Supporting Information

Single- and Multi-Walled Carbon Nanotubes covalently linked with Perylenebisimides: Synthesis, characterization and photophysical properties

Roberto Martín,[a] F. Javier Céspedes-Guirao,[b] Maykel de Miguel,[a] Fernando Fernández-Lázaro,[b] and Hermenegildo Garcia*,[a] and Ángela Sastre-Santos*,[b]

[a] *Instituto de Tecnología Química CSIC-UPV, Unversidad Politécnica de Valencia, Avenida de los Naranjos s/n, 46022 Valencia, Spain;E-mail: hgarcia@qim.upv.es*

[b] *División de Química Orgánica, Instituto de Bioingeniería, Universidad Miguel Hernández, Elche 03202 (Alicante), Spain. E-mail: asastre@umh.es*

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Instrumentation and Materials

All reagents were purchased from commercial suppliers and used without further purification unless otherwise noted. Commercial TLC plates (silica gel 60 F254, SDS) were used to monitor the progress of the reaction, with spots observed under UV light at 254 and 365 nm. Column chromatography was performed with silica gel 60A (particle size 40-63 μm, SDS). NMR spectra were taken using a 300 MHz Bruker AC-300. Ultraviolet–visible (UV-vis) absorption measurements were taken on a ThermoSpectronic Helios γ spectrophotometer. Infrared measurements were taken with a Fourier Transform (FT-IR) ThermoNicolet model IR 200 Spectrometer in transmission method with KBr. Mass spectra-MALDI were obtained from a Bruker Reflex III matrix-assisted laser desorption/ionization time of flight (MALDI-TOF) spectrometer using dithranol as a matrix. Mass spectra-electrospray were obtained from a QSTAR (Applied Biosystems) spectrometer using methanol as a solvent and as a ionizing phase. Elemental analyses were performed on a LECO CHNS-932 elemental analyzator.

Emission spectra were recorded on a PTI LPS-220B spectrofluorimeter having excitation and detection Czerny–Turner monochromators and a slit of 1 mm. Fluorescence spectra were recorded for optically matched solutions after nitrogen purging in septum capped cuvettes upon excitation at 550 nm in all cases. Relative quantum yields were determined from the relative areas of the emission spectra and the absolute quantum yields were determined using purified 2,4,6-triphenylpyrylium tetrafluoroborate as standard.

