Electronic Supplementary information for

Visible light-harvesting perylenebisimide-fullerene (C_{60}) dyads with bidirectional "ping-pong" energy transfer as triplet photosensitizers for photooxidation of 1,5-dihydroxynaphthalene

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Experimental

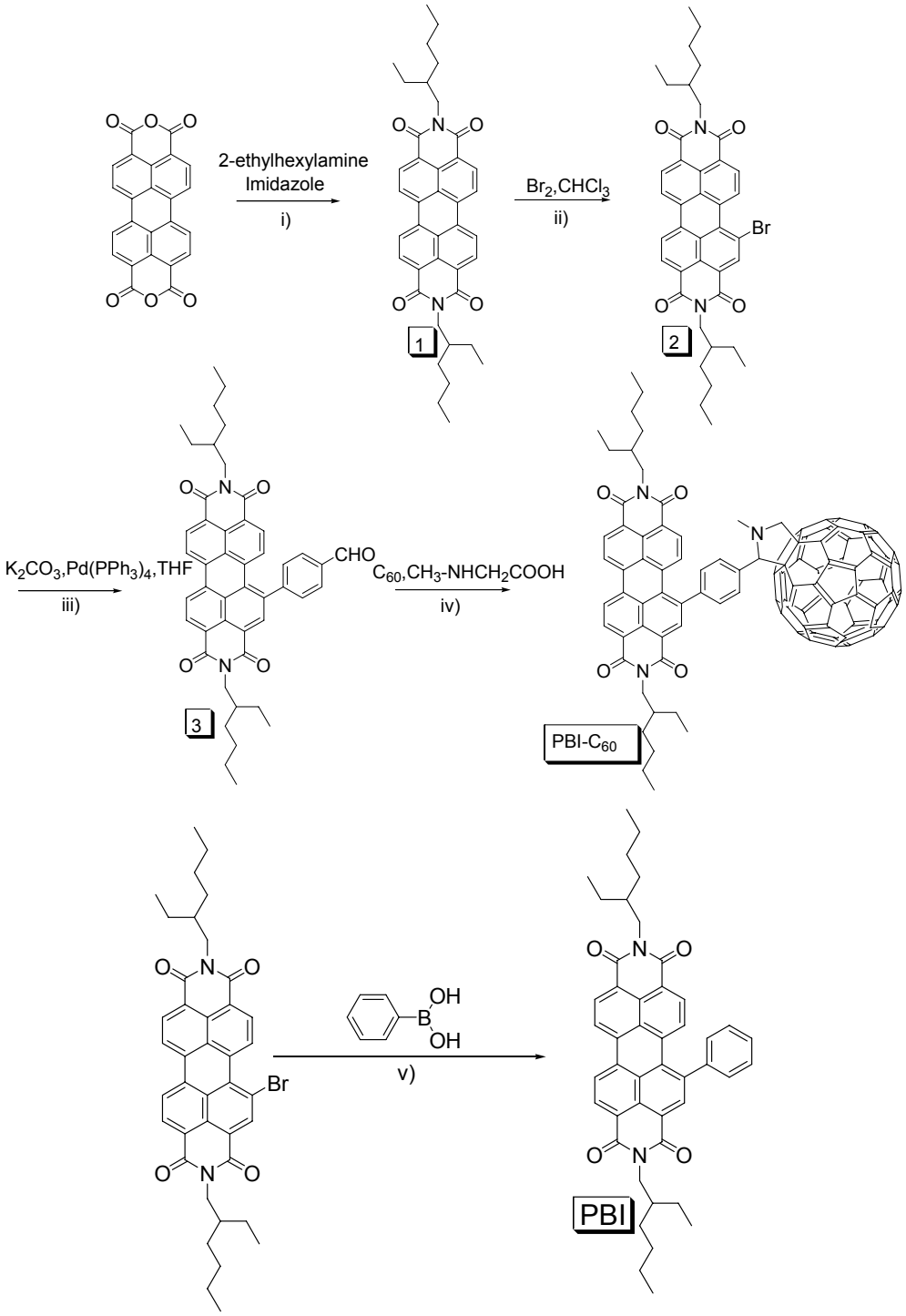
Photooxidation details:

A CH_2Cl_2 / MeOH (9:1, v/v) mixed solvent containing **DHN** (2.0×10^{-4} M) and triplet photosensitizer (10 mol % *vs.* **DHN**) was put into a two neck round bottom flask (25 mL), and O_2 was bubbled through the solution for 10 min. The solution was then irradiated using a 35 W xenon lamp through a cut off filter (0.72 M $NaNO_2$ aqueous solution, which is transparent for light with wavelength $\lambda > 385$ nm). UV-vis absorption spectra were recorded at intervals of 2–5 min. The **DHN** consumption was monitored by the decrease of the UV absorption at 301 nm, and the concentration of **DHN** was calculated based on its molar extinction coefficient ($\varepsilon = 7664$ M^{-1} cm^{-1}). On the other hand, the Juglone production was monitored by an increase in the absorption at 427 nm. The concentration of Juglone was calculated by using its molar extinction coefficient ($\varepsilon = 3811$ M^{-1} cm^{-1} at 427 nm), and the yield of Juglone was obtained by dividing the concentration of Juglone with the initial concentration of **DHN**.[2] The photostability experiments were carried out using the same method except without the substrate DHN (for the sensitizers).

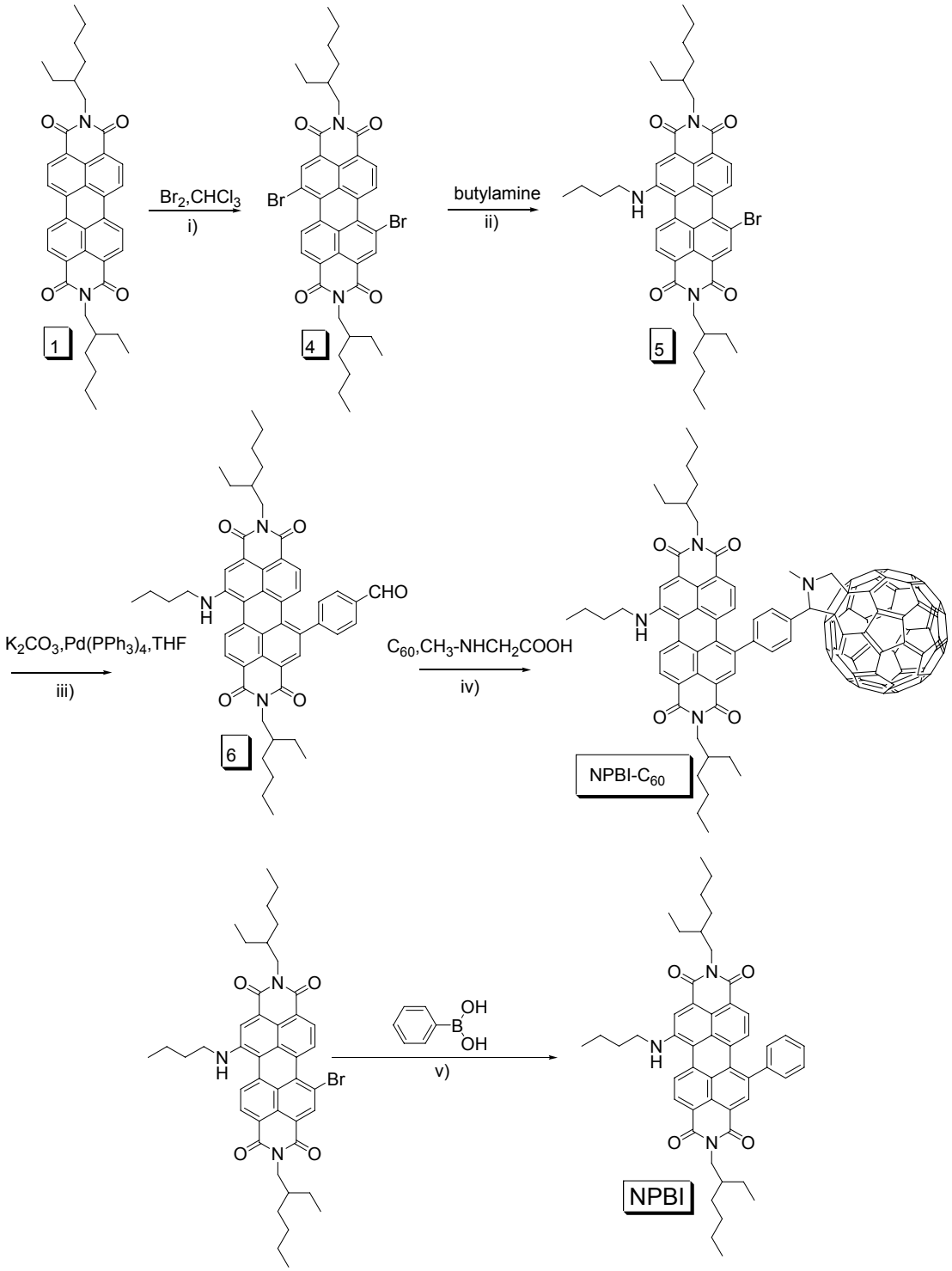
DFT calculations.

The density functional theory (DFT) calculations were used for optimization of the triplet states. The spin density surfaces of the complexes were calculated based on the optimized triplet state geometries. All the calculations were performed with Gaussian 09W.

Synthesis details



Scheme 1. *To be continued on the next page.*



Scheme 1. *As continued from the previous page.* Synthesis route of target molecules **PBI-C_{60} /PBI**. i) 2-ethylhexylamine, imidazole, argon atmosphere, 160 °C, 6 h, 77 %; ii) chloroform, room temperature, 48 h, 22 % iii) Na_2CO_3, 2-methoxyethanol/ water (3/1, v/v), $Pd(PPh_3)_4$, 100 °C, 8 h, 72 % iv) creatine, C_{60}, toluene, reflux, 20 h, 12% v) Na_2CO_3, 2-methoxyethanol/ water (3/1, v/v), $Pd(PPh_3)_4$, 100 °C, 8 h, 41%; Synthesis route of target molecules **NPBI-C_{60}/NPBI**. i) chloroform, 60 °C, 48h, 27 % ii) n-butylamine, room temperature, 8 h, 71 % iii) Na_2CO_3, 2-methoxyethanol/ water (3/1, v/v), $Pd(PPh_3)_4$, 100 °C, 8h, 40 % iv) creatine, C_{60}, toluene, reflux, 20 h, 12 % v) Na_2CO_3, 2-methoxyethanol/ water (3/1, v/v), $Pd(PPh_3)_4$, 100 °C, 8 h, 35 %.

Synthesis Procedures:

N,N'-Di-(2-ethylhexan-1-amine)-perylene-3,4,9,10-tetracarboxydianhydride (1)

The mixture of 3,4,9,10-perylenetetracarboxylic dianhydride (2.0 g, 5.1 mmol), imidazole (10.0 g, 146.9 mmol), and 2-ethylhexylamine (3.8 mL, 21.0 mmol) was stirred under argon atmosphere at 160 °C for 6 h. The mixture was cooled and chloroform was added. The organic layer was washed with water and dried over anhydrous Na_2SO_4. The solvent was removed and the residue was purified with column chromatography (silica gel; chloroform) to give 2.4 g (yield: 77 %) of red solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.63 (d, 2H, J = 8.0 Hz), 8.53 (d, 2H, J = 8.0 Hz), 4.09–4.19 (m, 2H), 1.95–1.98 (m, 1H), 1.39–1.42 (m, 8H), 0.98 (t, 3H, J = 7.2 Hz), 0.91 (t, 3H, J = 6.8 Hz). MS (MALDI) calcd for $C_{40}H_{42}N_2O_4$ [M^-]: 614.31, found: 614.50.

