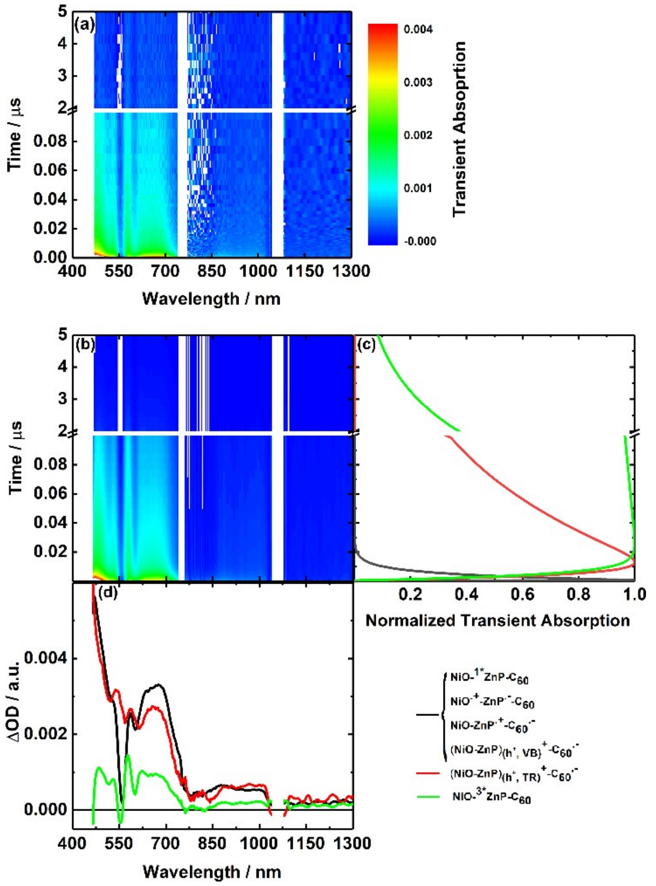


Figure S47. Transient absorption spectra obtained upon nanosecond laser flash photolysis (430 nm) of **C_{60}*tr*ZnPCOOH@NiO**. (a) Raw data measured (b) The data matrix is analyzed by SVD decomposition into three significant components that are related to each other through the kinetic scheme based on Figure 7 with optimized rate constants presented in Table 2. The fitting result is displayed in the middle 2D graph (b), and the time and spectral components are shown in the right (c) and bottom (d) panels, respectively.

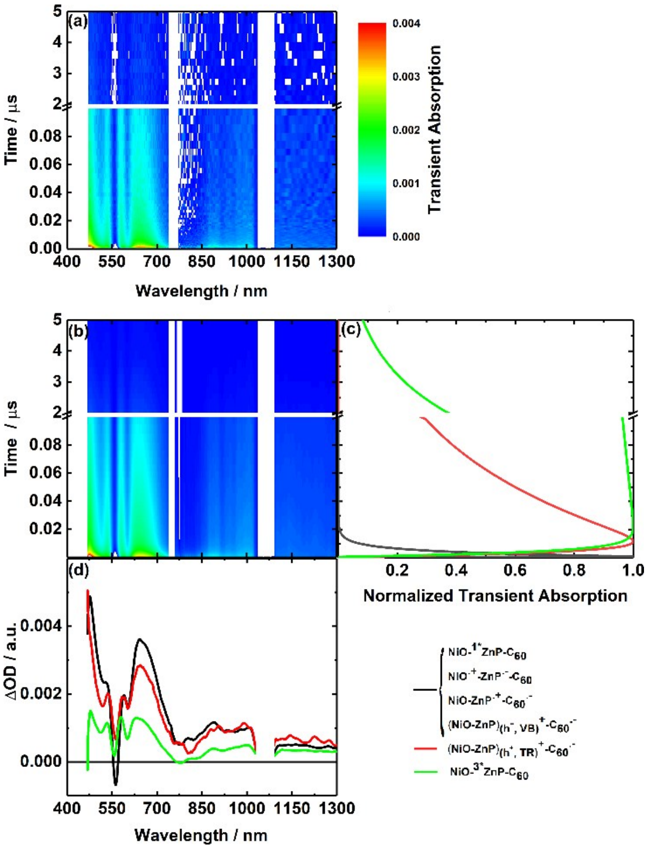


Figure S48. Transient absorption spectra obtained upon nanosecond laser flash photolysis (430 nm) of **C_{60}*tr*ZnP*tr*COOH@NiO**. (a) Raw data measured (b) The data matrix is analyzed by SVD decomposition into three significant components that are related to each other through the kinetic scheme based on Figure 7 with optimized rate constants presented in Table 2. The fitting result is displayed in the middle 2D graph (b), and the time and spectral components are shown in the right (c) and bottom (d) panels, respectively.

