Electronic supplementary information

Control of near infrared photoluminescence properties of single-walled carbon nanotubes by functionalization utilizing steric effect of dendron

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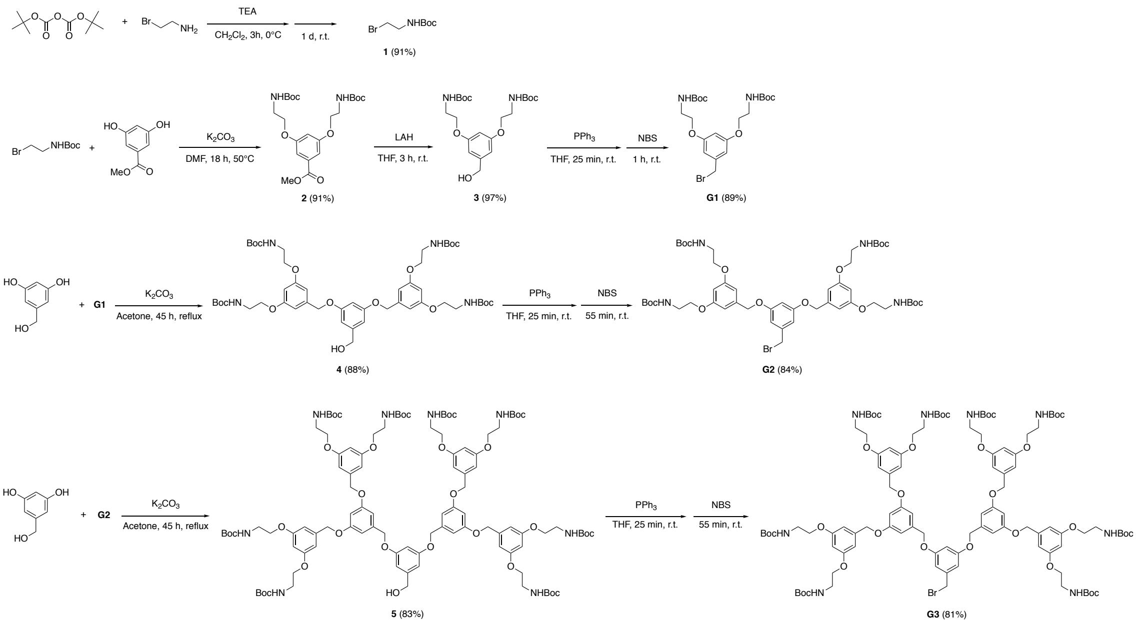
p.24**Fig. S15.** Molecular orbitals of 1,4-adducts of Bn-SWNT-H at the level of B3LYP/6-31G* (isovalue=0.01).

Fig. S16. Molecular orbitals of 1,4-adduct (L_{87}) of Bn-SWNT-Bn at the level of B3LYP/6-31G* (isovalue=0.01).

Scheme



Synthesis of 2-(Boc amino) ethyl bromide (1)[1]

A solution of (2-bromoethyl) amine (14.3 g, 70.0 mmol) and di-*t*-butyl dicarbonate (12.1 mL, 58.4 mmol) in dichloromethane (37 mL) were placed in a 100 mL round-bottom flask. Triethylamine (9.8 mL, 70.0 mmol) was added dropwise to the solution at 0°C and stirred for 3h. After 1 day stirring at r.t., the solution was washed by sat. NH_4Cl aq. (50 mL), sat. $NaHCO_3$ aq. (50 mL), and brine (50 mL). Organic layer was dried (Na_2SO_4) and filtered. Solvent was removed to give a light-yellow oil **1** (11.9 g, 91%).