N,N'-Di-(2-ethylhexan-1-amine)-1-bromoperylene-3,4,9,10-tetracarboxydianhydride (2)

The mixture of *N,N'*-di-(2-ethylhexan-1-amine)-perylene-3,4,9,10-tetracarboxydianhydride (2.0 g, 3.3 mmol), bromine (9.0 mL, 180.0 mmol), and chloroform (50 mL) was stirred at room temperature for 48 h. The mixture was washed with Na_2SO_3 saturated solution, the organic layer was dried over anhydrous Na_2SO_4 and then removed the solution. The residue was purified with column chromatography (silica gel; dichloromethane) to give 500 mg (yield: 22 %) of red solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.73 (d, 1H, J = 8.0 Hz), 8.84 (s, 1H), 8.64 (d, 3H, J = 7.2 Hz), 8.52 (d, 2H, J = 7.6 Hz), 4.07–4.20 (m, 4H), 1.94–1.97 (m, 2H), 1.32–1.42 (m, 16H), 0.90–0.97 (m, 12H). MS (MALDI) [M^-]calcd for $C_{40}H_{41}BrN_2O_4$: 692.22; found : 692.45.

N,N'-Di-(2-ethylhexan-1-amine)-[1-(4-aldehyde-phenyl)perylene]-3,4,9,10-tetracarboxydianhydride (3)

The mixture of compound 2 (200 mg, 0.29 mmol), Na_2CO_3 (100 mg, 0.94 mmol), 4-formylphenylboronic acid (90 mg, 0.60 mmol), $Pd(PPh_3)_4$ (20 mg, 0.08mmol), 2-methoxyethanol (6 mL) and water (2 mL) was stirred under argon atmosphere at 100 °C for 8 h. After cooled to room temperature, the solvent was removed and the residue was purified with column chromatography (silica gel; dichloromethane) to give 150 mg (yield: 72 %) of red solid. ^{1}H NMR (400 MHz, $CDCl_3$) 10.15 (s, 1H), 8.62–8.75 (m, 4H), 8.57 (s, 1H), 8.15 (d, 1H, J = 8.0 Hz), 8.07 (d, 2H, J = 8.0 Hz), 7.78 (d, 1H, J = 8.0 Hz), 7.71 (d, 2H, J = 8.0 Hz), 4.07–4.19 (m, 4H), 1.91–1.98 (m, 2H), 1.30–1.42 (m, 16H), 0.88–0.97 (m, 12H). ESI-HRMS ($[C_{47}H_{46}N_2O_5]^+$): calcd 718.3407, found 718.3411.

PBI-C_{60}

The mixture of compound **3** (50 mg, 0.07 mmol), creatine (21 mg, 0.25mmol), C_{60} (50 mg, 0.07 mmol) and toluene (50 mL) was reflux under argon atmosphere at 120 °C for 20 h. After removal of solvent in vacuum, the residue was purified with column chromatography (silica gel; dichloromethane/methanol, 100/1, v/v) to give 12mg (yield:12 %) of reddish brown solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.89 (s,1H), 8.40 (s,1H), 8.15 (d, 1H, J = 7.6 Hz), 7.76–7.79 (m, 2H), 7.49–7.53 (m, 1H), 7.42–7.46 (m, 3H), 7.28 (t, 1H J = 7.6 Hz), 4.33 (t, 2H, J = 7.2 Hz) 1.84–1.91 (m, 2H), 1.36–1.46 (m, 2H), 0.96 (t, 3H, J = 7.2 Hz). ESI-HRMS ($[C_{109}H_{51}N_3O_4]^+$): calcd 1465.3880, found 1465.3824.

PBI

The mixture of compound **2** (50 mg, 0.07 mmol), Na_2CO_3 (25 mg, 0.24mmol), phenylboronic acid (18 mg, 0.15 mmol), $Pd(PPh_3)_4$ (15 mg, 0.07 mmol), 2-methoxyethanol (6 mL) and water (2 mL) was stirred under argon atmosphere at 100 °C for 8 h. After cooled to room temperature, the solvent was removed and the residue was purified with column chromatography (silica gel; dichloromethane) to give 20 mg (yield: 41 %) of red solid. ^{1}H NMR (400 MHz,

$CDCl_3$) 8.58–8.70 (m, 5H), 8.13 (d, 1H, *J* = 8.0 Hz), 7.84 (d, 1H, *J* = 8.0 Hz), 7.47–7.53 (m, 5H), 4.08–4.17 (m, 4H), 1.92–1.97 (m, 2H), 1.30–1.41 (m, 16H), 0.88–0.95 (m, 12H). ^{13}C NMR (100 MHz, $CDCl_3/CD_3OD$) δ 163.9, 163.8, 142.6, 141.8, 136.2, 134.8, 134.7, 134.4, 132.5, 131.1, 130.9, 130.5, 130.2, 128.9, 128.8, 128.5, 128.3, 128.0, 127.5, 123.5, 123.3, 123.2, 122.7, 122.3, 44.5, 38.1, 30.9, 28.8, 24.2, 23.2, 14.3, 10.8. ESI-HRMS ($[C_{46}H_{46}N_2O_4 + H]^+$): calcd 691.3536, found 691.3501.

N,N'-Di-(2-ethylhexan-1-amine)-1,7-dibromoperylene-3,4,9,10-tetracarboxydianhydride (4)

The mixture of *N,N'*-di-(2-ethylhexan-1-amine)-perylene-3,4,9,10-tetracarboxydianhydride (2.0 g, 3.3 mmol), bromine (9.0 mL, 180.0 mmol), and chloroform (50 mL) was stirred at 60 °C for 48 h. The mixture was washed with Na_2SO_3 saturated solution, the organic layer was dried over anhydrous Na_2SO_4 and then removed the solution. The residue was purified with column chromatography (silica gel; dichloromethane) to give 685 mg (yield: 27 %) of red solid. ^{1}H NMR (400 M Hz, $CDCl_3$) δ 9.50 (d, 2H, *J* = 8.0 Hz), 8.93 (s, 1H), 8.71 (d, 2H, *J* = 8.4 Hz), 4.12–4.19 (m, 4H), 1.94–1.97 (m, 2H), 1.32–1.42 (m, 16H), 0.90–0.97 (m, 12H). MS (MALDI) [M^-](calcd for $C_{40}H_{40}Br_2N_2O_4$: 770.14; found: 770.11.

N,N'-Di-(2-ethylhexan-1-amine)-1-bromo-7-butylamino-perylene-3,4,9,10-tetracarboxydianhydride (5)

N,N'-Di-(2-ethylhexan-1-amine)-1,7-dibromoperylene-3,4,9,10-tetracarboxydianhydride (500 mg, 0.65 mmol) and n-butylamine (10 mL) was stirred at room temperature for 8 h, under argon. After remove the solution, the residue was purified with column chromatography (silica gel; dichloromethane) to give 352 mg (yield: 71%) of green solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.19 (d, 1H, *J* = 8.0 Hz), δ 8.79 (d, 1H, *J* = 8.4 Hz), 8.54 (s, 1H), 8.47 (d, 1H, *J* = 8.0 Hz), 8.29 (d, 1H, *J* = 8.4 Hz), 8.19 (s, 1H), 4.05–4.14 (m, 4H), 3.53 (t, 2H, *J* = 7.2 Hz), 1.84–1.93 (m, 4H), 1.32–1.40 (m, 18H), 0.89–0.98 (m, 15H). MS (MALDI) [M^-](calcd for $C_{44}H_{50}BrN_3O_4$: 763.2985; found: 763.3382

N,N'-Di-(2-ethylhexan-1-amine)-[1-(4-aldehyde-phenyl)-7-butylamino-perylene]-3,4,9,10-tetracarboxydianhydride (6)

The mixture of compound **5** (200 mg, 0.26 mmol), Na_2CO_3 (100 mg, 0.94 mmol), 4-formylphenylboronic acid (90 mg, 0.60 mmol), $Pd(PPh_3)_4$ (20 mg, 0.08 mmol), 2-methoxyethanol (6 mL) and water (2 mL) was stirred under argon atmosphere at 100 °C for 8 h. After cooled to room temperature, the solvent was removed and the residue was purified with column chromatography (silica gel; dichloromethane) to give 83 mg (yield: 40 %) of green solid. ^{1}H NMR (400 MHz, $CDCl_3$) 10.09 (s, 1H), δ 8.89 (d, 1H, *J* = 8.4 Hz), 8.62 (d, 1H, *J* = 8.0 Hz), 8.56 (d, 1H, *J* = 6.4 Hz), 8.23 (s, 1H), 7.96 (d, 2H, *J* = 8.4 Hz), 7.88 (d, 1H, *J* = 8.4 Hz), 7.61–7.66 (m, 3H), 4.07–4.17 (m, 4H), 3.56 (t, 2H, *J* = 7.2 Hz), 1.82–1.96 (m, 4H), 1.31–1.41 (m, 18H), 0.89–0.94 (m, 15H). ESI-HRMS ($[C_{51}H_{56}N_3O_5]^+$): calcd 790.4220, found 790.4241.

NPBI-C_{60}

The mixture of compound 6 (50mg, 0.06 mmol), creatine (21mg, 0.25mmol), C_{60} (50mg, 0.07mmol) and 50ml toluene was reflux under argon atmosphere at 120℃ for 20h. After removal of solvent in vacuum, the residue was purified with column chromatography (silica gel; dichloromethane/methanol, 100/1, v/v) to give 11mg (yield:12 %) of blackish green solid. 1H NMR (400 M Hz, $CDCl_3$) 8.85 (d, 1H, *J* = 8.0 Hz), 8.59 (d, 2H, *J* = 8.0 Hz), 8.17 (s, 1H), 7.49–7.56 (m, 6 H), 5.0 (s, 1H), 4.31 (d, 1H, *J* = 8.8 Hz), 4.12–4.18 (m, 4H), 3.49 (s, 2H), 2.85 (s, 2H), 1.77–1.81 (m, 4H), 1.32–1.40 (m, 18H), 0.89-0.96 (m, 15H). ESI-HRMS ($[C_{113}H_{60}N_4O_4]^-$): calcd 1536.4615, found 1536.4718.

NPBI

The mixture of compound 5 (50mg, 0.07 mmol), Na_2CO_3 (25mg, 0.24mmol), phenylboronic acid (18mg, 0.15mmol),

$Pd(PPh_3)_4$ (15mg, 0.07mmol), 2-methoxyethanol (6ml) and water (2ml) was stirred under argon atmosphere at 100 °C for 8 h. After cooled to room temperature, the solvent was removed and the residue was purified with column chromatography (silica gel; dichloromethane) to give 18 mg (yield: 35 %) of green solid. 1H NMR (400 M Hz, $CDCl_3$) 8.71 (d, 1H, *J* = 8.0 Hz), 8.40 (d, 1H, *J* = 8.0 Hz), 8.20 (s, 1H), 7.97 (s, 1H), 7.68 (d, 1H, *J* = 8.0 Hz), 7.43 (d, 1H, *J*=8.0 Hz), 7.13–7.23 (m, 5H), 4.02–4.11 (m, 4H), 3.47 (t, 2H, *J* = 6.8 Hz), 1.85-1.90 (m, 4H), 1.32–1.37 (m, 18H), 0.89–0.95 (m, 15H). ESI-HRMS ($[C_{50}H_{55}N_3O_4 + H]^+$): calcd 762.4271, found 762.4211.