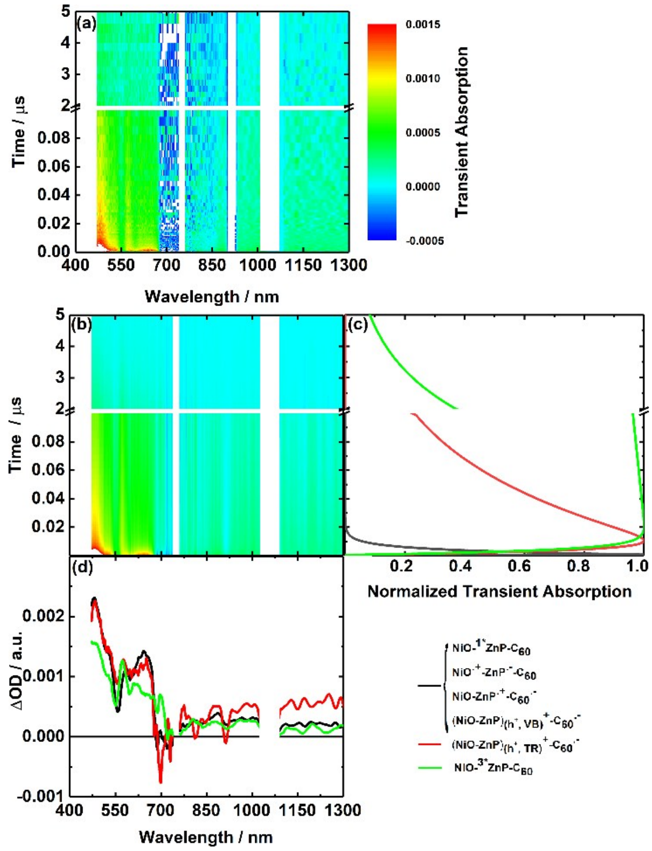


Figure S49. Transient absorption spectra obtained upon nanosecond laser flash photolysis (430 nm) of **C_{60}ZnPCOOH@NiO**. (a) Raw data measured (b) The data matrix is analyzed by SVD decomposition into three significant components that are related to each other through the kinetic scheme based on Figure 7 with optimized rate constants presented in Table 2. The fitting result is displayed in the middle 2D graph (b), and the time and spectral components are shown in the right (c) and bottom (d) panels, respectively.

Table S1. Crystal data, data collection, and refinement parameters for porphyrin **10**.

Crystal data	
Chemical formula	$C_{38}H_{34}N_4$
M_r	546.69
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	293
a, b, c (Å)	13.658 (3), 13.839 (3), 8.1732 (16)
β (°)	100.54 (3)
V (Å^3)	1518.7 (5)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.07
Data collection	
Diffractometer	STOE
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	5662, 3754, 2154
R_{int}	0.051
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.666
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.057, 0.137, 1.16
No. of reflections	3754
No. of parameters	190
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.27, −0.26

Table S2. Bond lengths [Å] and angles [°] for porphyrin **10**.

N(1)-C(1)	1.372(2)
N(1)-C(4)	1.373(2)
N(2)-C(9)	1.363(2)
N(2)-C(6)	1.379(2)
C(1)-C(10)#1	1.388(2)
C(1)-C(2)	1.423(3)
C(2)-C(3)	1.360(3)
C(3)-C(4)	1.430(3)
C(4)-C(5)	1.398(2)
C(5)-C(6)	1.402(3)
C(5)-C(11)	1.504(2)
C(6)-C(7)	1.456(2)
C(7)-C(8)	1.343(3)
C(8)-C(9)	1.452(3)
C(9)-C(10)	1.395(3)
C(10)-C(1)#1	1.388(2)
C(11)-C(16)	1.406(3)
C(11)-C(12)	1.410(3)
C(12)-C(13)	1.387(3)
C(12)-C(17)	1.518(3)
C(13)-C(14)	1.382(3)
C(14)-C(15)	1.389(3)
C(14)-C(18)	1.517(3)
C(15)-C(16)	1.395(3)
C(16)-C(19)	1.507(3)
C(1)-N(1)-C(4)	110.48(15)

C(9)-N(2)-C(6)	105.59(14)
N(1)-C(1)-C(10)#1	126.31(17)
N(1)-C(1)-C(2)	106.67(15)
C(10)#1-C(1)-C(2)	127.01(17)
C(3)-C(2)-C(1)	108.28(17)
C(2)-C(3)-C(4)	108.27(16)
N(1)-C(4)-C(5)	125.87(17)
N(1)-C(4)-C(3)	106.28(15)
C(5)-C(4)-C(3)	127.85(17)
C(4)-C(5)-C(6)	124.29(16)
C(4)-C(5)-C(11)	115.79(16)
C(6)-C(5)-C(11)	119.92(16)
N(2)-C(6)-C(5)	124.97(15)
N(2)-C(6)-C(7)	110.04(16)
C(5)-C(6)-C(7)	124.98(17)
C(8)-C(7)-C(6)	106.80(17)
C(7)-C(8)-C(9)	106.81(17)
N(2)-C(9)-C(10)	126.00(16)
N(2)-C(9)-C(8)	110.75(16)
C(10)-C(9)-C(8)	123.19(17)
C(1)#1-C(10)-C(9)	128.36(17)
C(16)-C(11)-C(12)	119.92(17)
C(16)-C(11)-C(5)	120.63(17)
C(12)-C(11)-C(5)	119.39(16)
C(13)-C(12)-C(11)	118.83(18)
C(13)-C(12)-C(17)	119.91(19)
C(11)-C(12)-C(17)	121.25(18)
C(14)-C(13)-C(12)	122.5(2)
C(13)-C(14)-C(15)	117.77(18)
C(13)-C(14)-C(18)	121.6(2)

C(15)-C(14)-C(18)	120.7(2)
C(14)-C(15)-C(16)	122.39(19)
C(15)-C(16)-C(11)	118.51(18)
C(15)-C(16)-C(19)	120.62(18)
C(11)-C(16)-C(19)	120.87(17)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y+1,-z

Table S3. Absorption features of all studied derivatives in Benzonitrile solutions

Dye	Absorption λ_{max}/nm
C_{60}*tr*ZnPCOOH	330, 432, 562 and 602
C_{60}*tr*ZnP*tr*COOH	330, 431, 561 and 602
C_{60}ZnPCOOH	330, 432, 562 and 605
Ph*tr*ZnPCOOH	425, 555 and 595
C_{60}*tr*ZnPCOOCH$_3$	330, 432, 563 and 605
C_{60}*tr*ZnP*tr*COOCH$_3$	330, 431, 560 and 605
C_{60}ZnPCOOCH$_3$	330, 432, 562 and 606
Ph*tr*ZnPCOOCH$_3$	431, 560 and 605