^{1}H NMR (400 MHz, $CDCl_3$): $\delta = 1.45$ (s, 9H; $C(CH_3)_3$), 3.46 (t, $J = 5.5$ Hz, 2 H; $BrCH_2$), 3.53 (t, $J = 5.5$ Hz, 2 H, CH_2NH), 4.95 (br.s, 1H; N*H*)

^{13}C-NMR (100 MHz, $CDCl_3$): δ=28.48 [$C(CH_3)_3$], 33.05 ($BrCH_2$), 42.46 (CH_2NH), 85.33 [$C(CH_3)$], 146.87 (C=O)

IR: 3500-3200 (O-H), 2978 (C-H), 1700 cm^{-1}(C=O)

Synthesis of benzoic acid, 3,5-bis[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethoxy]-, methyl ester (2)[2]

A mixture of **1** (14.1 g, 63.0 mmol), methyl 3,5-dihydroxybenzoate (4.24 g, 25.2 mmol), K_2CO_3 (13.9 g, 100.8 mmol), and dry DMF (41 mL) was stirred at 50°C for 18 h. The mixture was cooled and extracted with ethyl acetate (50 mL). The solution was washed by water (50 mL×2) and brine (50 mL). The organic layer was dried (Na_2SO_4), filtered, and evaporated. Purification by column chromatography (SiO_2, dichloromethane/methanol = 99:1) gave **2** (10.4 g, 91%) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.45 [s, 18H; $C(CH_3)_3$], 3.54 (d, *J* = 5.49 Hz, 4H; C*H*$_2$NH), 3.90 (s, 3H; OCH_3), 4.04 (t, *J* = 5.04 Hz, 4H; OCH_2), 4.95 (br, s, 2H; NH), 6.64 (t, *J* = 2.28 Hz1H; Ph C^4-H),7.18 (d, *J* = 2.28 Hz, 2H; Ph $C^{2,6}$-H)

^{13}C-NMR (100 MHz, $CDCl_3$): δ= 28.40 [C(*C*H_3)$_3$], 39.91($NHCH_2$), 52.42 (OCH_3), 67.76 (OCH_2), 79.65 [I(CH_3)$_3$], 112.41, 113.01, 115.38 (Ph $C^{2,4,6}$), 132.18 (Ph C^1), 155.82 (C=O), 159.22, 165.95 (Ph $C^{3,5}$)

IR: 3336 (N-H), 2979, 2937, 2874 (C-H), 1689 (C=O), 1167 cm^{-1}(C-O)

Synthesis of carbamic acid, *N,N'*-[[5-(hydroxymethyl)-1,3-phenylene]bis(oxy-2,1-ethanediyl)] bis-, *C,C'*-(1,1-dimethylethyl) ester (3)[3]

A solution of **2** (1.36 mg, 2.99 mmol) in THF (35.3 mL) was added dropwise to a solution of LAH (0.280 g, 7.46 mmol) in THF (3.9 mL) and stirred at r.t. After 3h, methanol (1mL) was slowly added followed by water (3 drops). The resulting mixture was filtered through Celite and evaporated. Column chromatography (SiO_2, dichloromethane/ethyl acetate = 1:1) gave **3** (1.24 g, 97%) as a white solid.

^{1}H-NMR, ppm (400 MHz, $CDCl_3$): δ=1.45 (s, 18H; $C(CH_3)_3$), 3.52 (m, 4H; NHC*H*$_2$), 4.01(t, *J* = 5.62 Hz, 2H; OCH_2), 4.63 (d, *J* = 5.62 Hz, 2H; Ph-C*H*$_2$), 4.97 (br. s, 2H; N*H*), 6.37(t, *J* = 2.08 Hz, 1H; Ph-C^4-*H*), 6.53(d, *J* = 2.08 Hz, 2H; Ph-$C^{2.6}$-*H*)

^{13}C-NMR (100 MHz, $CDCl_3$) δ= 14.21, 21.08, 28.39, 40.03, 60.42, 65.11, 67.24, 76.72, 77.03, 77.34, 79.59, 100.50, 105.36, 143.66, 155.90, 159.91, 171.22

Synthesis of carbamic acid, *N,N'*-[[5-(bromomethyl)-1,3-phenylene]bis(oxy-2,1-ethanediyl)]bis-, *C,C'*-bis(1,1-dimethylethyl) ester (G1)[3]

A solution of **3** (6.69 g, 15.7 mmol), PPh_3 (6.17 g, 23.5 mmol) in THF (83.5 mL) in a 100 mL heat-dried two-necked round-bottomed flask were stirred at r.t. After 25 min, NBS (4.47 g, 25.0 mmol) was added. After 1h, H_2O was added to the mixture. The resulting aqueous layer was extracted with dichloromethane (80 mL×3). The combined organic layer was dried (Na_2SO_4), filtered, and evaporated. Column chromatography (SiO_2, ethyl acetate/hexane = 6:4) gave **G1** (6.83 g, 89%) as a white solid.