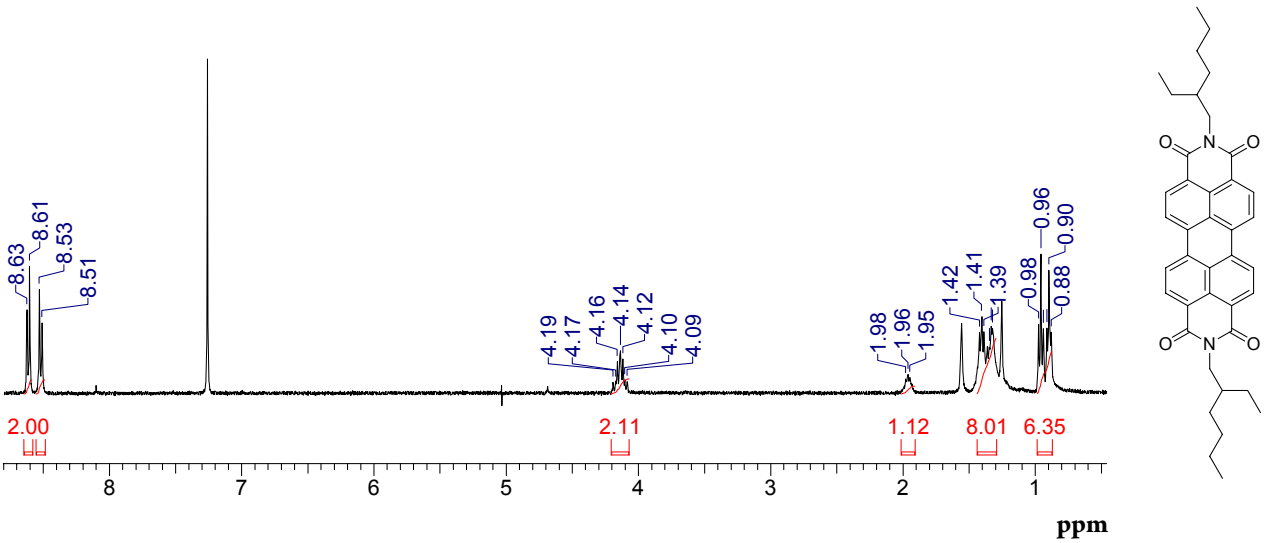


Figure S1. ^1H NMR of **1** ($CDCl_3$, 400 MHz).

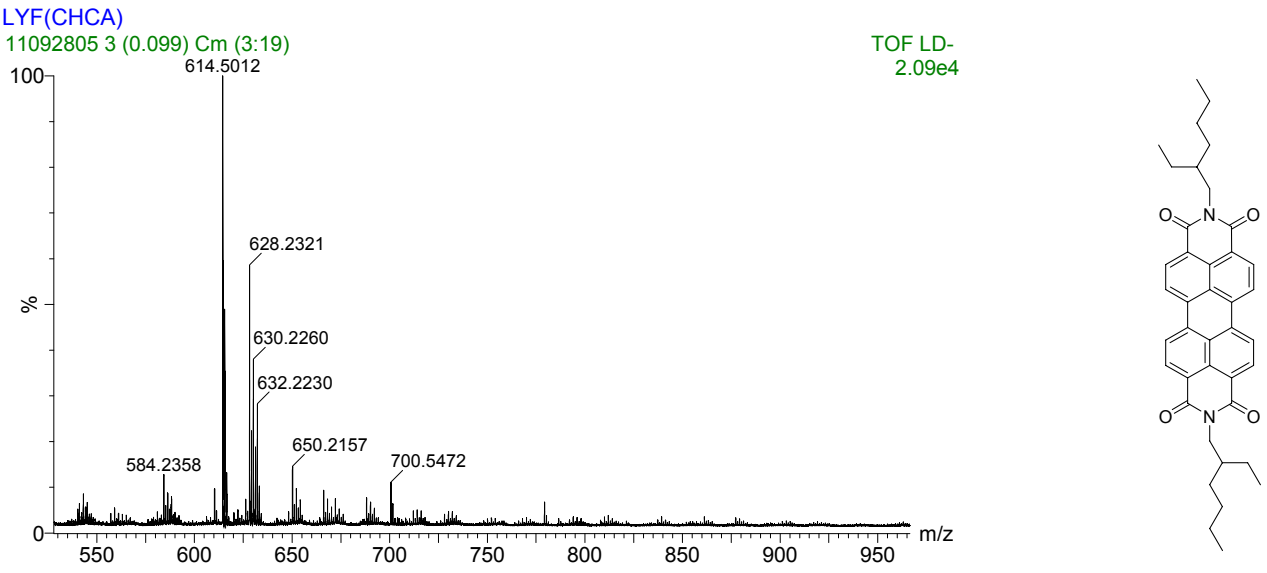


Figure S2. MS of **1** ($CHCl_3$).

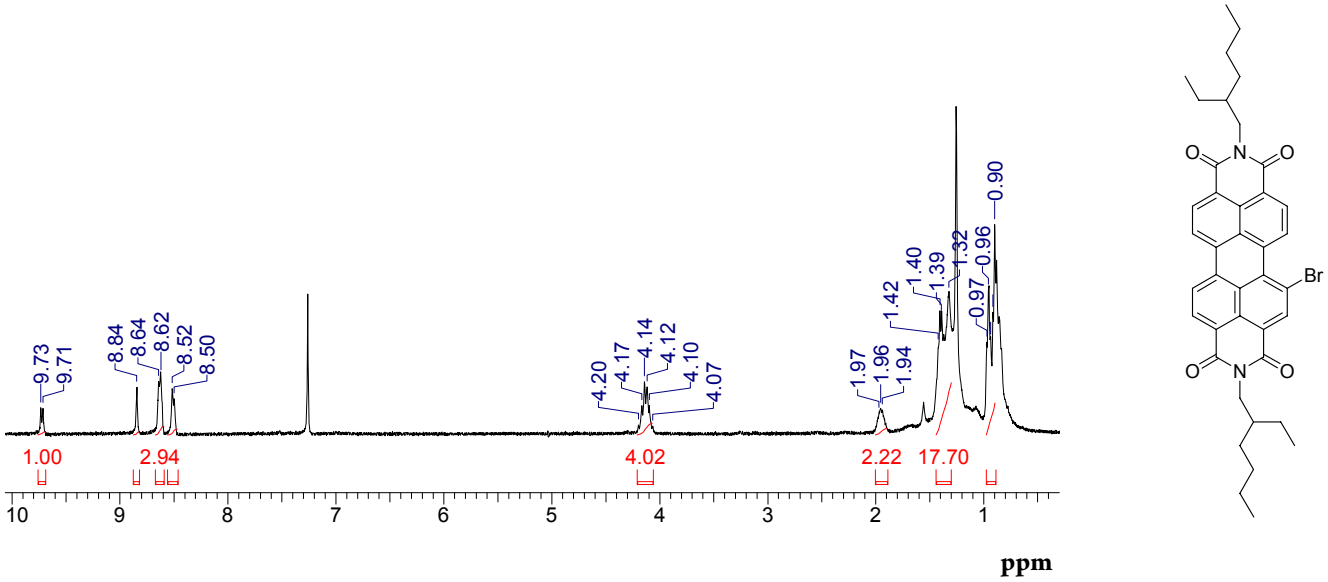


Figure S3. ^{1}H NMR of **2** ($CDCl_3$, 400 MHz).

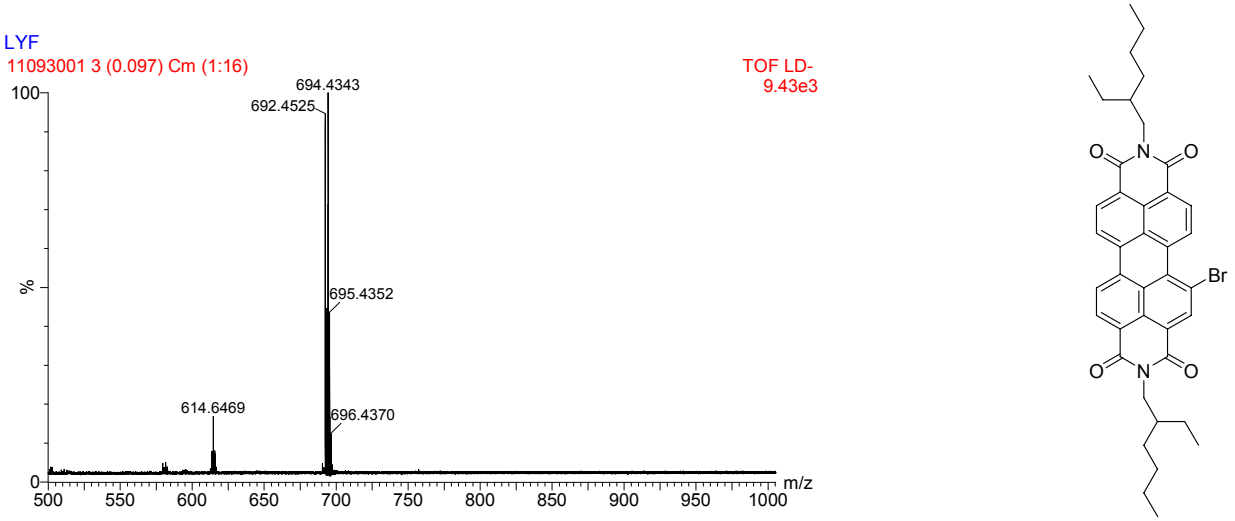


Figure S4. MS of **2** (CH_2Cl_2).