Table S4. Fluorescence quantum yields

	toluene	anisole	THF	benzonitrile	DMSO
C_{60}*tr*ZnPCOOH	---	0.0054	0.0043	0.0073	0.0124
C_{60}*tr*ZnP*tr*COOH	---	0.0089	0.0074	0.0117	0.0106
C_{60}ZnPCOOH	---	0.0119	0.0064	0.0175	0.0198
Ph*tr*ZnPCOOH	---	0.0158	0.0182	0.0198	0.0212
C_{60}*tr*ZnPCOOCH$_3$	0.0024	0.0031	0.0012	0.0021	---
C_{60}*tr*ZnP*tr*COOCH$_3$	0.0033	0.0027	0.0015	0.0023	---
C_{60}ZnPCOOCH$_3$	0.0065	0.0094	0.0013	0.0073	---
Ph*tr*ZnPCOOCH$_3$	0.0219	0.0260	0.0177	0.0260	---

Table S5. Singlet first excited state lifetimes

	toluene	anisole	THF	benzonitrile	DMSO
C_{60}*tr*ZnPCOOH	---	176 ps	135 ps	81 ps	67 ps
C_{60}*tr*ZnP*tr*COOH	---	125 ps	90 ps	85 ps	<10 ps
C_{60}ZnPCOOH	---	<10 ps	<5 ps	<5 ps	<5 ps
Ph*tr*ZnPCOOH	---	1.93 ns	2.02 ns	2.03 ns	2.18 ns
C_{60}*tr*ZnPCOOCH$_3$	151 ps	269 ps	142 ps	96 ps	---
C_{60}*tr*ZnP*tr*COOCH$_3$	200 ps	150 ps	95 ps	80 ps	---
C_{60}ZnPCOOCH$_3$	20 ps	31 ps	26 ps	12 ps	---
Ph*tr*ZnPCOOCH$_3$	2.09 ns	2.27 ns	2.33 ns	2.28 ns	---

Table S6. Charge separated state lifetimes

	toluene	anisole	THF	benzonitrile	DMSO
C_{60}*tr*ZnPCOOH	---	2200 ps	2450 ps	1260 ps	500 ps
C_{60}*tr*ZnP*tr*COOH	---	2200 ps	2400 ps	1350 ps	550 ps
C_{60}ZnPCOOH	---	2100 ps	300 ps	180 ps	25 ps
C_{60}*tr*ZnPCOOCH$_3$	1460 ps	2330 ps	1760 ps	1030 ps	---
C_{60}*tr*ZnP*tr*COOCH$_3$	2100 ps	2550 ps	2600 ps	1250 ps	---
C_{60}ZnPCOOCH$_3$	2480 ps	1910 ps	850 ps	217 ps	---

Table S7. Summary of the electrochemical redox data of **C_{60}*tr*ZnPCOOH**, **C_{60}*tr*ZnP*tr*COOH**, **C_{60}ZnPCOOH** and **Ph*tr*ZnPCOOH** in THF. All potentials are reported vs. SCE. FcH/FcH$^+$ was used as an internal standard and its oxidation potential was 0.62 V.

	Oxidation		**Reduction**				
Dyes	$E_{1/2}$ (ZnP) (V)	$E_{1/2}$ (ZnP) (V)	$E_{1/2}$ (C_{60}) (V)	$E_{1/2}$ (C_{60}) (V)	$E_{1/2}$ (ZnP) (V)	$E_{1/2}$ (ZnP) (V)	$E_{1/2}$ (C_{60}) (V)
C_{60}*tr*ZnPCOOH	1.06	1.37	–0.40	–1.00	–1.40	–1.64	–1.86
C_{60}*tr*ZnP*tr*COOH	1.06	1.41	–0.38	–0.95	–1.28	–1.58	–1.75
C_{60}ZnPCOOH	1.08	1.39	–0.37	–0.94	–1.39	-	-
Ph*tr*ZnPCOOH	1.09	1.40	-	-	–1.32	–1.58	-

Table S8: Coordinates of gas phase geometry optimized structure of **C_{60}*tr*ZnPCOOH** calculated by DFT at the B3LYP/LANL2DG/6-31G* level with energy E = -5332.9185836 Hartree/particle.

	x	y	z
C	0.244219000	-0.586840000	-1.372750000
C	1.127243000	-1.401949000	-2.015134000
C	2.399663000	-0.715337000	-2.040760000
N	2.271605000	0.500468000	-1.409807000
C	0.968895000	0.605825000	-0.983776000
C	1.516305000	4.939560000	0.917872000
C	0.541179000	3.994818000	0.800487000
C	1.100052000	2.895138000	0.041231000
N	2.406015000	3.184801000	-0.275278000
C	2.688592000	4.426928000	0.244531000
C	0.412716000	1.707227000	-0.295578000
C	7.234421000	4.486519000	-1.152068000
C	6.355163000	5.298291000	-0.500031000
C	5.088134000	4.602652000	-0.452874000
N	5.216032000	3.384867000	-1.080287000
C	6.513808000	3.285488000	-1.521227000
C	3.922559000	5.103711000	0.160759000
C	5.987863000	-1.075011000	-3.365918000
C	6.961972000	-0.129123000	-3.251416000
C	6.392967000	0.982491000	-2.517115000
N	5.084327000	0.697285000	-2.208920000
C	4.807217000	-0.551873000	-2.714327000
C	3.570619000	-1.224043000	-2.639131000
C	7.071919000	2.178834000	-2.198423000
C	4.004035000	6.470948000	0.786850000
C	8.506396000	2.283807000	-2.614039000