= solvents and water

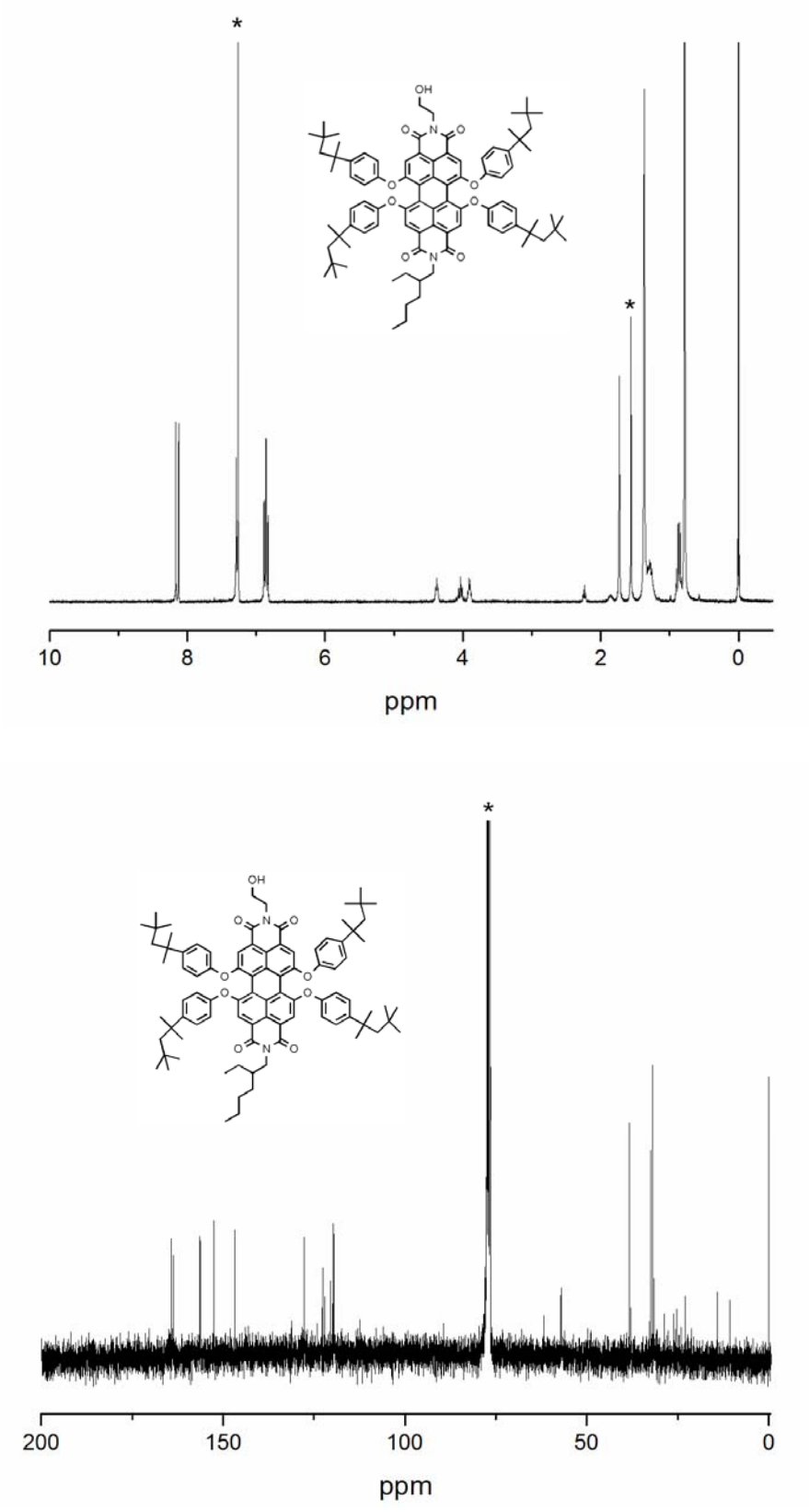

Figure S1. ^{1}H NMR and ^{13}C NMR spectrum of **PBI-1** in $CDCl_3$.