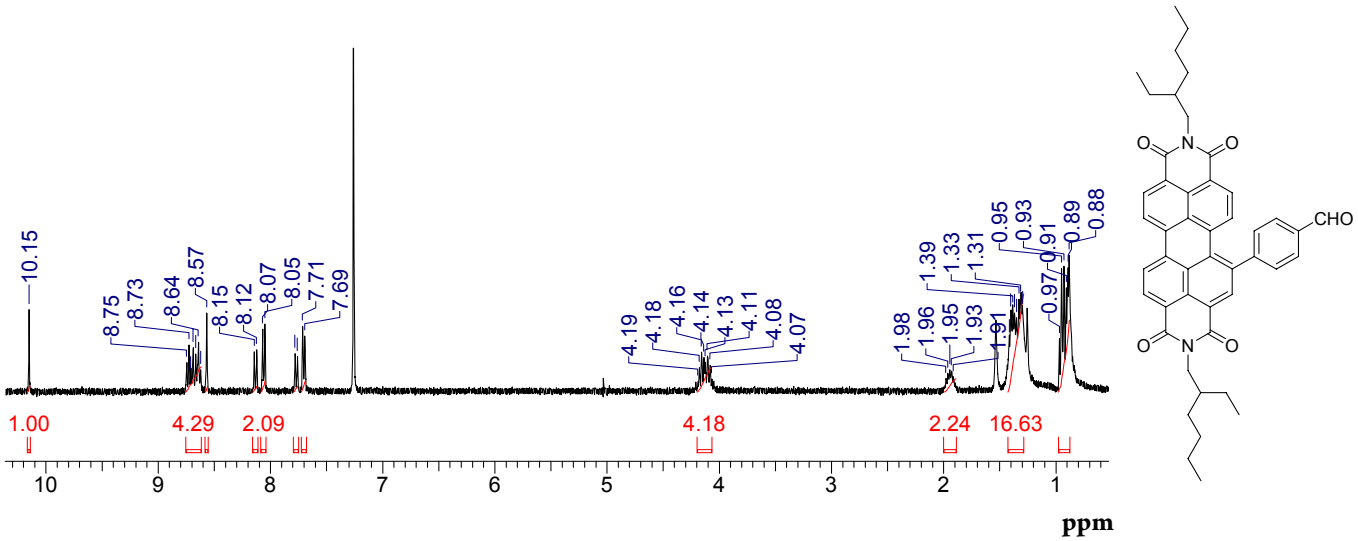
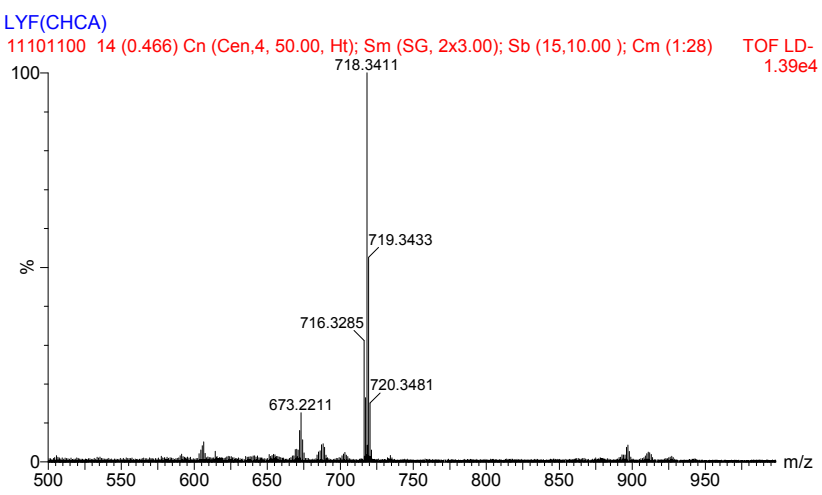


Figure S5. ^{1}H NMR of **3** ($CDCl_3$, 400 MHz).



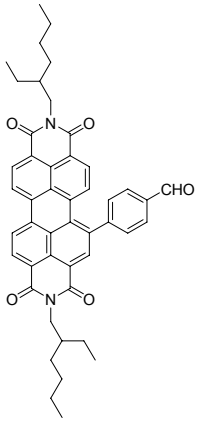


Figure S6. TOF HRMS (ESI) of **3**.

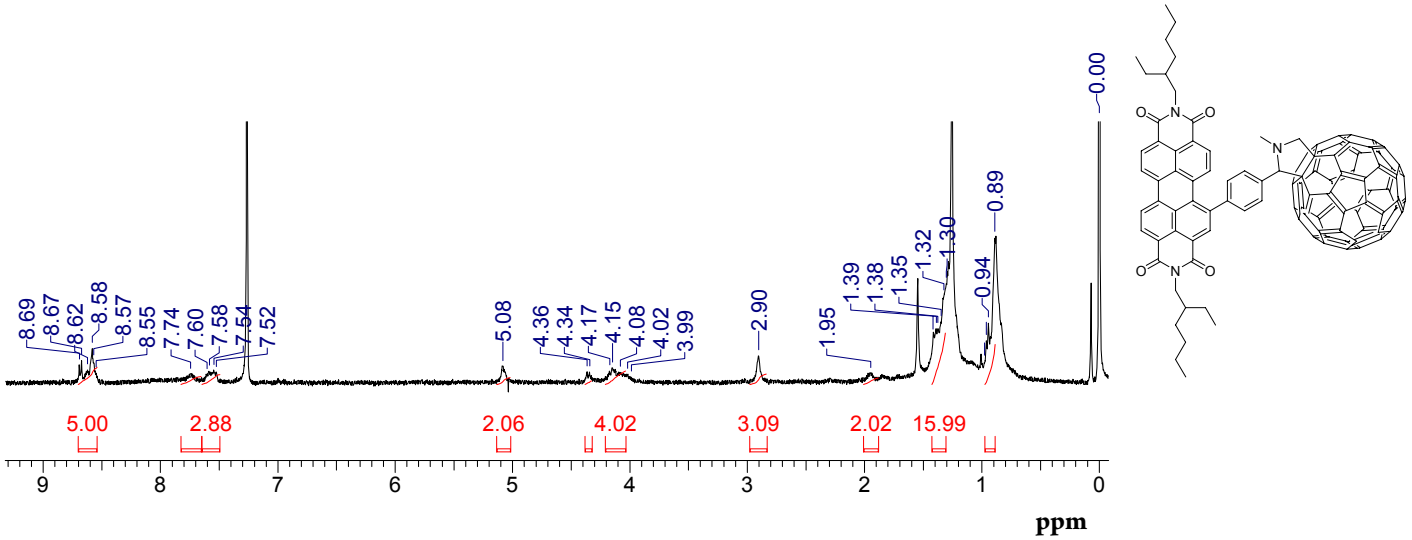
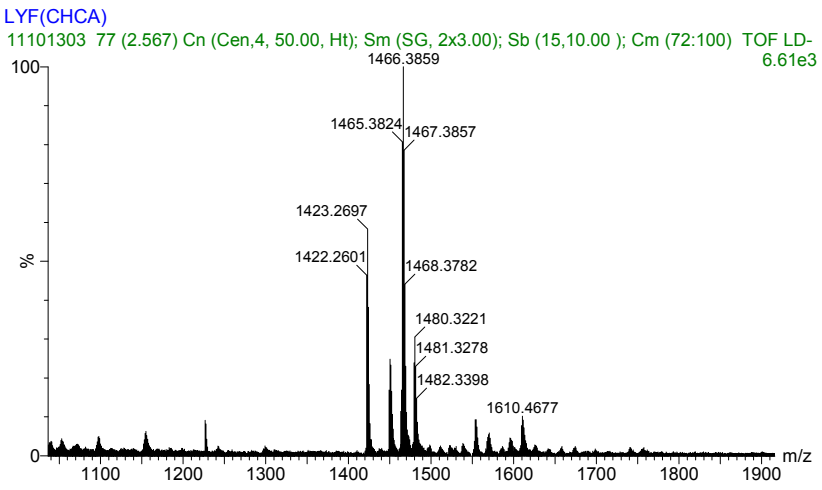


Figure S7. ^{1}H NMR of **PBI-C$_{60}$** ($CDCl_3$, 400 MHz).



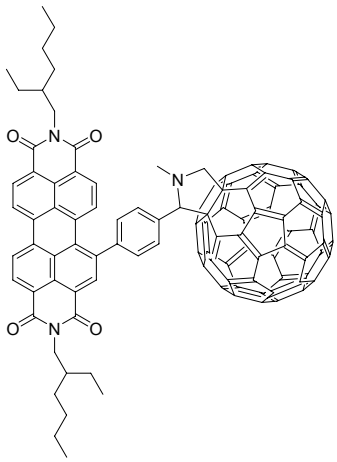


Figure S8. TOF HRMS (ESI) of **PBI-C$_{60}$**.

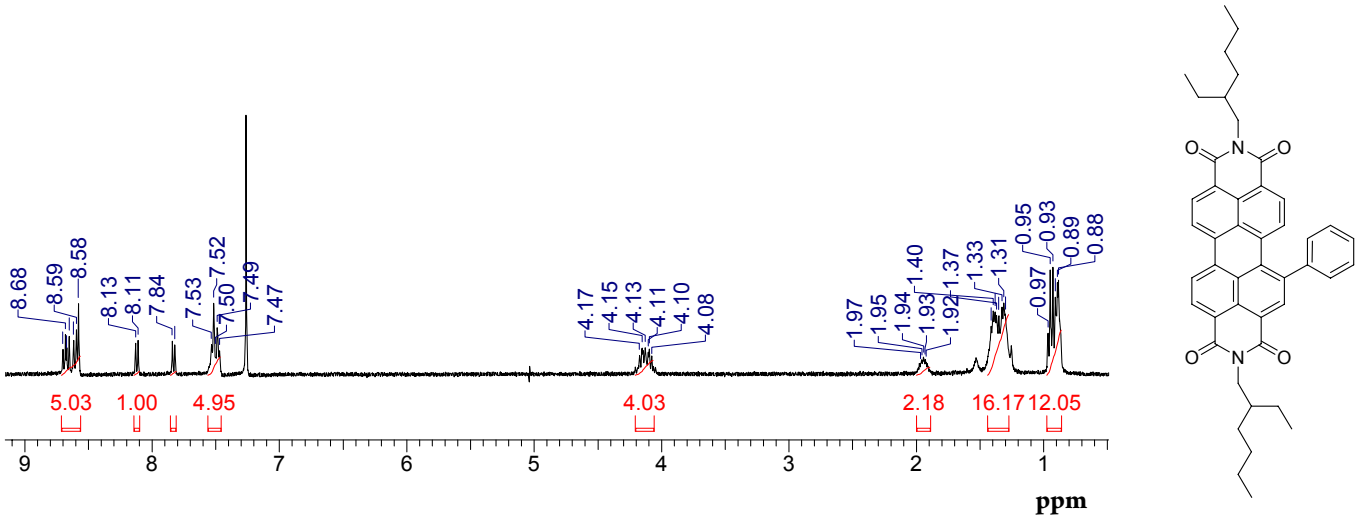


Figure S9. ^{1}H NMR of **PBI** ($CDCl_3$, 400 MHz).

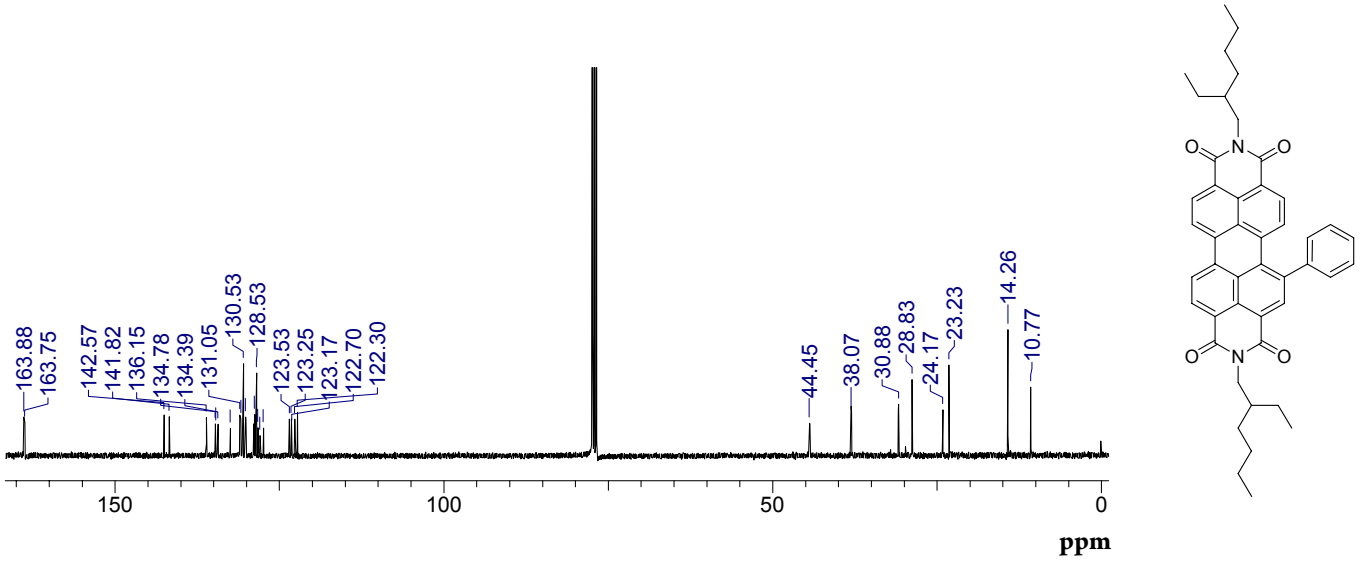


Figure S10. ^{13}C NMR of **PBI** ($CDCl_3$, 100 MHz).