C	3.491171000	-2.594962000	-3.257264000
C	-1.023677000	1.607422000	0.112093000
C	4.386860000	6.610858000	2.136514000
C	4.454094000	7.893472000	2.695391000
C	4.153265000	9.039462000	1.956494000
C	3.777867000	8.877624000	0.618274000
C	3.696679000	7.616882000	0.020155000
C	9.489176000	1.459610000	-2.038285000
C	10.821167000	1.555141000	-2.427806000
C	11.214557000	2.491105000	-3.394125000
C	10.238495000	3.308699000	-3.981727000
C	8.903204000	3.204566000	-3.596818000
C	3.785310000	-3.734955000	-2.482139000
C	3.707170000	-5.000939000	-3.076270000
C	3.346359000	-5.168987000	-4.414541000
C	3.058205000	-4.023824000	-5.165381000
C	3.123467000	-2.741274000	-4.613555000
C	-1.450055000	0.636060000	1.033910000
C	-2.782407000	0.542442000	1.425800000
C	-3.721349000	1.427131000	0.886469000
C	-3.326155000	2.393114000	-0.043041000
C	-1.986934000	2.481028000	-0.417463000
C	4.219641000	10.415013000	2.579389000
C	3.283751000	7.499317000	-1.430658000
C	4.724840000	5.404479000	2.984830000
C	4.183721000	-3.613570000	-1.027587000
C	2.802077000	-1.536763000	-5.470954000
C	3.268162000	-6.542686000	-5.040034000
N	-5.079638000	1.336458000	1.292851000
Zn	3.744934000	1.940485000	-1.242274000

N	-5.612696000	0.140558000	1.669270000
N	-6.849550000	0.351494000	1.997602000
C	-7.154334000	1.682121000	1.846910000
C	-6.015710000	2.319636000	1.390480000
C	-8.481938000	2.216546000	2.168603000
C	-9.513990000	1.347067000	2.555664000
C	-10.774625000	1.844796000	2.874679000
C	-11.043034000	3.218674000	2.832190000
C	-10.013491000	4.086814000	2.441842000
C	-8.755549000	3.592941000	2.109650000
C	-14.009645000	5.419242000	3.226535000
C	-12.403472000	3.739795000	3.244224000
N	-12.826908000	4.941487000	2.524306000
C	-13.069066000	4.731771000	1.102412000
C	-15.220566000	6.068964000	10.936313000
C	-14.933264000	7.355197000	10.317600000
C	-13.696337000	7.964046000	10.522065000
C	-12.968471000	6.084051000	11.949066000
C	-14.257781000	5.446418000	11.730206000
C	-15.540904000	7.359880000	8.995460000
C	-13.006806000	8.600001000	9.410817000
C	-11.953292000	5.048534000	11.978651000
C	-14.034594000	4.013214000	11.621927000
C	-16.000258000	5.286063000	9.991458000
C	-10.697532000	5.283022000	11.413952000
C	-10.409982000	6.561651000	10.793084000
C	-14.873391000	7.963595000	7.924634000
C	-11.580283000	8.357021000	9.565652000
C	-13.582106000	8.590981000	8.140167000
C	-12.609902000	3.765879000	11.778626000

C	-14.775350000	3.260622000	10.710555000
C	-15.773777000	3.909795000	9.876239000
C	-16.200166000	6.083403000	8.797975000
C	-14.122512000	2.226045000	9.924576000
C	-15.729636000	3.294015000	8.567437000
C	-16.165839000	5.473166000	7.539449000
C	-11.984157000	2.768255000	11.031664000
C	-12.755184000	8.331940000	6.972084000
C	-14.699081000	2.243872000	8.597735000
C	-15.918733000	4.056075000	7.426756000
C	-15.474741000	6.104861000	6.431964000
C	-14.841668000	5.063866000	5.622123000
C	-10.748463000	7.082108000	6.343324000
C	-15.080978000	3.843898000	6.230349000
C	-14.068182000	2.812753000	6.259866000
C	-12.825952000	3.010158000	5.680394000
C	-13.907699000	2.007588000	7.486025000
C	-10.674824000	3.011916000	10.443716000
C	-11.514457000	6.304322000	5.447155000
C	-12.754904000	1.976472000	10.086844000
C	-11.927467000	1.725530000	8.924334000
C	-12.910222000	6.571626000	5.261491000
C	-9.747536000	6.452093000	7.167415000
C	-9.560767000	5.071226000	7.067581000
C	-13.652042000	5.335562000	4.733077000
C	-12.504689000	4.164172000	4.763626000
C	-12.500118000	1.736150000	7.647730000
C	-11.822408000	2.380629000	6.539913000
C	-11.271127000	4.897978000	5.308534000
C	-10.643876000	2.365054000	9.140652000

C	-9.350580000	4.274162000	8.266102000
C	-10.329055000	4.294966000	6.123975000
C	-9.996683000	2.989259000	8.069361000
C	-10.595426000	2.986907000	6.746958000
C	-11.382438000	8.119437000	7.119062000
C	-10.784679000	8.126783000	8.441998000
C	-9.766093000	7.088476000	8.472211000
C	-14.849969000	7.326021000	6.620556000
C	-13.519558000	7.550918000	6.026957000
C	-12.692423000	7.317924000	11.355376000
C	-11.390961000	7.562270000	10.764243000
C	-9.584873000	6.321772000	9.624534000
C	-10.047236000	4.242486000	10.630404000
C	-9.365632000	4.886500000	9.518916000
C	12.664828000	2.536969000	-3.770290000
O	13.435414000	1.630643000	-3.557509000
O	13.105730000	3.672346000	-4.379275000
H	-0.804068000	-0.772259000	-1.189548000
H	0.937420000	-2.375458000	-2.444735000
H	1.457555000	5.892395000	1.424780000
H	-0.460264000	4.033622000	1.203383000
H	8.278540000	4.677871000	-1.352879000
H	6.544072000	6.275131000	-0.077501000
H	6.053166000	-2.036531000	-3.855265000
H	7.969959000	-0.176187000	-3.637310000
H	4.750936000	7.995779000	3.737280000
H	3.541142000	9.756857000	0.021556000
H	9.199249000	0.743029000	-1.275450000
H	11.579172000	0.914896000	-1.988762000
H	10.496043000	4.003161000	-4.778948000