^{1}H-NMR (400 MHz, $CDCl_3$): δ =1.45 (s, 18H; $C(CH_3)_3$), 3.52 (q, *J* = 5.20 Hz, 4H; C*H*$_2$NH), 4.00 (t, *J* = 5.20 Hz, 4H; OCH_2), 4.40 (s, 2H; CH_2Br), 4.96 (br. s, 2H, NH), 6.38 (t, *J* = 2.17 Hz, 1H; Ph-C^4-H), 6.54 (d, *J* = 2.17 Hz, 2H; Ph-$C^{2,6}$-H)

^{13}C-NMR (100 MHz, $CDCl_3$): δ = 28.38, 33.33, 39.99, 67.33, 79.61, 101.33, 107.80, 139.96, 155.85, 159.85

IR: 3367 (N-H), 2977, 2933 (C-H), 1597 (C=O), 1172 cm^{-1} (C-O)

Synthesis of carbamic acid, *N,N',N'',N'''*-[[5-(hydroxymethyl)-1,3-phenylene]bis[oxymethylene-5,1,3-benzenetriyl bis(oxy-2,1ethanediyl)]]tetrakis-*C,C',C'',C'''*-tetrakis(1,1-dimethylethyl)

ester (4)[3]

G1 (2.36 g, 4.82 mmol), methyl 3,5-dihydroxy benzylalcohol (0.290 g, 2.09 mmol), K_2CO_3 (1.16 g, 8.37 mmol) were placed in a 100 mL heat-dried two-necked round-bottomed flask. Dry acetone (40 mL) was added and the mixture was stirred under reflux. After 45 h, the mixture was cooled, filtered, and evapoarted. Column chromatography (SiO_2, dichloromethane/ethyl acetate = 8:2) gave **4** (1.75 g, 88%) as a white solid.

^{1}H-NMR (400 MHz, $CDCl_3$): δ = 1.45 (s, 36H), 3.52 (m, 8H), 4.00 (t, *J* = 5.04 Hz, 8H), 4.62 (d, *J* = 5.00 Hz, 2H), 4.97 (s, 2H), 5.00 (br. s, 4H), 6.39 (t, *J* = 2.00 Hz, 2H), 6.50 (t, *J* = 2.00 Hz, 1H), 6.56 (d, *J* = 2.00 Hz, 4H), 6.61 (d, *J* = 2.00 Hz, 2H)

^{13}C-NMR (100 MHz, $CDCl_3$): δ = 28.40, 40.13, 53.44, 65.01, 65.19, 67.27, 69.68, 69.76, 79.62, 100.33, 100.74, 101.25, 101.44, 105.82, 105.94, 106.05, 106.53, 139.45, 143.61, 155.93, 159.91

IR: 3600-3200 (OH, N-H), 2977 2933, 2876 (C-H), 1598 (C=O), 1167 cm^{-1}(C-O)

Synthesis of carbamic acid, *N,N',N'',N'''*-[[5-(bromomethyl)-1,3-phenylene]bis[oxymethylene-5,1,3-benzenetriyl bis(oxy-2,1ethanediyl)]]tetrakis-*C,C',C'',C'''*-tetrakis(1,1-dimethylethyl) ester (G2)[3]

A solution of **4** (3.59 g, 3.75 mmol), PPh_3 (1.48 g, 5.62 mmol) in THF (20 mL) in a 100 mL heat-dried two-necked round-bottomed flask was stirred at r.t. After 25 min, NBS(1.61 g, 5.99 mmol) was added. After 55 min, H_2O was added to the mixture. The resulting aqueous layer was extracted with dichloromethane (20 mL×3). The combined organic layer was dried (Na_2SO_4), filtered, and evaporated. Column chromatography (SiO_2, ethyl acetate/hexane = 2:8) gave **G2** (3.22 g, 84%) as a white solid.