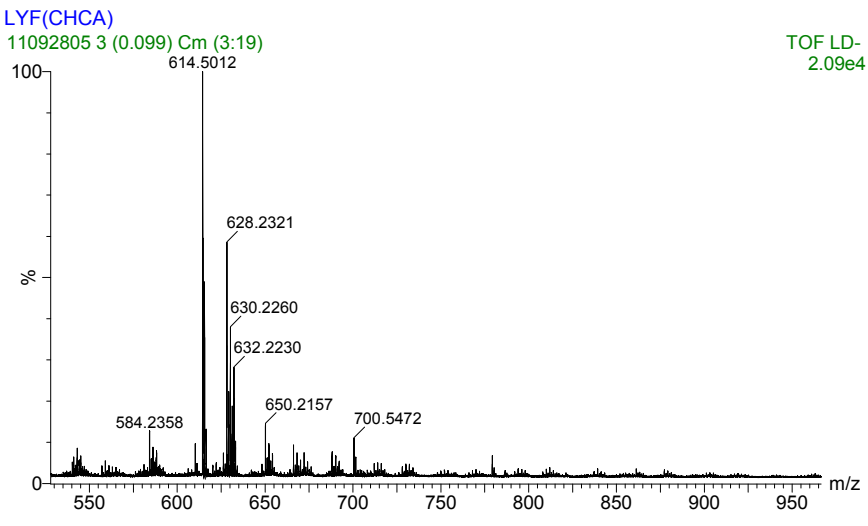


Figure S11. TOF HRMS (ESI) of **PBI**.

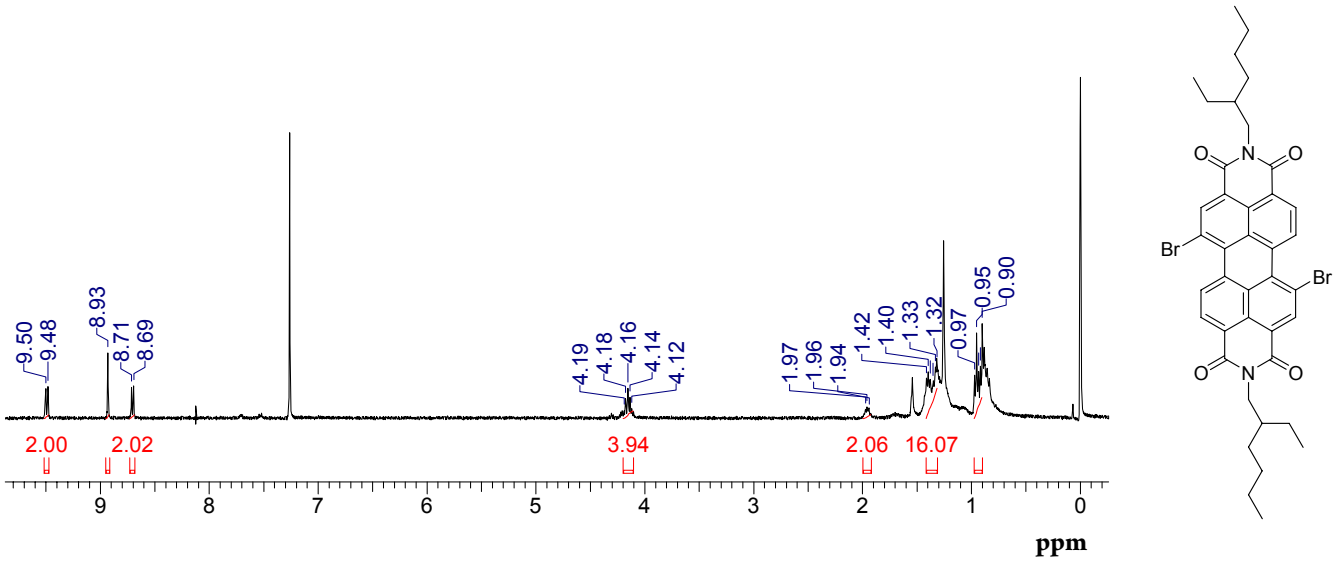


Figure S12. ^{1}H NMR of **4** ($CDCl_3$, 400 MHz).

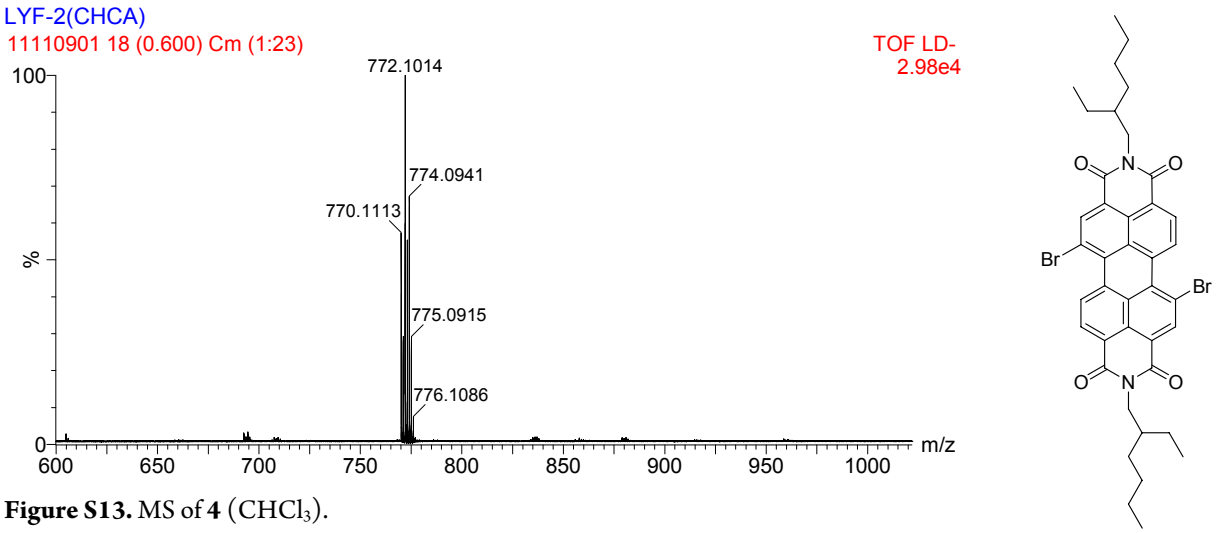


Figure S13. MS of **4** ($CHCl_3$).

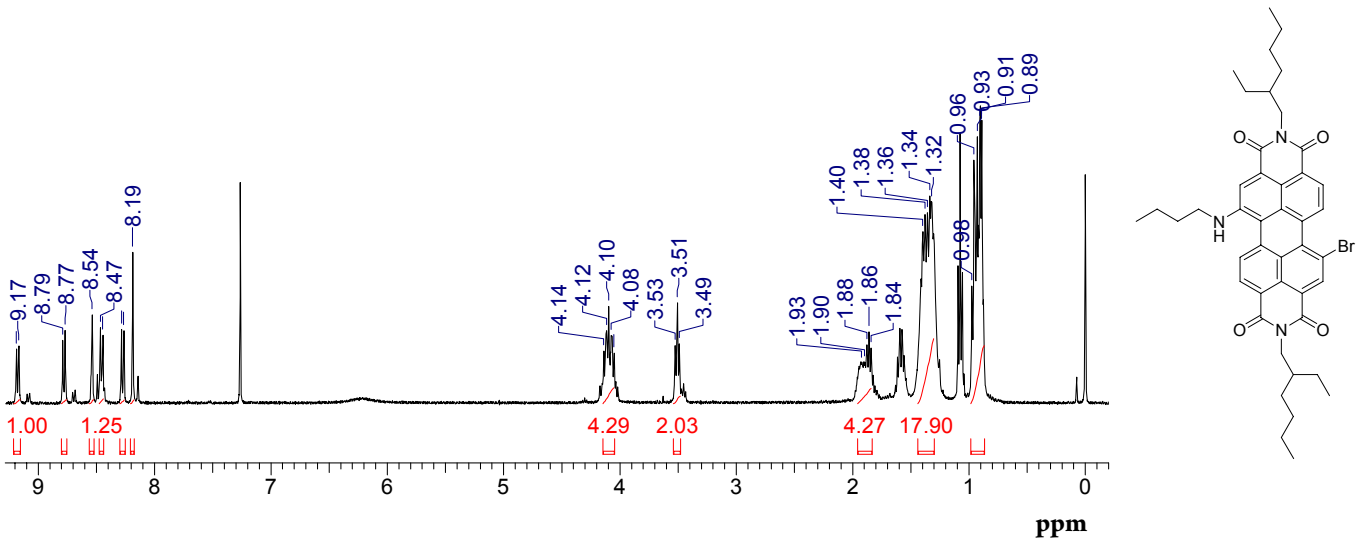


Figure S14. ^{1}H NMR of **5** ($CDCl_3$, 400 MHz).

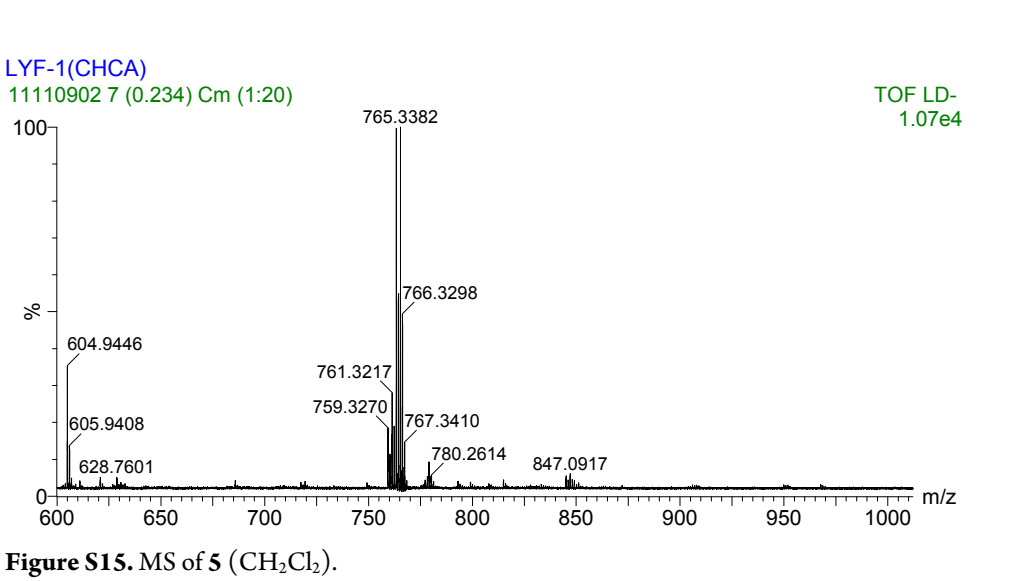


Figure S15. MS of **5** (CH_2Cl_2).