H	8.153840000	3.831066000	-4.071258000
H	3.935911000	-5.877406000	-2.473231000
H	2.774367000	-4.130581000	-6.210880000
H	-0.720767000	-0.044555000	1.462644000
H	-3.103984000	-0.200383000	2.146397000
H	-4.060830000	3.053427000	-0.493339000
H	-1.685394000	3.226438000	-1.147064000
H	4.647151000	10.378112000	3.586416000
H	3.222046000	10.866083000	2.658912000
H	4.832580000	11.098024000	1.978818000
H	3.091095000	8.486440000	-1.862203000
H	2.373760000	6.897953000	-1.542767000
H	4.060171000	7.012902000	-2.032909000
H	5.562058000	4.836676000	2.562113000
H	3.877309000	4.712679000	3.056877000
H	5.000619000	5.706415000	3.999941000
H	3.403477000	-3.121267000	-0.435162000
H	5.095869000	-3.016894000	-0.908075000
H	4.366722000	-4.599877000	-0.590187000
H	2.537196000	-1.841838000	-6.488045000
H	3.654058000	-0.849643000	-5.535563000
H	1.962600000	-0.962871000	-5.060993000
H	3.516899000	-7.325988000	-4.317042000
H	2.262030000	-6.750617000	-5.425207000
H	3.960448000	-6.637076000	-5.886118000
H	-5.793596000	3.350319000	1.166739000
H	-9.314000000	0.281844000	2.599607000
H	-11.562126000	1.154102000	3.167365000
H	-10.211096000	5.153255000	2.398320000
H	-7.976107000	4.290222000	1.812990000

H	-14.892181000	4.779628000	3.029159000
H	-14.260178000	6.440925000	2.921636000
H	-13.140297000	2.923127000	3.106009000
H	-13.365393000	5.679907000	0.641443000
H	-13.868391000	3.990201000	0.911868000
H	-12.154187000	4.383996000	0.615976000
H	12.420778000	4.359262000	-4.342279000

Table S9: Coordinates of gas phase geometry optimized structure of **C_{60}*tr*ZnP*tr*COOH** calculated by DFT at the B3LYP/LANL2DG/6-31G* level with energy E = -5804.9985093 Hartree/particle.

	x	**y**	**z**
C	-3.912320000	4.993706000	-1.561323000
C	-3.506678000	3.699098000	-1.689087000
C	-2.065376000	3.690175000	-1.566502000
N	-1.619955000	4.975547000	-1.361881000
C	-2.724081000	5.794095000	-1.346836000
C	-0.248041000	9.805235000	-0.661168000
C	-1.550058000	9.418329000	-0.772643000
C	-1.552517000	7.989133000	-1.007218000
N	-0.256145000	7.532526000	-1.020801000
C	0.563553000	8.618187000	-0.815491000
C	-2.709088000	7.195307000	-1.172242000
C	4.628980000	6.155490000	-0.985753000
C	4.222948000	7.448733000	-0.844226000
C	2.776813000	7.446238000	-0.869325000
N	2.328640000	6.154410000	-1.020922000
C	3.435125000	5.341955000	-1.088847000
C	1.972015000	8.598232000	-0.758307000
C	0.951737000	1.312949000	-1.627135000

C	2.253892000	1.699116000	-1.515509000
C	2.262441000	3.142997000	-1.400080000
N	0.968579000	3.605621000	-1.431337000
C	0.145431000	2.512412000	-1.572400000
C	-1.261872000	2.534980000	-1.651230000
C	3.419164000	3.939829000	-1.255476000
C	2.674682000	9.915791000	-0.562949000
C	4.741820000	3.238028000	-1.283942000
C	-1.963929000	1.216731000	-1.843507000
C	-4.030195000	7.899715000	-1.162920000
C	2.980165000	10.368265000	0.740090000
C	3.635024000	11.593001000	0.898226000
C	3.998472000	12.385660000	-0.196212000
C	3.686495000	11.919409000	-1.474852000
C	3.030447000	10.698938000	-1.679773000
C	5.551027000	3.167903000	-0.137752000
C	6.785062000	2.523723000	-0.158982000
C	7.225823000	1.923357000	-1.342384000
C	6.433294000	1.966141000	-2.492715000
C	5.206688000	2.626437000	-2.458428000
C	-2.393134000	0.474516000	-0.722188000
C	-3.046652000	-0.745790000	-0.923882000
C	-3.286755000	-1.254265000	-2.203951000
C	-2.857703000	-0.500598000	-3.299862000
C	-2.198919000	0.724347000	-3.144631000
C	-4.957699000	7.690378000	-0.128810000
C	-6.183537000	8.349732000	-0.108193000
C	-6.508290000	9.231035000	-1.144713000
C	-5.609092000	9.443935000	-2.193687000
C	-4.379831000	8.787968000	-2.191746000