* = solvents and water

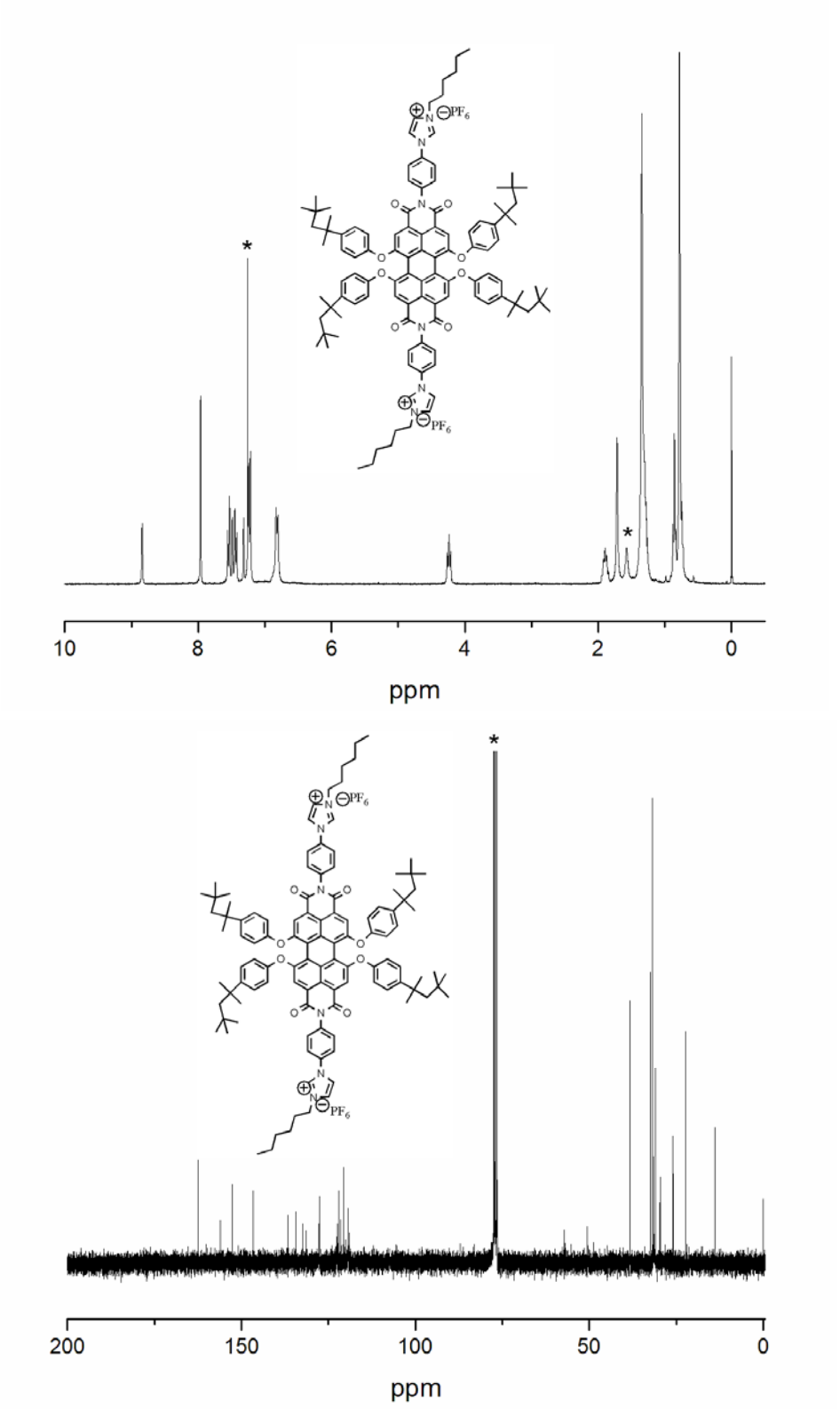

Figure S2. ^{1}H NMR and ^{13}C NMR spectrum of **PBI-2** in $CDCl_3$.

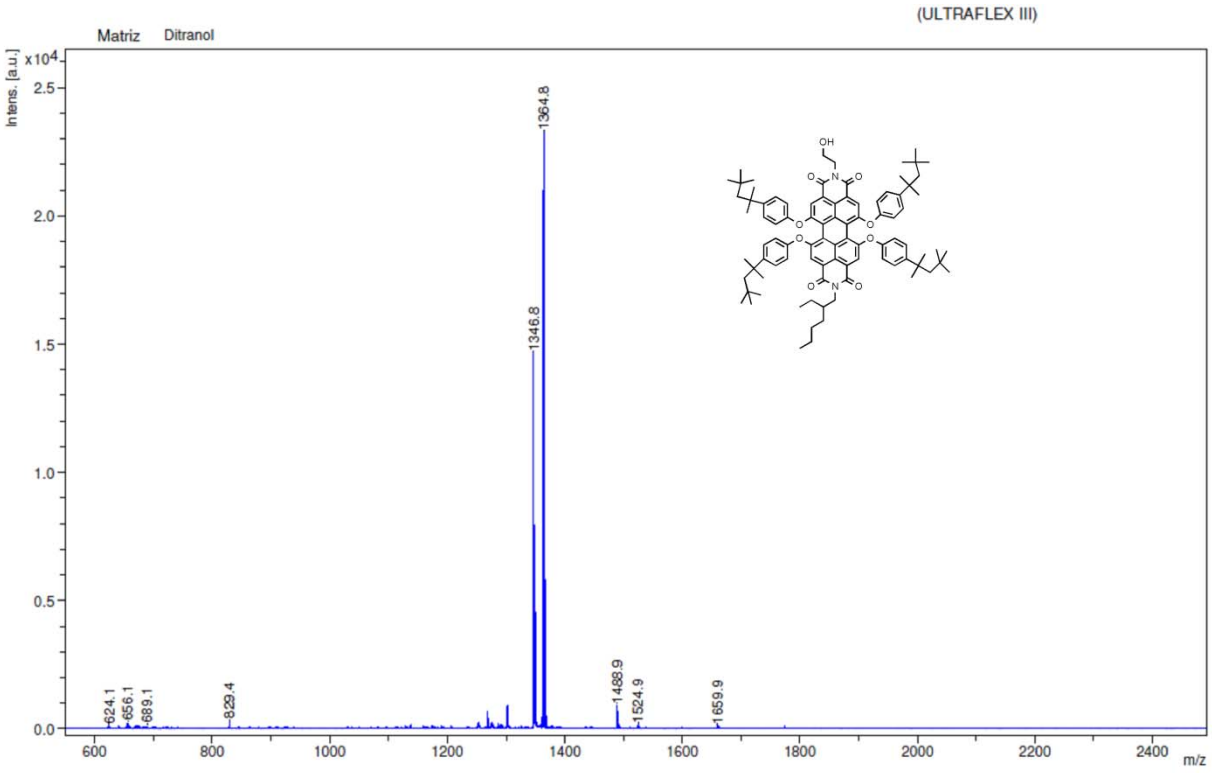

Figure S3. MALDI mass spectra of **PBI-1** (positive mode).