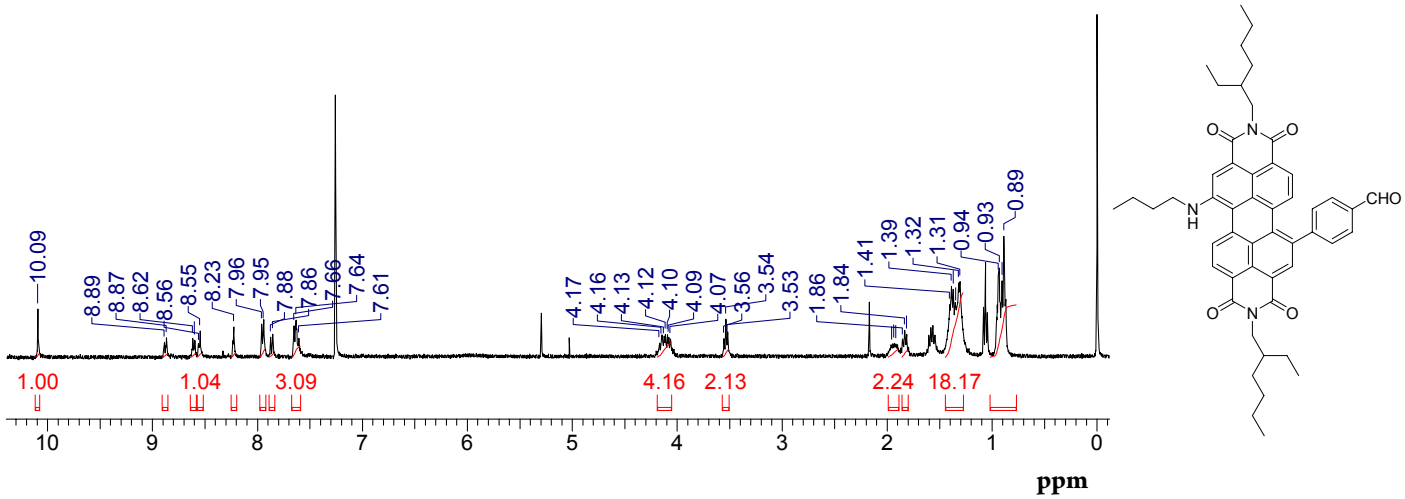


Figure S16. ^{1}H NMR of **6** ($CDCl_3$, 400 MHz).

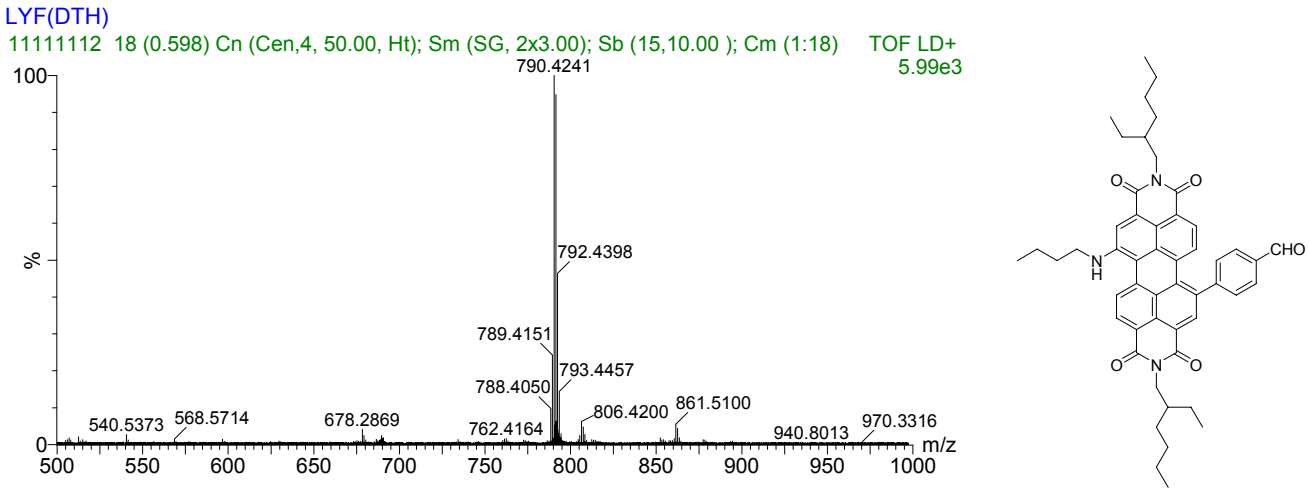


Figure S17. TOF HRMS (ESI) of **6**.

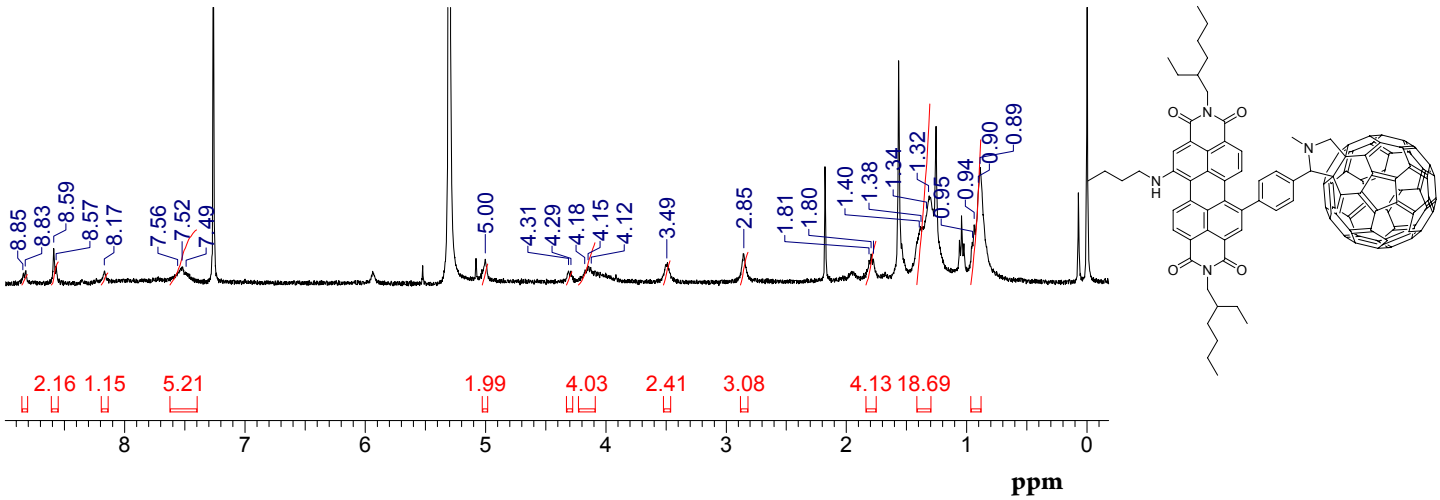


Figure S18. ^{1}H NMR of **NPBI-C$_{60}$** ($CDCl_3$, 400 MHz).

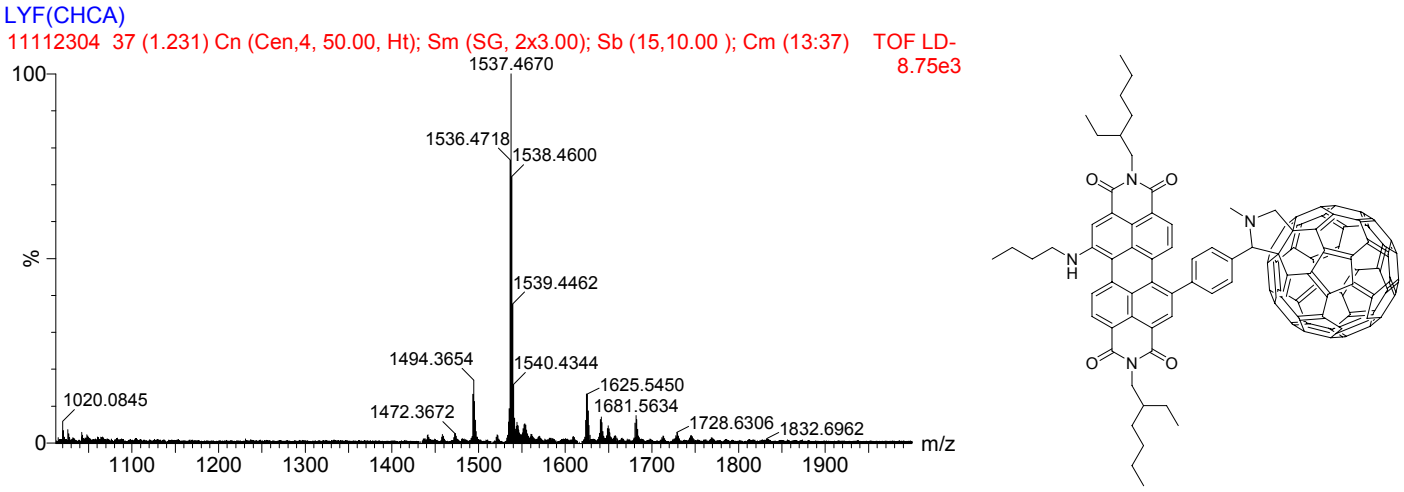


Figure S19. TOF HRMS (ESI) of **NPBI-C$_{60}$**.

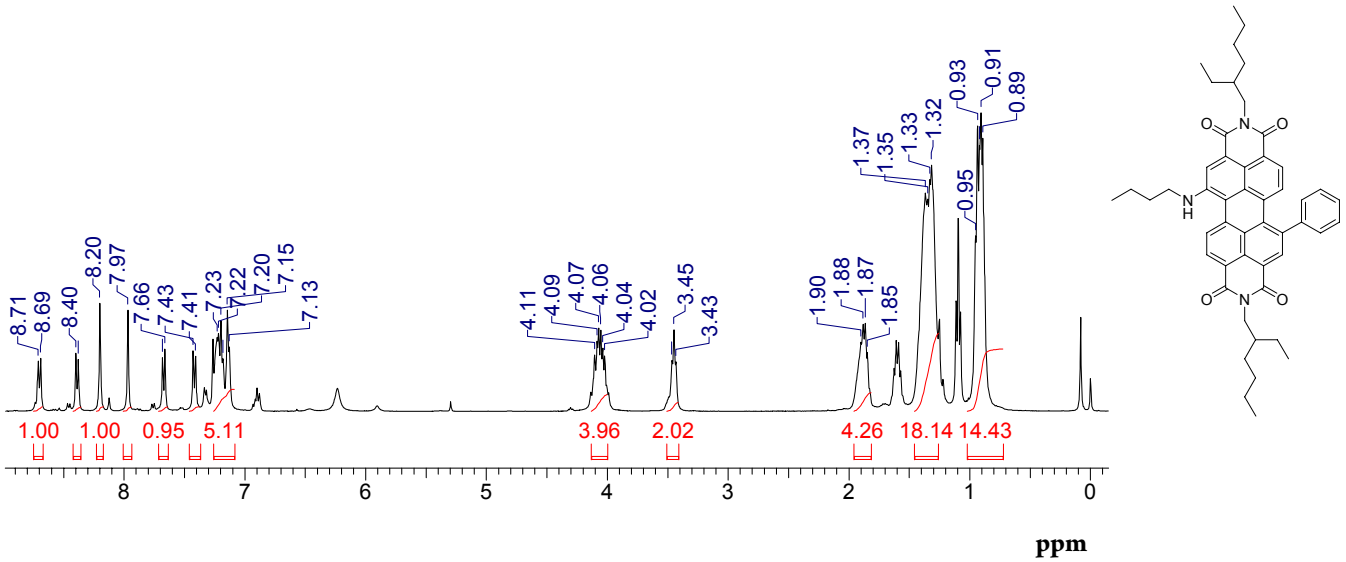


Figure S20. ^{1}H NMR of **NPBI** ($CDCl_3$, 400 MHz).