C	4.705546000	13.705960000	0.007464000
C	2.718872000	10.242048000	-3.087975000
C	2.609578000	9.551468000	1.958440000
C	-2.160563000	0.978502000	0.685180000
C	-1.756641000	1.498747000	-4.366822000
C	-3.967412000	-2.590113000	-2.394539000
N	-7.758215000	9.906091000	-1.122278000
Zn	0.354788000	5.566424000	-1.207111000
N	-8.813328000	9.388286000	-0.432911000
N	-9.813006000	10.200856000	-0.580028000
C	-9.440544000	11.264054000	-1.365679000
C	-8.116594000	11.077543000	-1.715832000
C	-10.369479000	12.348963000	-1.699061000
C	-9.990725000	13.409219000	-2.539063000
C	-10.882512000	14.432054000	-2.846098000
C	-12.181059000	14.432697000	-2.316429000
C	-12.555754000	13.379324000	-1.473106000
C	-11.669805000	12.348601000	-1.170116000
C	-13.617684000	17.691667000	-3.366659000
C	-13.172388000	15.523944000	-2.659401000
N	-12.567557000	16.848044000	-2.814203000
C	-11.999115000	17.394086000	-1.588344000
N	8.486741000	1.265664000	-1.363739000
N	9.015760000	0.744425000	-0.220422000
N	10.156091000	0.209985000	-0.525668000
C	10.400618000	0.365901000	-1.867556000
C	9.326328000	1.046948000	-2.410374000
C	11.625039000	-0.138986000	-2.494573000
C	12.583318000	-0.815187000	-1.717666000
C	13.747501000	-1.301612000	-2.297484000

C	14.001849000	-1.110739000	-3.663548000
C	13.042552000	-0.447581000	-4.443284000
C	11.869562000	0.029484000	-3.867214000
C	-17.611231000	17.597952000	-6.062399000
C	-16.225386000	17.947934000	-5.817077000
C	-15.395757000	18.253694000	-6.882461000
C	-17.242624000	17.873986000	-8.482885000
C	-18.114118000	17.558953000	-7.367445000
C	-15.732244000	17.143159000	-4.699685000
C	-14.019128000	17.726243000	-6.895182000
C	-17.577635000	16.983985000	-9.584207000
C	-18.985382000	16.473906000	-7.771518000
C	-17.947041000	16.554729000	-5.123707000
C	-16.572749000	16.478016000	-10.406924000
C	-15.184259000	16.833688000	-10.160239000
C	-14.266269000	16.848224000	-4.494171000
C	-13.706402000	17.377816000	-8.262131000
C	-13.543721000	16.961909000	-5.843587000
C	-18.660492000	16.116849000	-9.142501000
C	-19.317929000	15.471858000	-6.852822000
C	-18.781431000	15.519060000	-5.509499000
C	-16.748578000	16.291651000	-4.303207000
C	-19.355966000	14.080036000	-7.271601000
C	-18.495508000	14.137765000	-5.089118000
C	-16.466844000	14.935206000	-3.890763000
C	-18.690549000	14.780875000	-9.541049000
C	-12.771657000	15.787630000	-6.123604000
C	-18.860270000	13.258591000	-6.178897000
C	-17.388479000	13.859519000	-4.304448000
C	-15.172329000	14.443398000	-3.875399000

C	-15.213821000	13.051251000	-4.325757000
C	-12.453205000	14.076751000	-7.876992000
C	-16.595436000	12.683416000	-4.567501000
C	-16.931340000	11.830286000	-5.624367000
C	-15.887805000	11.307967000	-6.485087000
C	-18.087081000	12.123249000	-6.447286000
C	-17.644876000	14.252727000	-10.403474000
C	-12.824654000	13.092663000	-6.957564000
C	-19.052018000	13.741401000	-8.590055000
C	-18.234663000	12.571127000	-8.868691000
C	-13.138965000	13.445824000	-5.594004000
C	-12.961170000	14.027295000	-9.236287000
C	-13.809773000	12.989664000	-9.625871000
C	-14.218647000	12.548974000	-5.146300000
C	-14.557494000	11.669788000	-6.250648000
C	-17.765550000	11.777437000	-7.822397000
C	-16.399541000	11.274225000	-7.846676000
C	-13.691577000	11.999244000	-7.367933000
C	-17.363855000	12.891570000	-9.989188000
C	-14.971830000	13.272277000	-10.446792000
C	-14.176820000	11.950666000	-8.674542000
C	-16.053338000	12.409279000	-10.012623000
C	-15.563078000	11.584510000	-8.917563000
C	-12.430508000	15.454139000	-7.452804000
C	-12.905783000	16.268456000	-8.544082000
C	-13.243184000	15.392830000	-9.651874000
C	-13.946040000	15.310613000	-4.021374000
C	-13.090012000	14.763305000	-5.171891000
C	-15.906398000	18.208655000	-8.240454000
C	-14.861738000	17.673620000	-9.094454000

C	-14.362335000	15.665674000	-10.440558000
C	-16.605544000	15.084268000	-10.827269000
C	-15.243254000	14.587468000	-10.847540000
C	15.275726000	-1.664386000	-4.223203000
O	15.918145000	-2.534043000	-3.683278000
O	15.707114000	-1.137641000	-5.403858000
H	-4.922438000	5.372964000	-1.616236000
H	-4.121340000	2.826513000	-1.860149000
H	0.133896000	10.800044000	-0.479779000
H	-2.428879000	10.041282000	-0.691728000
H	5.643976000	5.787309000	-1.024364000
H	4.841161000	8.329415000	-0.741194000
H	0.564787000	0.308564000	-1.726307000
H	3.127279000	1.063362000	-1.499848000
H	3.867843000	11.936519000	1.904641000
H	3.960053000	12.519092000	-2.340750000
H	5.206737000	3.627102000	0.783999000
H	7.405725000	2.472063000	0.727731000
H	6.758240000	1.475270000	-3.404717000
H	4.595630000	2.663679000	-3.355154000
H	-3.377772000	-1.312629000	-0.055731000
H	-3.040716000	-0.873458000	-4.305855000
H	-4.705576000	7.011855000	0.680630000
H	-6.889857000	8.194134000	0.698536000
H	-5.872120000	10.094986000	-3.021304000
H	-3.687241000	8.952121000	-3.011782000
H	5.644723000	13.576090000	0.559495000
H	4.088831000	14.405414000	0.585963000
H	4.943429000	14.183955000	-0.948130000
H	3.183999000	9.274148000	-3.309213000