^{1}H-NMR (400 MHz, $CDCl_3$): δ = 1.45 (s, 36H), 3.52 (m, 8H), 4.00 (t, *J* = 4.8 Hz, 8H), 4.41 (s, 2H), 4.95 (s, 4H), 5.03 (m, 4H), 6.40 (t, *J* = 1.84 Hz, 2H), 6.51 (s, 1H), 6.56 (d, *J* = 2.32 Hz, 4H), 6.63 (d, 2H, *J* = 2.32 Hz)

^{13}C-NMR (100 MHz, $CDCl_3$): δ = 10.96, 14.05, 14.21, 21.04, 55.99, 23.77, 28.41, 28.94, 30.38, 33.50, 38.76, 40.07, 53.42, 60.39, 67.33, 68.17, 69.94, 79.58, 100.90, 102.19, 106.07, 108.27, 128.81, 130.88, 139.23, 139.85, 155.88, 159.93, 160.00, 171.14

IR: 3358 (N-H), 2977, 2933, 2978 (C-H), 1597 (C=O), 1166 cm^{-1}(C-O)

Synthesis of carbamic acid, *N,N',N'',N''',N'''',N''''',N'''''',N'''''''*-[[5-(hydroxymethyl)-1,3-phenylene]bis[oxymethylene-5,1,3-benzenetriylbis[oxymethylene-5,1,3-benzenetriylbis(oxy-2,1-ethanediyl,)]]]tetrakis-*C,C',C'',C''',C'''',C''''',C'''''',C'''''''*-octakis(1,1-dimethylethyl) ester (5)[3]

G2 (2.87 g, 2.81 mmol), methyl 3,5-dihydroxy benzyl alcohol (0.170 g, 1.22 mmol), K_2CO_3 (0.89 g, 4.98 mmol) were placed in a 100 mL heat-dried two-necked round-bottomed flask. Dry acetone (40 mL) was added and the mixture was stirred under reflux. After 45 h, the mixture was cooled, filtered, and evapoarted. Column chromatography (SiO_2, dichloromethane/ethyl acetate = 8:2 to 6:4) gave **5**

(2.04 g, 83%) as a white solid.

^{1}H-NMR (400 MHz, $CDCl_3$): δ =1.44 (s, 72H), 3.50 (d, *J* = 5.28 Hz, 16H), 3.98 (t, *J* = 5.28 Hz, 16H), 4.62 (d, *J* = 5.84 Hz, 2H), 4.95 (s, 6H), 4.97 (m, 3H), 5.04 (s, 6H), 6.38 (t, *J* = 2.45 Hz, 4H), 6.49 (t, *J* = 2.85, 1H), 6.52 (s, 2H), 6.55 (d, *J* = 2.45 Hz, 8H), 6.59 (d, *J* = 2.85 Hz, 2H), 6.64 (d, *J* = 2.30 Hz, 4H)

^{13}C-NMR (100 MHz, $CDCl_3$): δ = 14.25, 21.10, 28.45, 29.33, 31.79, 40.09, 53.48, 53..85, 60.45, 65.09, 67.34, 69.91, 79.61, 100.88, 101.23, 101.63, 105.85, 106.04, 106.37, 139.44, 143.78, 155.97, 159.99, 171.21

Synthesis of Carbamic acid, *N,N',N'',N''',N'''',N''''',N'''''',N'''''''*-[[5-(bromomethyl)-1,3-phenylene]bis[oxymethylene-5,1,3-benzenetriylbis[oxymethylene-5,1,3-benzenetriylbis(oxy-2,1-ethanediyl,)]]]tetrakis-*C,C',C'',C''',C'''',C''''',C'''''',C'''''''*-octakis(1,1-dimethylethyl) ester (G3)[3]

A solution of **5** (2.89 g, 1.44 mmol), PPh_3 (0.57 g, 2.15 mmol) in THF (10 mL) in a 100 mL heat-dried two-necked round-bottomed flask was stirred at r.t. After 25 min, NBS (0.410 g, 2.30 mmol) was added. After 55 min, H_2O was added to the mixture. The resulting aqueous layer was extracted with dichloromethane (20 mL×3). The combined organic layer was dried (Na_2SO_4), filtered, and evaporated. Column chromatography (SiO_2, ethyl acetate/hexane = 1:1 to1:2) gave **G2** (2.43 g, 81%) as a white solid.