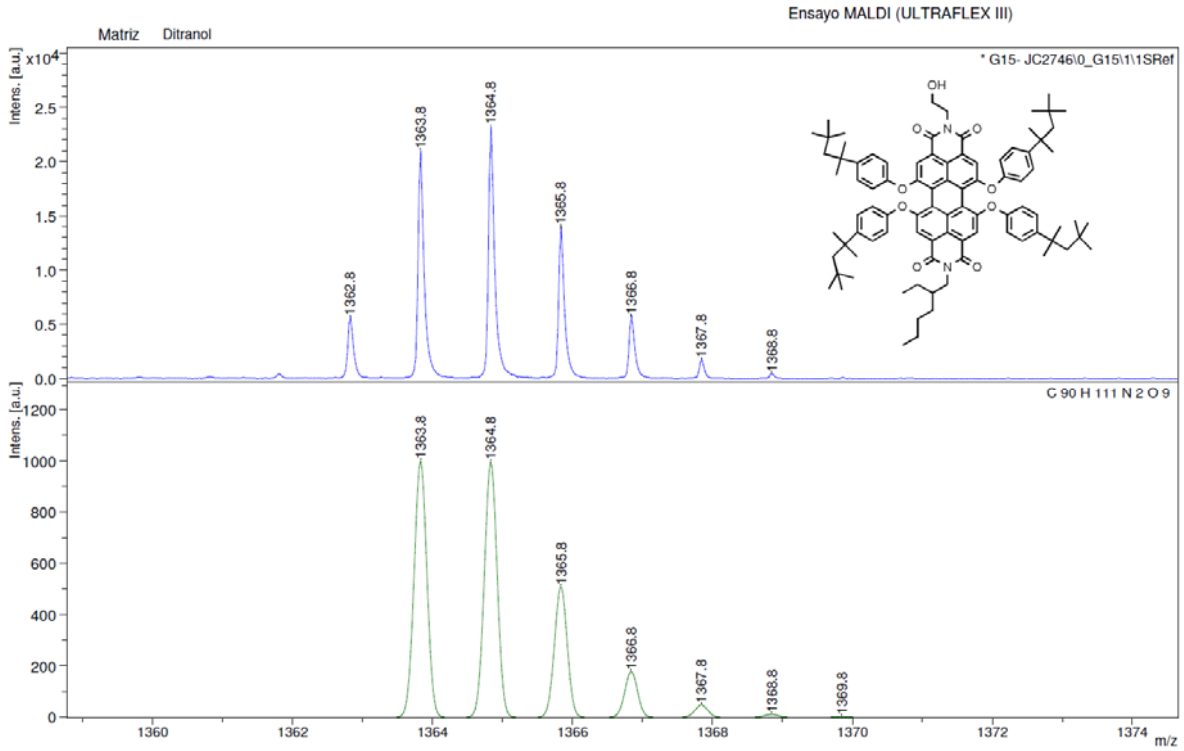

Figure S4. Isotopic distribution of **PBI-1** (mass spectra).