H	1.640393000	10.117118000	-3.241568000
H	3.082316000	10.967120000	-3.822765000
H	2.915857000	10.060992000	2.877247000
H	3.088526000	8.565335000	1.943440000
H	1.528478000	9.377150000	2.012918000
H	-2.536043000	0.262585000	1.422796000
H	-1.094574000	1.140926000	0.883649000
H	-2.664510000	1.936867000	0.858465000
H	-2.047457000	0.978120000	-5.284462000
H	-0.668535000	1.633563000	-4.385885000
H	-2.200240000	2.501029000	-4.391516000
H	-4.713441000	-2.775527000	-1.614010000
H	-3.243462000	-3.415148000	-2.352520000
H	-4.470725000	-2.648911000	-3.365421000
H	-7.422105000	11.673057000	-2.285009000
H	-8.990202000	13.436207000	-2.963252000
H	-10.576108000	15.247318000	-3.493780000
H	-13.556018000	13.365385000	-1.046246000
H	-11.970484000	11.537041000	-0.516201000
H	-14.389001000	17.937675000	-2.610632000
H	-13.205441000	18.633021000	-3.745372000
H	-13.949067000	15.541512000	-1.868512000
H	-11.562027000	18.375995000	-1.798132000
H	-11.207330000	16.737061000	-1.219607000
H	-12.752894000	17.515462000	-0.786988000
H	9.113947000	1.404538000	-3.404606000
H	12.394340000	-0.953296000	-0.658699000
H	14.482977000	-1.835520000	-1.704944000
H	13.178045000	-0.332161000	-5.516610000
H	11.137168000	0.529321000	-4.494994000

H	15.186762000	-0.348932000	-5.626470000

Table S10: Coordinates of gas phase geometry optimized structure of $\mathbf{C_{60}ZnPCOOH}$ calculated by DFT at the B3LYP/LANL2DG/6-31G* level with energy E = -4860.8372509

Hartree/particle.

	x	**y**	**z**
C	-0.799311000	-0.140756000	-0.326703000
C	0.250422000	-0.998944000	-0.187957000
C	1.457885000	-0.204259000	-0.227985000
N	1.123467000	1.120064000	-0.391354000
C	-0.247477000	1.191250000	-0.464050000
C	-0.382638000	5.928933000	-0.937590000
C	-1.255006000	4.882243000	-0.924862000
C	-0.477479000	3.680195000	-0.703244000
N	0.852017000	4.016452000	-0.602820000
C	0.941484000	5.382229000	-0.741117000
C	-1.006056000	2.371984000	-0.627654000
C	5.687738000	5.564998000	-0.489743000
C	4.637175000	6.424311000	-0.611200000
C	3.430187000	5.627593000	-0.588361000
N	3.765437000	4.301117000	-0.444215000
C	5.136500000	4.229992000	-0.377994000
C	2.126448000	6.146102000	-0.720373000
C	5.278467000	-0.512804000	0.037624000
C	6.151714000	0.532688000	0.000882000
C	5.368253000	1.737027000	-0.182837000
N	4.036347000	1.403526000	-0.245195000
C	3.949149000	0.036751000	-0.113550000
C	2.762920000	-0.724385000	-0.108262000

C	5.895071000	3.045473000	-0.252664000
C	1.987188000	7.638671000	-0.864111000
C	7.384281000	3.188782000	-0.191373000
C	2.902598000	-2.216251000	0.041834000
C	1.826479000	8.444463000	0.283168000
C	1.689983000	9.828441000	0.129252000
C	1.710785000	10.438711000	-1.128106000
C	1.867660000	9.621469000	-2.251286000
C	2.007958000	8.233381000	-2.143817000
C	8.004127000	3.816156000	0.903578000
C	9.387494000	3.951912000	0.957753000
C	10.186424000	3.463033000	-0.084757000
C	9.580489000	2.834748000	-1.181567000
C	8.195184000	2.700557000	-1.230035000
C	2.912842000	-2.801760000	1.326133000
C	3.048599000	-4.189548000	1.440310000
C	3.177515000	-5.015397000	0.319540000
C	3.158976000	-4.415346000	-0.942496000
C	3.025092000	-3.031579000	-1.103162000
C	1.592541000	11.939038000	-1.267382000
C	2.173345000	7.396558000	-3.393283000
C	1.795114000	7.836399000	1.668125000
C	2.776385000	-1.955557000	2.572785000
C	3.011689000	-2.435531000	-2.493628000
C	3.357186000	-6.508475000	0.470215000
Zn	2.444087000	2.710870000	-0.418772000
C	-2.490491000	2.225018000	-0.751707000
C	-3.363456000	2.776112000	0.198185000
C	-4.745279000	2.660231000	0.051537000
C	-5.312507000	1.988980000	-1.041247000