^{1}H-NMR (400 MHz, $CDCl_3$): δ = 1.44 (s, 72H), 3.51 (m, 16H), 3.99 (t, *J* = 5.04 Hz, 16H), 4.41 (s, 2H), 4.95 (s, 8H), 4.97 (s, 4H), 5.05 (br.s, 8H), 6.39 (m, 4H), 6.54-6.56 (m, 11H), 6.63 (d, *J* = 2.32 Hz, 2H), 6.66 (d, *J* = 2.32 Hz, 4H)

^{13}C-NMR (100 MHz, $CDCl_3$): δ = 28.39, 29.57, 40.03, 67.57, 69.86, 70.02, 79.55, 100.76, 101.56, 102.20, 106.00, 108.21, 139.06, 139.30, 139.81, 155.88, 159.93, 160.01

Ref.1. Brouwer, A. J. et al., *Eur. J. Org. Chem.* 2001*,* **2001***,* 1903.
Ref.2. Avlonitis, N. et al., *Org. Bimol. Chem.* 2013*,* **11**, 4414.
Ref.3. Sigwalt, D. et al., *Chem. Commun*. 2011, **47**, 4640.

Table S1. Relative energies and absorption energies of (6,5) SWNT and its derivatives calculated at the level of B3LYP/6-31G* except for G3'-SWNT-H with B3LYP/3-21G.

Compound	Addition position	Relative energy	Absorption energy		Oscillator strength
		ΔE (kcal mol^{-1})	E_{abs}(eV)	λ_{abs}(nm)	
SWNT			1.536	807	2.2963
Me-SWNT-Me	1,2-adduct (L_{-33})	0.4	1.350	919	0.3962
	1,2-adduct (L_{87})	7.1	1.293	959	0.6756
	1,2-adduct (L_{27})	3.2	1.071	1158	0.8586
	1,4-adduct (L_{-33})	7.0	1.080	1148	0.9555
	1,4-adduct (L_{87})	0.0	1.214	1021	0.8499
	1,4-adduct (L_{27})	5.1	1.430	867	0.3494
	1,6-adduct (L_{-33})	16.9	1.070	1159	0.1092
	1,6-adduct (L_{87})	16.3	0.882	1406	0.2085
	1,6-adduct (L_{27})	22.4	0.629	1970	0.6282
	1,8-adduct (L_{-33})	19.7	0.768	1614	0.8734
	1,8-adduct (L_{87})	13.6	1.016	1221	0.4517
	1,8-adduct (L_{27})	14.0	1.207	1028	0.2126
	1,10-adduct (L_{-33})	21.8	0.742	1672	0.1598
	1,10-adduct (L_{87})	18.4	0.841	1475	0.1020
	1,10-adduct (L_{27})	29.2	0.452	2745	0.5100
Bn-SWNT-Bn	1,2-adduct (L_{-33})	8.4	1.340	925	0.3429
	1,2-adduct (L_{87})	8.4	1.289	962	0.6655
	1,2-adduct (L_{27})	13.1	1.052	1179	0.8434
	1,4-adduct (L_{-33})	5.9	1.068	1161	0.9262
	1,4-adduct (L_{87})	0.0	1.202	1031	0.8144
	1,4-adduct (L_{27})	4.6	1.428	868	0.4088
	1,6-adduct (L_{-33})	16.3	1.053	1177	0.1145
	1,6-adduct (L_{87})	13.1	0.867	1430	0.1947
	1,6-adduct (L_{27})	22.3	0.616	2013	0.6161
	1,8-adduct (L_{-33})	16.6	0.752	1649	0.8286
	1,8-adduct (L_{87})	13.5	0.998	1243	0.4269
	1,8-adduct (L_{27})	10.9	1.184	1047	0.2303
	1,10-adduct (L_{-33})	21.1	0.728	1702	0.1739
	1,10-adduct (L_{87})	15.0	0.830	1493	0.0995
	1,10-adduct (L_{27})	29.0	0.442	2802	0.5058
Bn-SWNT-H	1,2-adduct (L_{-33})	0.0	1.365	909	0.4651
	1,2-adduct (L_{87})	3.4	1.308	948	0.6838
	1,2-adduct (L_{27})	2.5	1.079	1149	0.8767
	1,4-adduct (L_{-33})	7.1	1.070	1159	0.9498
	1,4-adduct (L_{87})	4.2	1.215	1020	0.8456
	1,4-adduct (L_{27})	3.8	1.406/1.428	882/868	0.1856/0.3466
G2'-SWNT-H	1,2-adduct (L_{-33})	0.0	1.365	908	0.4827
	1,2-adduct (L_{87})	3.4	1.307	948	0.6776
	1,2-adduct (L_{27})	2.5	1.082	1146	0.8806