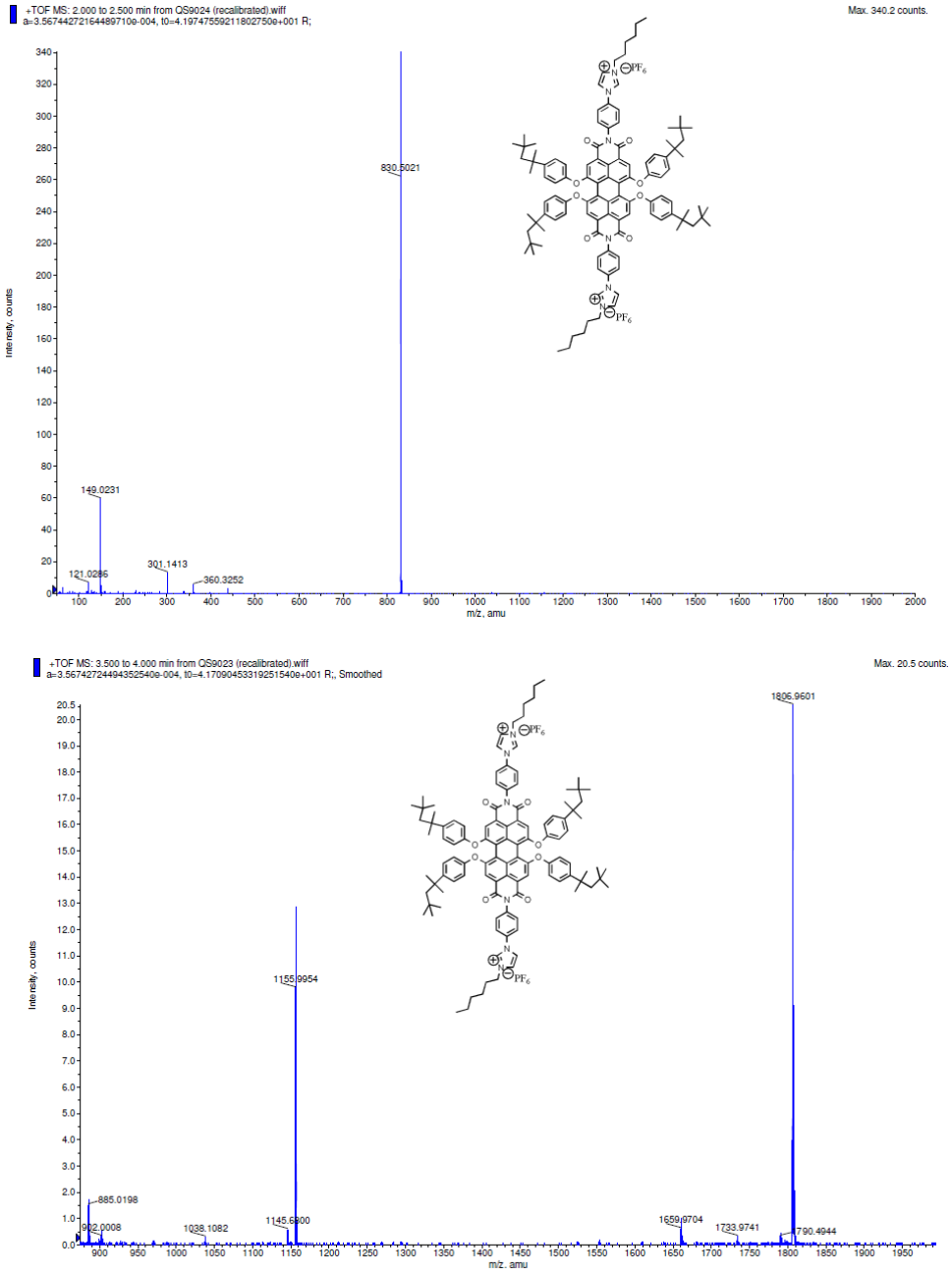

Figure S5. HR-ESI-MS of **PBI-2** (positive mode).