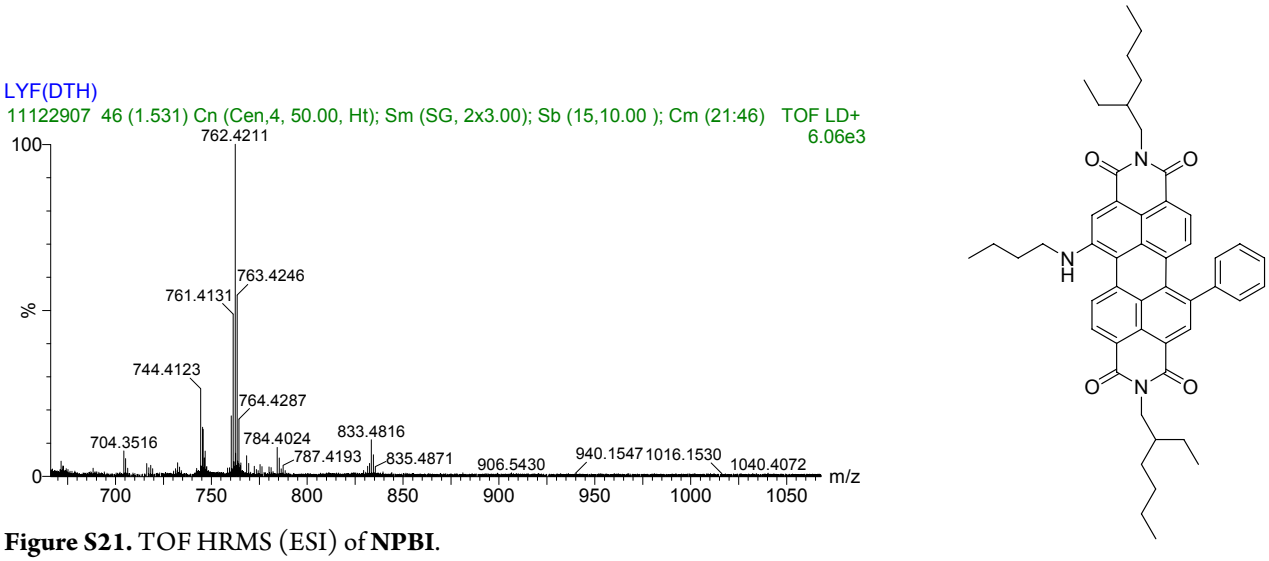


Figure S21. TOF HRMS (ESI) of **NPBI**.

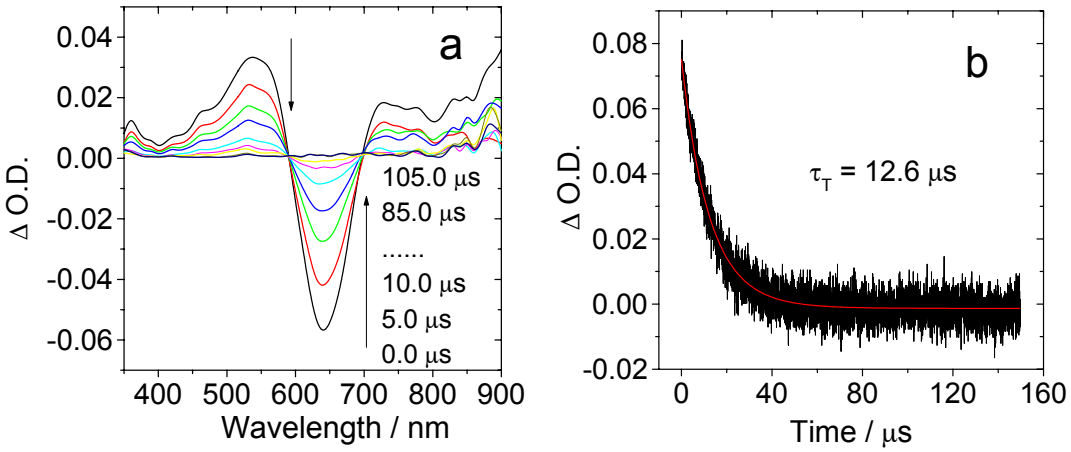


Figure S22. Transient absorption difference spectra of **NPBI-C_{60}** in deaerated toluene at room temperature after pulsed excitation (λ_{ex} = 532 nm). (a) Transient absorption at different delay times.(b)Decay trace at 640 nm, triplet excited state life (τ_T) is 12.6 μs. 20 °C.

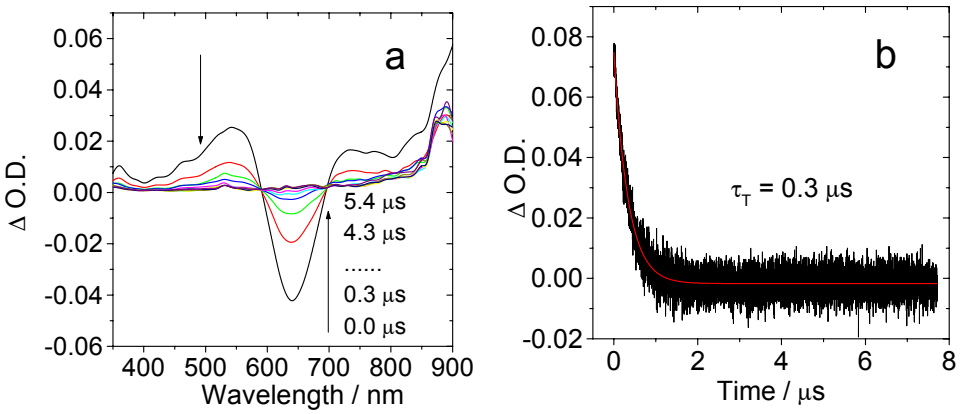


Figure S23. Transient absorption difference spectra of **NPBI-C_{60}** in toluene under air atmosphere at room temperature after pulsed excitation (λ_{ex} = 532 nm). (a)Transient absorption at different delay times. (b) Decay trace at 640 nm, triplet excited state life (τ_T) is 0.3 μs. 20 °.

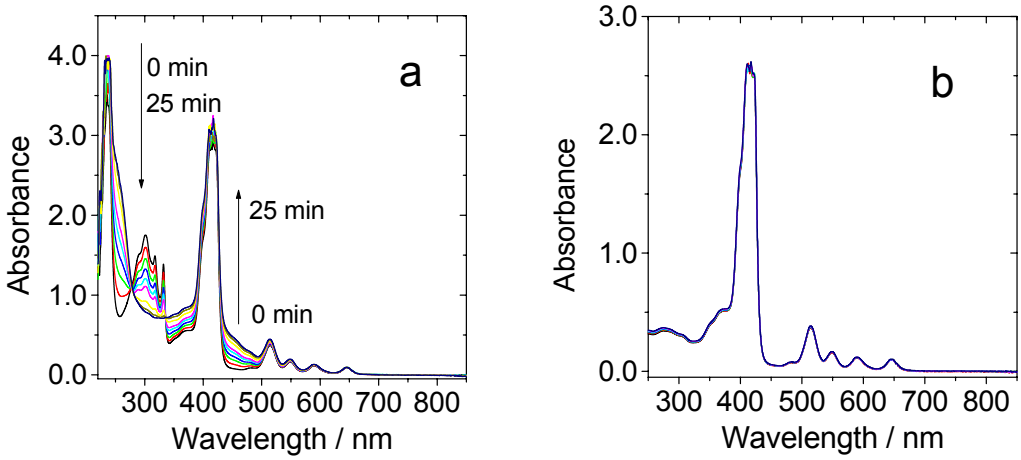


Figure S24. (a) Absorption spectral change for the photooxidation of DHN using **TPP** as sensitizer. c [TPP] = 2.0×10^{-5} mol L^{-1}, c [DHN] = 2.0×10^{-4} mol L^{-1}. (b) The stability of **TPP** was studied with continuous illumination for 1 hour at the same condition without **DPA**.

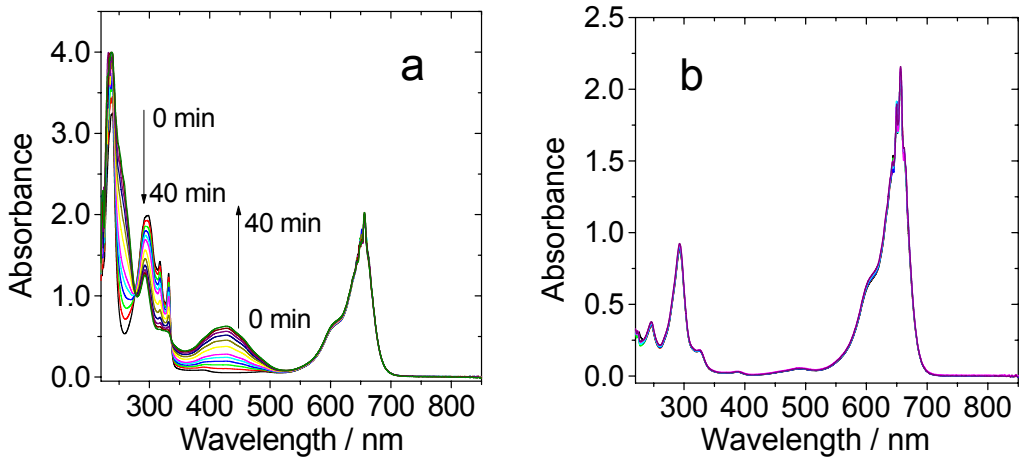


Figure S25. (a) Absorption spectral change for the photooxidation of DHN using **MB** as sensitizer. c [MB] = 2.0×10^{-5} mol L^{-1}, c [DHN] = 2.0×10^{-4} mol L^{-1}. (b) The stability of **MB** was studied with continuous illumination for 1 hour at the same condition without **DPA**.

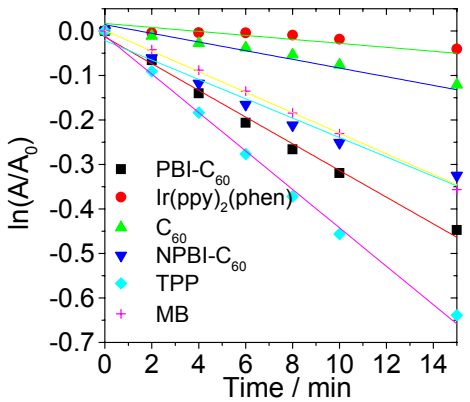


Figure S26. Plots of $\ln(A/A_0)$ *vs.* irradiation time (t) for the photooxidation of DHN using **PBI-C_{60}, NPBI-C_{60}, C_{60}, Ir(ppy)$_2$(phen), TPP** and **MB** as sensitizers.