G2'-SWNT-H	1,4-adduct (L_{-33})	7.2	1.070	1159	0.9401
	1,4-adduct (L_{87})	4.2	1.215	1020	0.8439
	1,4-adduct (L_{27})	3.8	1.408/1.427	881/869	0.2174/0.3178
G3'-SWNT-H	1,2-adduct (L_{-33})	0.0	1.401	885	0.5799
	1,2-adduct (L_{87})	2.3	1.333	930	0.7024
	1,2-adduct (L_{27})	2.7	1.116	1111	0.9652
	1,4-adduct (L_{-33})	4.9	1.067	1162	0.9442
	1,4-adduct (L_{87})	4.5	1.212	1023	0.8494
	1,4-adduct (L_{27})	1.6	1.401/1.424	885/871	0.1925/0.3868

Table S2. Relative energies and absorption energies of (6,5) SWNT and its derivatives calculated at the level of B3LYP/3-21G.

Compound	Addition position	Relative energy	Absorption energy		Oscillator strength
		ΔE (kcal mol^{-1})	E_{abs}(eV)	λ_{abs}(nm)	
SWNT			1.570	790	2.3662
Me-SWNT-Me	1,2-adduct (L_{-33})	0.9	1.393	890	0.5109
	1,2-adduct (L_{87})	7.1	1.320	939	0.7129
	1,2-adduct (L_{27})	3.4	1.108	1119	0.9438
	1,4-adduct (L_{-33})	7.0	1.112	1115	1.0267
	1,4-adduct (L_{87})	0.0	1.247	994	0.9344
	1,4-adduct (L_{27})	5.1	1.451	854	0.3873
	1,6-adduct (L_{-33})	17.6	1.121	1106	0.1021
	1,6-adduct (L_{87})	17.0	0.929	1335	0.2527
	1,6-adduct (L_{27})	23.3	0.663	1871	0.7066
	1,8-adduct (L_{-33})	20.5	0.805	1541	0.9752
	1,8-adduct (L_{87})	14.5	1.059	1171	0.5385
	1,8-adduct (L_{27})	14.7	1.257	987	0.1958
	1,10-adduct (L_{-33})	22.5	0.797	1556	0.1985
	1,10-adduct (L_{87})	19.4	0.882	1406	0.1262
	1,10-adduct (L_{27})	30.4	0.473	2623	0.5569
Bn-SWNT-Bn	1,2-adduct (L_{-33})	8.3	1.338	894	0.4899
	1,2-adduct (L_{87})	8.1	1.316	942	0.7060
	1,2-adduct (L_{27})	12.7	1.086	1141	0.9395
	1,4-adduct (L_{-33})	5.3	1.101	1126	0.9993
	1,4-adduct (L_{87})	0.0	1.223	1005	0.9006
	1,4-adduct (L_{27})	3.9	1.453	853	0.3384
	1,6-adduct (L_{-33})	16.8	1.106	1121	0.1053
	1,6-adduct (L_{87})	13.6	0.914	1356	0.2350
	1,6-adduct (L_{27})	23.2	0.650	1908	0.6966
	1,8-adduct (L_{-33})	17.3	0.789	1572	0.9271
	1,8-adduct (L_{87})	14.2	1.041	1191	0.5121
	1,8-adduct (L_{27})	11.5	1.235	1004	0.2187
	1,10-adduct (L_{-33})	21.7	0.782	1586	0.2204
	1,10-adduct (L_{87})	16.0	0.871	1424	0.1222
	1,10-adduct (L_{27})	30.0	0.464	2673	0.5543
Bn-SWNT-H	1,2-adduct (L_{-33})	0.0	1.402	884	0.5693
	1,2-adduct (L_{87})	3.3	1.335	929	0.7176
	1,2-adduct (L_{27})	2.5	1.113	1114	0.9626
	1,4-adduct (L_{-33})	6.0	1.100	1127	1.0205
	1,4-adduct (L_{87})	3.0	1.244	997	0.9235
	1,4-adduct (L_{27})	2.7	1.443/1.455	859/852	0.2803/0.3193