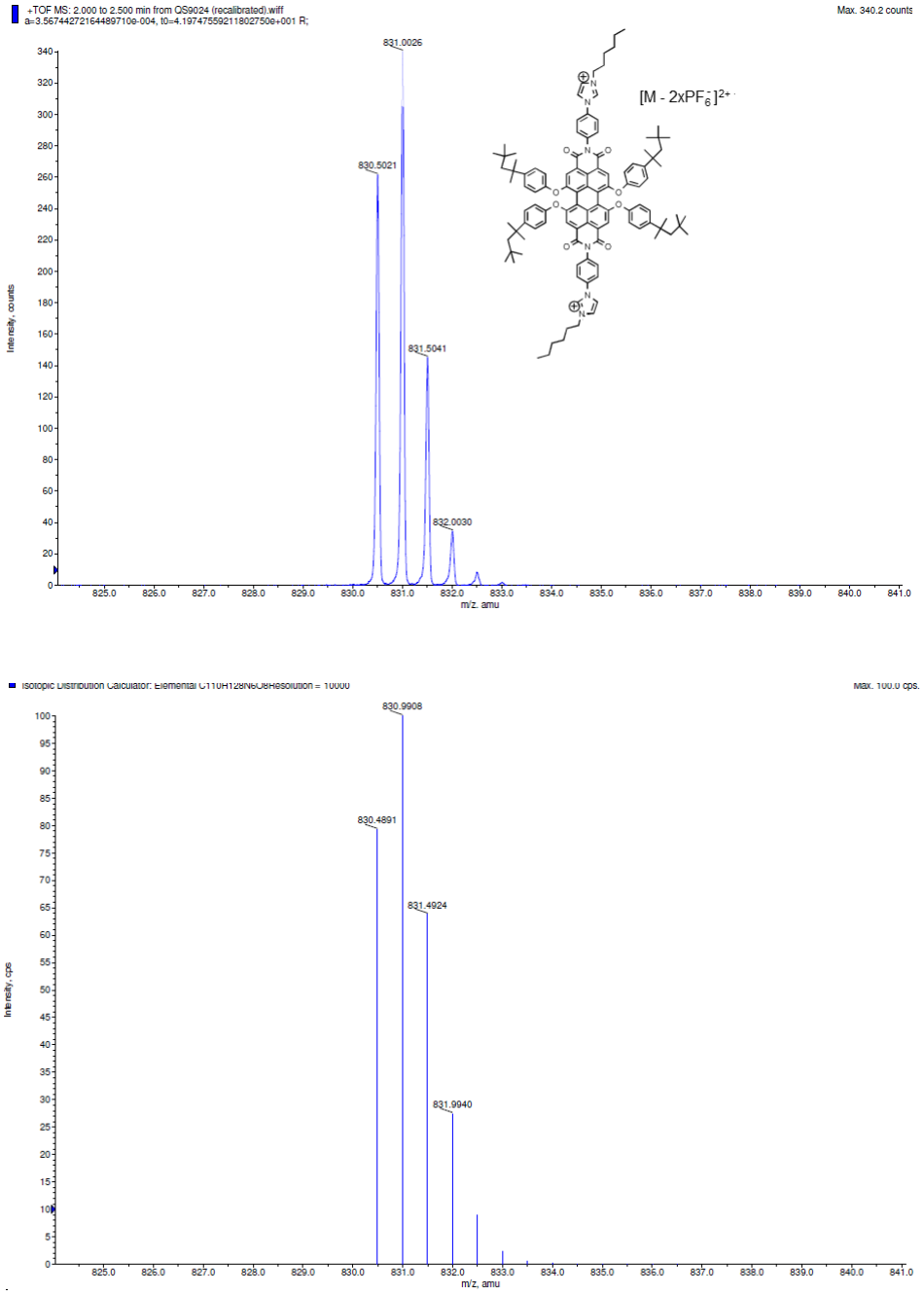

Figure S6. Isotopic distribution of **PBI-2** (mass spectra).

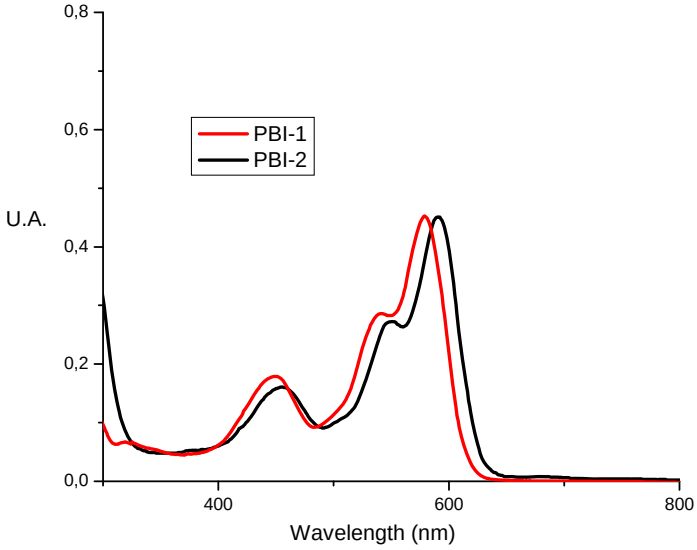

Figure S7. Normalized UV-vis absorption spectra of **PBI-1** (red) and **PBI-2** (black) in CH_2Cl_2.