C	-4.437051000	1.424871000	-1.982491000
C	-3.055704000	1.542009000	-1.840364000
C	-8.859521000	0.862613000	-1.170315000
C	-6.823209000	1.926821000	-1.146599000
N	-7.456099000	0.635778000	-0.893604000
C	-6.888981000	-0.564984000	-1.505003000
C	-8.656222000	5.280564000	-8.856744000
C	-9.625859000	6.257892000	-8.385862000
C	-9.265940000	7.174034000	-7.394901000
C	-6.991526000	6.217994000	-7.293057000
C	-7.367078000	5.262157000	-8.324714000
C	-10.927044000	5.617750000	-8.345381000
C	-10.192263000	7.483507000	-6.322792000
C	-6.117727000	5.536644000	-6.350133000
C	-6.727193000	3.995231000	-8.011116000
C	-9.362958000	4.033631000	-9.103829000
C	-6.222898000	5.807300000	-4.982158000
C	-7.197250000	6.775699000	-4.511417000
C	-11.822442000	5.917344000	-7.316071000
C	-9.429046000	7.651109000	-5.100185000
C	-11.449189000	6.865648000	-6.283815000
C	-5.957069000	4.166412000	-6.794859000
C	-7.413449000	2.796540000	-8.235693000
C	-8.754820000	2.816229000	-8.796867000
C	-10.768046000	4.241913000	-8.791329000
C	-7.358495000	1.738391000	-7.249336000
C	-9.528976000	1.756417000	-8.170558000
C	-11.512810000	3.223474000	-8.196674000
C	-5.907247000	3.133741000	-5.852246000
C	-11.985284000	6.393502000	-5.020856000

C	-8.676629000	1.089415000	-7.209235000
C	-10.884153000	1.950896000	-7.882947000
C	-12.446502000	3.535409000	-7.124345000
C	-12.391956000	2.450692000	-6.155958000
C	-11.182659000	5.478474000	-2.876413000
C	-11.428351000	1.474716000	-6.626519000
C	-10.595983000	0.823974000	-5.709475000
C	-10.684487000	1.119681000	-4.291660000
C	-9.196454000	0.637813000	-6.007006000
C	-6.013703000	3.418300000	-4.434552000
C	-11.842466000	4.273416000	-3.127217000
C	-6.628090000	1.906469000	-6.083852000
C	-7.157973000	1.451035000	-4.787451000
C	-12.622752000	4.106944000	-4.343178000
C	-9.846891000	5.445351000	-2.331882000
C	-9.228353000	4.206399000	-2.056366000
C	-12.473722000	2.732995000	-4.788576000
C	-11.611339000	2.046417000	-3.844349000
C	-8.448391000	0.811556000	-4.749616000
C	-9.338075000	1.072387000	-3.718099000
C	-11.209826000	3.013703000	-2.809613000
C	-6.765748000	2.336375000	-3.791343000
C	-7.832866000	4.012047000	-2.333642000
C	-9.938024000	2.975981000	-2.266149000
C	-7.502893000	2.523021000	-2.492694000
C	-8.968027000	1.802814000	-2.454165000
C	-11.252433000	6.558651000	-3.844504000
C	-9.947552000	7.200379000	-3.885232000
C	-9.086913000	6.509927000	-2.941584000
C	-12.595986000	4.852521000	-6.693515000

C	-12.689521000	5.145017000	-5.272260000
C	-7.920992000	7.151678000	-6.838437000
C	-8.024196000	7.440422000	-5.416938000
C	-7.744072000	6.289659000	-3.255071000
C	-6.157044000	4.729065000	-4.012753000
C	-7.114859000	5.028758000	-2.936056000
C	11.657792000	3.635474000	0.021825000
O	12.231553000	4.173077000	0.948849000
O	12.332804000	3.124377000	-1.040704000
H	-1.851606000	-0.384678000	-0.324800000
H	0.216659000	-2.071852000	-0.060494000
H	-0.607385000	6.976514000	-1.080704000
H	-2.325394000	4.919221000	-1.064469000
H	6.739650000	5.810914000	-0.486109000
H	4.669979000	7.499465000	-0.717914000
H	5.506266000	-1.561720000	0.165298000
H	7.226774000	0.493821000	0.100154000
H	1.562265000	10.444497000	1.017396000
H	1.879649000	10.074222000	-3.240970000
H	7.390333000	4.190568000	1.717525000
H	9.870025000	4.430398000	1.803725000
H	10.193997000	2.459514000	-1.993245000
H	7.728555000	2.220496000	-2.085157000
H	3.053147000	-4.635423000	2.433234000
H	3.250753000	-5.039369000	-1.829503000
H	1.121010000	12.218109000	-2.215895000
H	1.000347000	12.372091000	-0.453981000
H	2.579548000	12.420531000	-1.241944000
H	2.165014000	8.026439000	-4.288239000
H	1.369559000	6.657489000	-3.492711000

H	3.117081000	6.838535000	-3.381545000
H	2.720585000	7.291765000	1.889534000
H	0.972876000	7.118887000	1.774534000
H	1.668472000	8.610625000	2.431246000
H	1.836125000	-1.391611000	2.575582000
H	2.798685000	-2.579317000	3.471793000
H	3.586395000	-1.220790000	2.651246000
H	3.116954000	-3.216082000	-3.253569000
H	3.828531000	-1.717224000	-2.631453000
H	2.078567000	-1.894823000	-2.691152000
H	2.814154000	-6.892527000	1.340764000
H	4.415121000	-6.770148000	0.607613000
H	3.002249000	-7.046419000	-0.415319000
H	-2.954858000	3.299598000	1.057697000
H	-5.396134000	3.099159000	0.803920000
H	-4.829707000	0.907043000	-2.849954000
H	-2.402203000	1.112285000	-2.594029000
H	-9.318707000	1.395550000	-0.328209000
H	-9.394016000	-0.079504000	-1.309867000
H	-7.213674000	2.590491000	-0.364471000
H	-6.893582000	-0.565821000	-2.605862000
H	-7.468168000	-1.427953000	-1.162289000
H	-5.860076000	-0.696678000	-1.163131000
H	13.275336000	3.296096000	-0.858243000