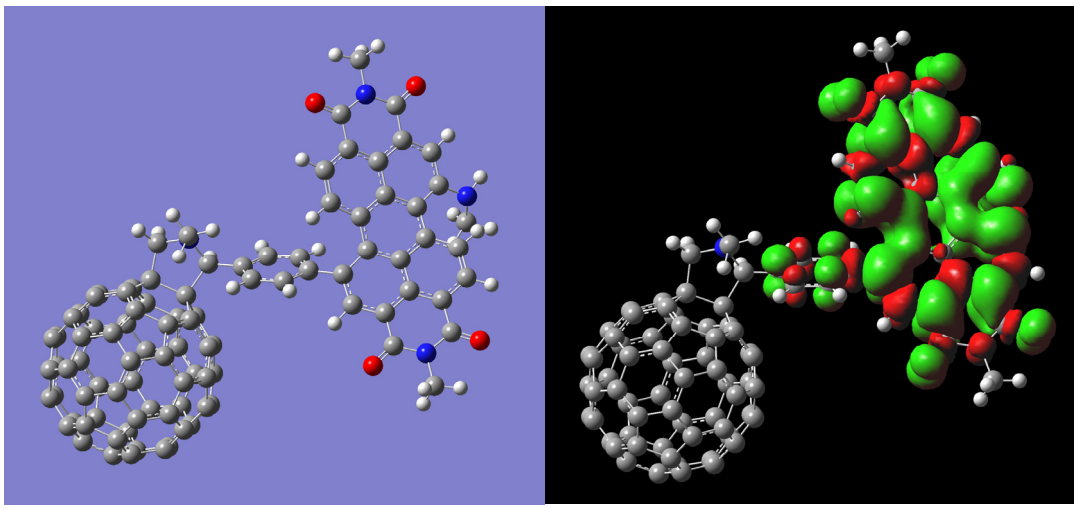
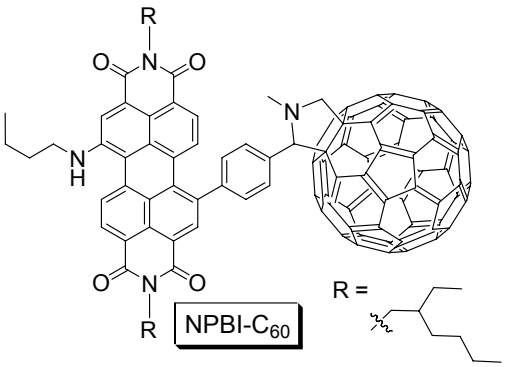


Figure S27. Spin density of the triplet state of **NPBI-C_{60}.** Calculated at B3LYP/6-31G(d) level with Gaussian 09W on the optimized triplet state geometry. Note the alkyl chains were simplified as methyl group, in order to reduce the computation cost.



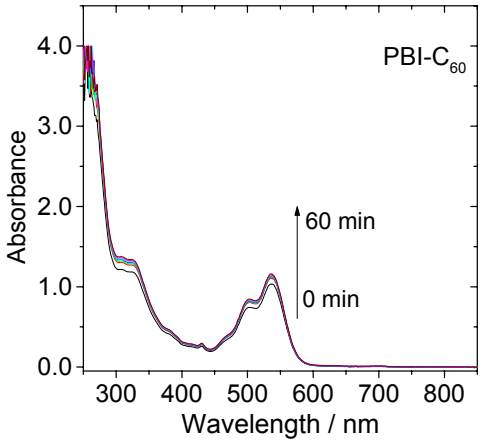


Figure S28. The stability of **PBI-C_{60}** within 1 hour of continues illumination. A CH_2Cl_2-CH_3OH (9:1) solution containing PBI-C_{60} (2.0×10^{-5}M) was irradiated by xenon arc lamp (The light intensity at the photoreactor is13 mW/cm^2).

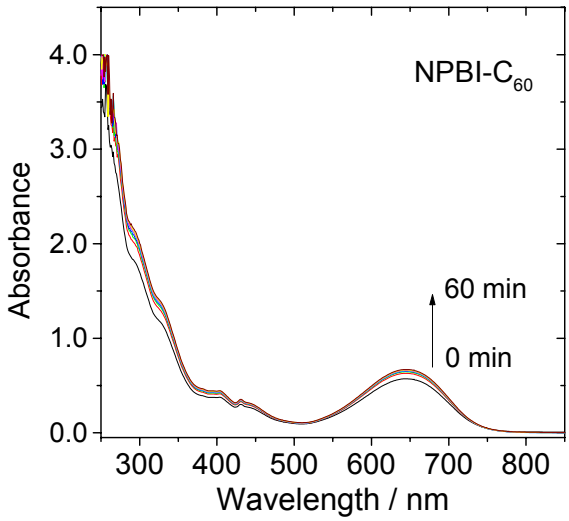


Figure S29. The stability of **NPBI-C_{60}** within 1 hour of continues illumination. A CH_2Cl_2-CH_3OH (9:1) solution containing NPBI-C_{60} (2.0×10^{-5}M) was irradiated by xenon lamp (The light intensity at the photoreactor is13 mW/cm^2).

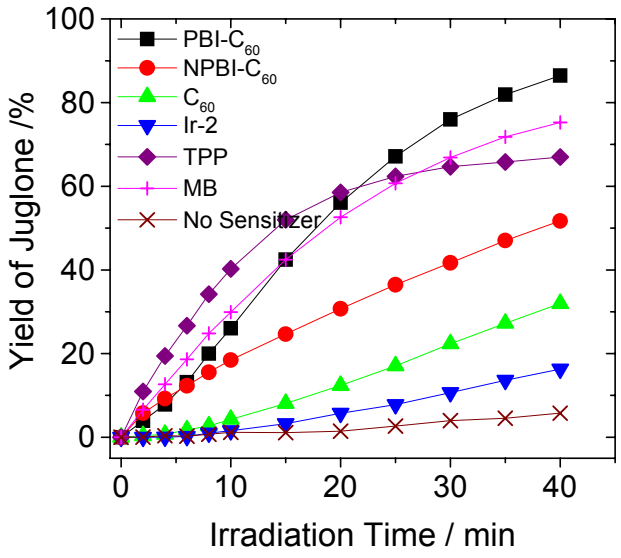


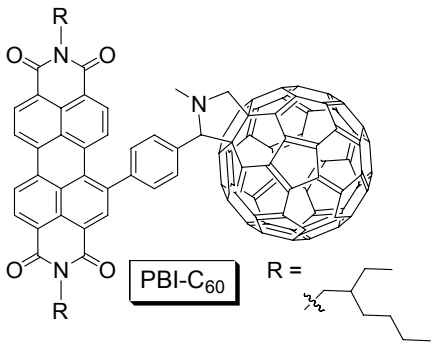
Figure S30. Plots of chemical yield as a function irradiation time for the photooxidation **of DHN** using complex PBI-C_{60}, NPBI-C_{60}, C_{60}, Ir-2, TPP, MB as sensitizers in CH_2Cl_2-CH_3OH (9:1) solution. c[sensitizer]=2.0×10^{-5}M. The light intensity at the photoreactor is13 mW/cm^2.

Z-matrix of the optimized triplet state geometry of PBI-C_{60}.

(Please note the alkyl chains have been simplified as methyl groups to reduce the computation cost)

0 3

C	2.71235400	0.36772773	-1.49291111
C	1.57516592	-0.43707997	-1.39497647
H	2.83622286	1.01366775	-2.35613712
C	2.37713078	-1.30340949	0.70582183
C	1.38230862	-1.28680235	-0.28954591
H	0.83441151	-0.39174050	-2.18322823
H	2.24987279	-1.94568069	1.57173580
C	-2.97409140	0.74952131	-2.75307866
C	-4.24292888	0.31609970	-3.32440365
C	-5.38188275	1.11500629	-3.19462587
C	-5.30284447	2.38408809	-2.47667217
C	-4.08533971	2.80521670	-1.93309395



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H	1.42762742	-2.90583010	-2.54587112
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124 125 1.0
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Z-matrix of the optimized triplet state geometry of NPBI-C_{60}.

(Please note the alkyl chains have been simplified as methyl groups to reduce the computation cost)

0 3

C	2.42699068	0.36181319	-1.56509742
C	1.28288491	-0.42462139	-1.44683814
H	2.54045852	1.01057606	-2.42905947
C	2.11842121	-1.31829402	0.61865272
C	1.10224557	-1.27969883	-0.34839222
H	0.52581446	-0.36212762	-2.22005089
H	2.00504256	-1.96703750	1.48340759
C	-3.29721071	0.74119584	-2.75314764
C	-4.57103699	0.30239081	-3.29323967
C	-5.70633609	1.10032428	-3.15152980
C	-5.61542174	2.37061973	-2.44944243
C	-4.39015865	2.79785783	-1.93351098
C	-3.20758463	1.97174390	-2.09513844
C	-2.59149496	-0.41696757	-2.24830656
C	-3.45039713	-1.59737923	-2.48484232
C	-4.66315788	-1.13606154	-3.12531020
C	-5.89606386	-1.72333819	-2.82196568
C	-6.98392554	0.49053437	-2.81902691
C	-6.82946960	2.53992123	-1.67511083
C	-6.77417312	3.12573452	-0.40851620
C	-5.50070940	3.56782835	0.13199529
C	-4.33197136	3.40855359	-0.61524966
C	-3.11298719	2.95643752	0.03303756
C	-2.42434179	2.06572631	-0.88752348
C	-1.76944712	0.92797946	-0.40363085
C	-1.81742725	-0.32854374	-1.10876292
C	-3.49461892	-2.61607306	-1.55819969
C	-2.51137456	-2.76824990	-0.39358287
C	-1.57010468	-1.48956029	-0.13728528
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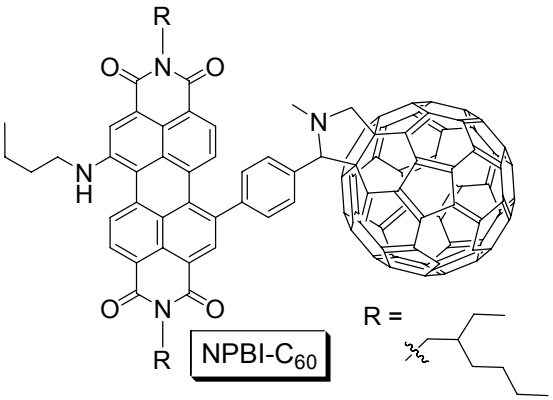

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C	-5.49574084	3.28463306	1.55841358
C	-7.67537939	1.37710732	-1.90300855
C	-7.65781795	0.47927199	2.61622844
C	-8.42225550	0.38993575	1.45104060
C	-8.52091065	-0.87433202	0.74346440
C	-7.85326846	-2.00044897	1.22932658
C	-7.05654697	-1.90652040	2.44233036
C	-5.68061728	-0.25037791	3.65084473
C	-5.59335309	1.19205969	3.48799122
C	-6.81255123	1.64219689	2.84492820
C	-6.76559495	2.66740278	1.89768166
C	-7.55666064	2.56961951	0.68252234
C	-8.36760430	1.45502280	0.46397567
C	-8.52603801	-0.59130322	-0.68281193
C	-7.86335944	-1.44551924	-1.56652729
C	-7.16581403	-2.61398468	-1.05880047
C	-7.16183223	-2.88592368	0.30866354
C	-5.93979184	-3.33345009	0.95760236
C	-5.87638100	-2.73393119	2.26826706
C	-4.64037218	-2.30590779	2.76519084
C	-4.54532256	-1.04062822	3.47081342
C	-4.37104611	1.78569742	3.16598253
C	-3.18787135	0.96227171	2.99221971
C	-3.27320571	-0.42723927	3.13398732
C	-2.57224439	-1.30464474	2.22098969
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