Table 1

NAME	Laser flash photolysis lifetimes				Fluorescence Quantum yield (ϕ_{fl})[a]
	380 nm		660 nm		
	τ_1	τ_2	τ_1	τ_2	
PBIs					0.3541
T-PBI-SWNT	2.47 (73.7%)	32 (26.3%)	2.47 (73.7%)	32 (26.3%)	0.0009
T-PBI-MWNT	4.6 (74.2%)	63.5 (25.7%)	2.58 (80%)	50.70(20%)	0.0106
W-PBI-SWNT	2.86 (88.5%)	30,2 (11.4%)	2.52 (88%)	32 (11.7%)	<0.0001
W-PBI-MWNT	3.43 (80%)	58.57 (20%)	3.43 (80%)	58.6 (20%)	0.0003

[a] Fluorescence Quantum Yields of the PBI-CNTs under study measured by taking tris(bipyridine)ruthenium(II) chloride as standard (φ_{fl} = 0.042)

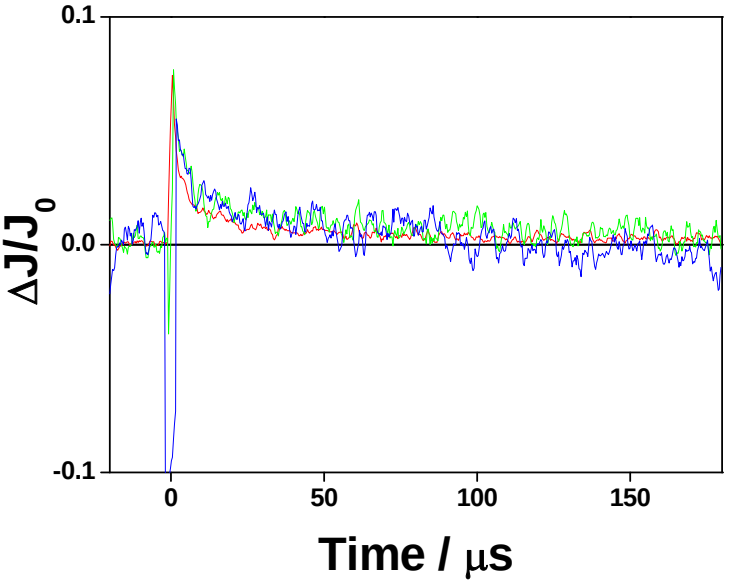

Figure S8. Normalized decay of the transient signal monitored at 380, 500 and 660 nm upon 532 nm laser excitation of N_2-purged benzonitrile solution of W-PBI-MWNT.

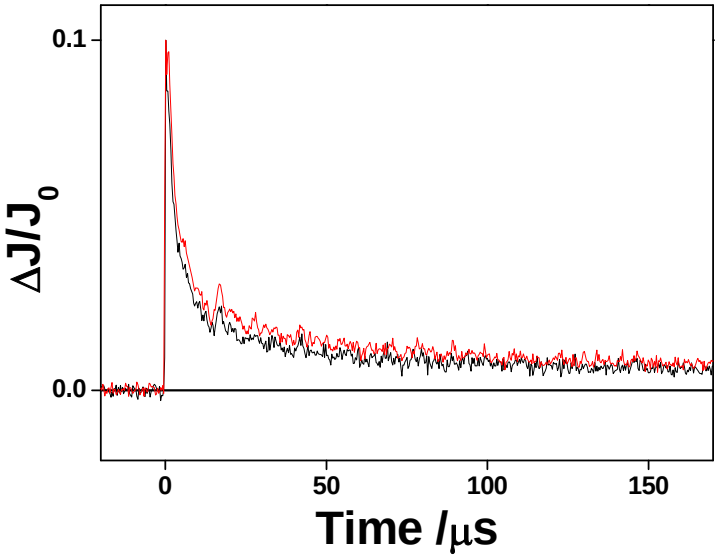

Figure S9. Normalized decay of the transient signal monitored at 380 and 660 nm upon 532 nm laser excitation of N_2-purged benzonitrile solution of W-PBI-SWNT.

References:

1. M. Planells, F. J. Céspedes-Guirao, A. Forneli, A. Sastre-Santos, F. Fernández-Lázaro and E. Palomares, *J. Mater. Chem.*, 2008, **18**, 5802–5808.
2. F. J. Céspedes-Guirao, L. Martín-Gomis, K. Ohkubo, S. Fukuzumi, F. Fernández-Lázaro and Á. Sastre-Santos, *Chem. Asian J.* 2011, DOI:10.1002/asia.2011320.