Synthesis and Characterization of Boron Azadipyrromethene Single-Wall Carbon Nanotube Electron Donor-Acceptor Conjugates

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Scheme S1: Deprotection of Boc-protected [1].

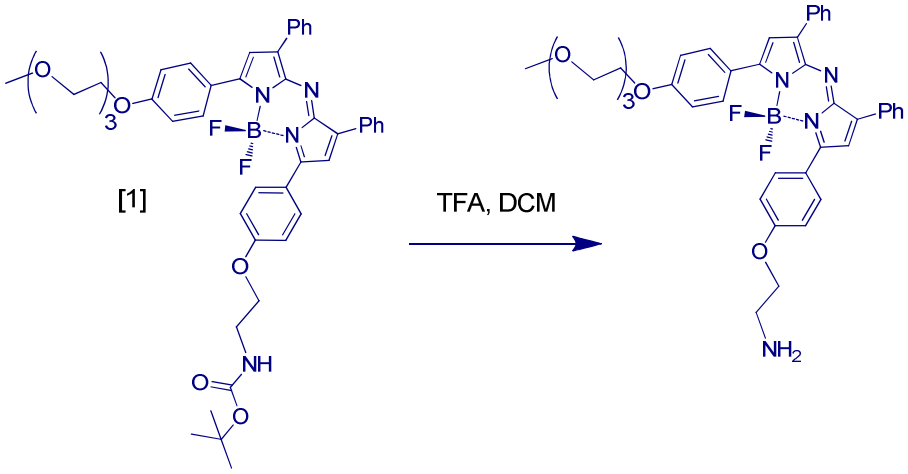

Table S1: XPS C 1s, O 1s, B 1s and N 1s data for [2-5] used for the estimation of efficiency of functionalisation reactions.

r-SWNTs [2]

Name	At. %	Atomic Ratio
C1s	96.93	100.00
O1s	2.17	2.24

p-SWNTs [3]

Name	At. %	Atomic Ratio
C1s	86.85	100.00
O1s	10.96	12.62

f-SWNTs [4]

Name	At. %	Atomic Ratio
C1s	75.35	100.00
O1s	15.32	20.33

f-SWNTs [5]

Name	At. %	Atomic Ratio
C1s	83.83	100.00
B1s	0.50	0.60
N1s	2.28	2.72

Table S2: Using atomic ratios for *f*-SWNT [4] (first column), by subtracting O 1s peak of *f*-SWNT [4] from *f*-SWNT [3] we could estimate the number of benzoic acid groups in the sample. We can subsequently estimate the relative amounts of carbon related to benzoic acid groups attached to the nanotube surface ($C_{attached}$ = 7 carbons per added 2 oxygen atoms) and from the nanotube body (C_{nt} = total carbon amount after $C_{attachment}$ subtraction). We renormalized atomic ratios on benzoic acid (second column) and results indicated that there is one group attached every 18.4 carbon nanotube atoms.

XPS Atomic Ratio	*f*-SWNTs [4]	Atoms per benzoic acid group
C 1s $_{f\text{-SWNTs [4]}}$	100.0	26.3
O 1s $_{f\text{-SWNTs [4]}}$	20.3	5.3
O 1s $_{p\text{-SWNTs [3]}}$	12.6	3.3
O 1s$_{f\text{-SWNTs [4]}}$ **- O 1s** $_{p\text{-SWNTs [2]}}$ **= O 1s** $_{Tour}$	7.7	2.0
O 1s $_{Tour}$ **/2 = number of benzoic acid groups**	3.8	**1.0**
O 1s $_{Tour}$ **/2 X 7 =** $C_{attached}$	30.0	7.9
C_{total} **-** $C_{attached}$ **=** C_{nt}	70.0	**18.4**

Table S3: Using atomic ratios for *f*-SWNT [5] (first column), we could estimate from N 1s the quantity of [1] present in the sample. We can subsequently estimate the relative amounts of carbon related to the fluorophore groups attached to the nanotube ($C_{attached}$ = 48C per attached fluorophore) and from the nanotube body (C_{nt} = total carbon amount after $C_{attachment}$ subtraction). We renormalized atomic ratios on [1] (second column) and results indicated that there is one fluorophore attached every 99.1 carbon nanotube atoms.

XPS Atomic Ratio	*f*-SWNTs [5]	Atoms per attached fluorophore
C 1s $_{f\text{-SWNTs [5]}}$	100	147.1
N 1s $_{f\text{-SWNTs [5]}}$	2.7	4.0
N 1s $_{f\text{-SWNTs [5]}}$ /4 = number of molecules of [1]	0.7	**1.0**
number of dye molecules X 48C = $C_{attached}$	32.6	47.9
C_{total} - $C_{attached}$ = C_{nt}	67.4	**99.1**

Table S3: Using atomic ratios for *f*-SWNT [5] (first column), we could estimate from the B 1s peak the quantity of boron present in the sample. We can subsequently estimate the relative amounts of carbon related to the boron chelated fluorophore groups attached to the nanotube ($C_{attached}$ = 48C per attached fluorophore) and from the nanotube body (C_{nt} = total carbon amount after $C_{attachment}$ subtraction). We renormalized atomic ratios on boron chelated [1] (second column) and results indicated that there is one fluorophore attached every 112.3 carbon nanotube atoms.

XPS Atomic Ratio	*f*-SWNTs [5]	Atoms per attached fluorophore
C 1s $_{f\text{-SWNTs [5]}}$	100	166.7
B 1s $_{f\text{-SWNTs [5]}}$	0.6	1.0
B 1s $_{f\text{-SWNTs [5]}}$ /1 = number of dye molecules	0.6	**1.0**
number of dye molecules X 48C = $C_{attached}$	32.6	54.3
C_{total} - $C_{attached}$ = C_{nt}	67.4	**112.3**

Figure S1: Steady state absorption and emission spectra for raw, purified and functionalised SWNTs.