G2'-SWNT-H	1,2-adduct (L_{-33})	0.0	1.401	885	0.5727
	1,2-adduct (L_{87})	3.0	1.333	930	0.7142
	1,2-adduct (L_{27})	2.4	1.114	1113	0.9640
	1,4-adduct (L_{-33})	5.7	1.100	1127	1.0205
	1,4-adduct (L_{87})	2.9	1.243	998	0.9161
	1,4-adduct (L_{27})	2.3	1.444/1.454	859/853	0.3434/0.2519
G3'-SWNT-H	1,2-adduct (L_{-33})	0.0	1.401	885	0.5799
	1,2-adduct (L_{87})	2.3	1.333	930	0.7024
	1,2-adduct (L_{27})	2.7	1.116	1111	0.9652
	1,4-adduct (L_{-33})	4.9	1.067	1162	0.9442
	1,4-adduct (L_{87})	4.5	1.212	1023	0.8494
	1,4-adduct (L_{27})	1.6	1.401/1.424	885/871	0.1925/0.3868

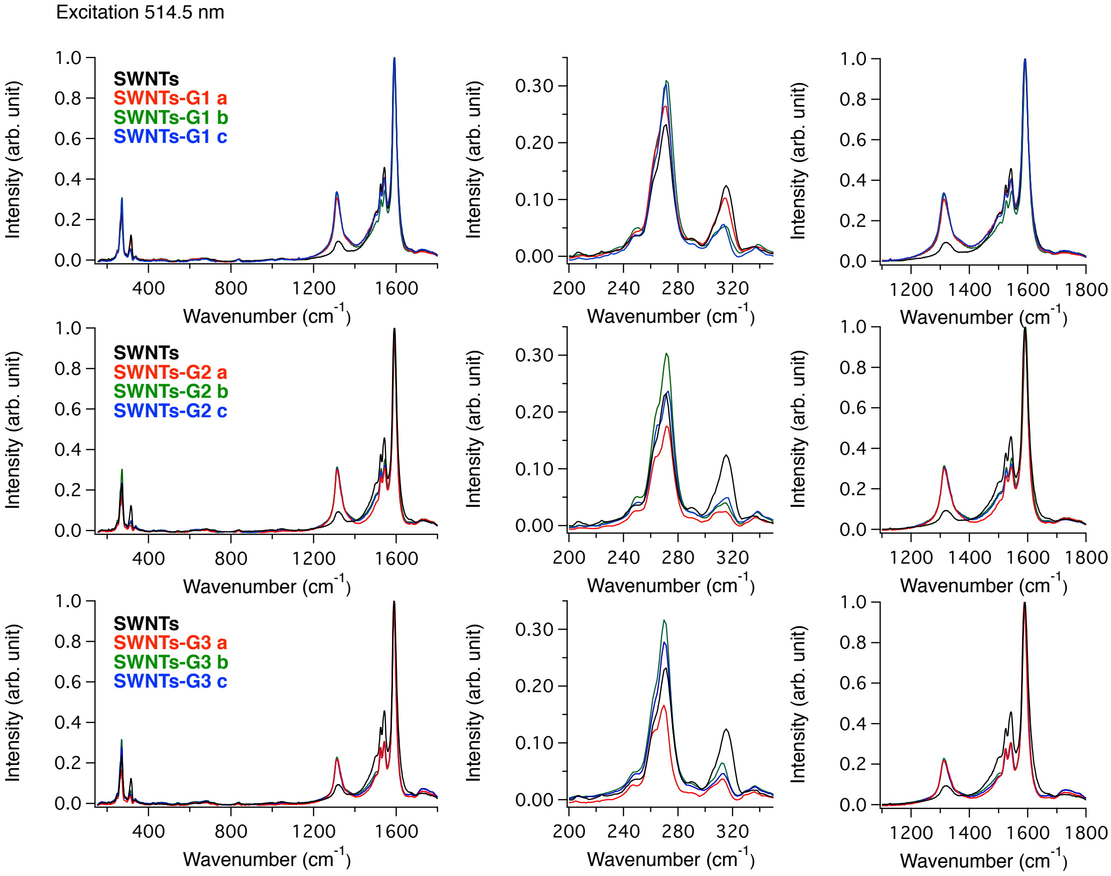


Fig. S1. Raman spectra of SWNTs derivatives at excitation wavelength of 514.5 nm. Each functionalized SWNTs-a, -b, and -c was prepared individually under the same reaction condition.

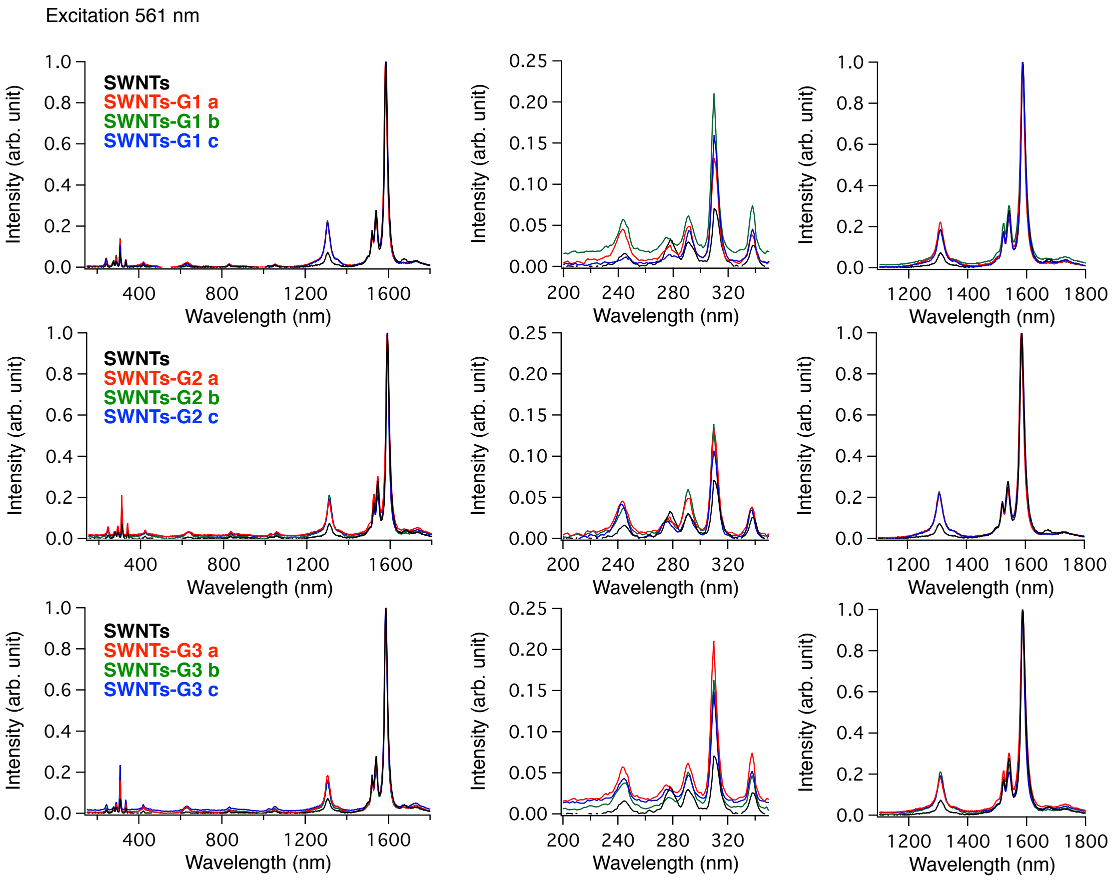


Fig. S2. Raman spectra of SWNTs derivatives at excitation wavelength of 561 nm. Each functionalized SWNTs-a, -b, and -c was prepared individually under the same reaction condition.

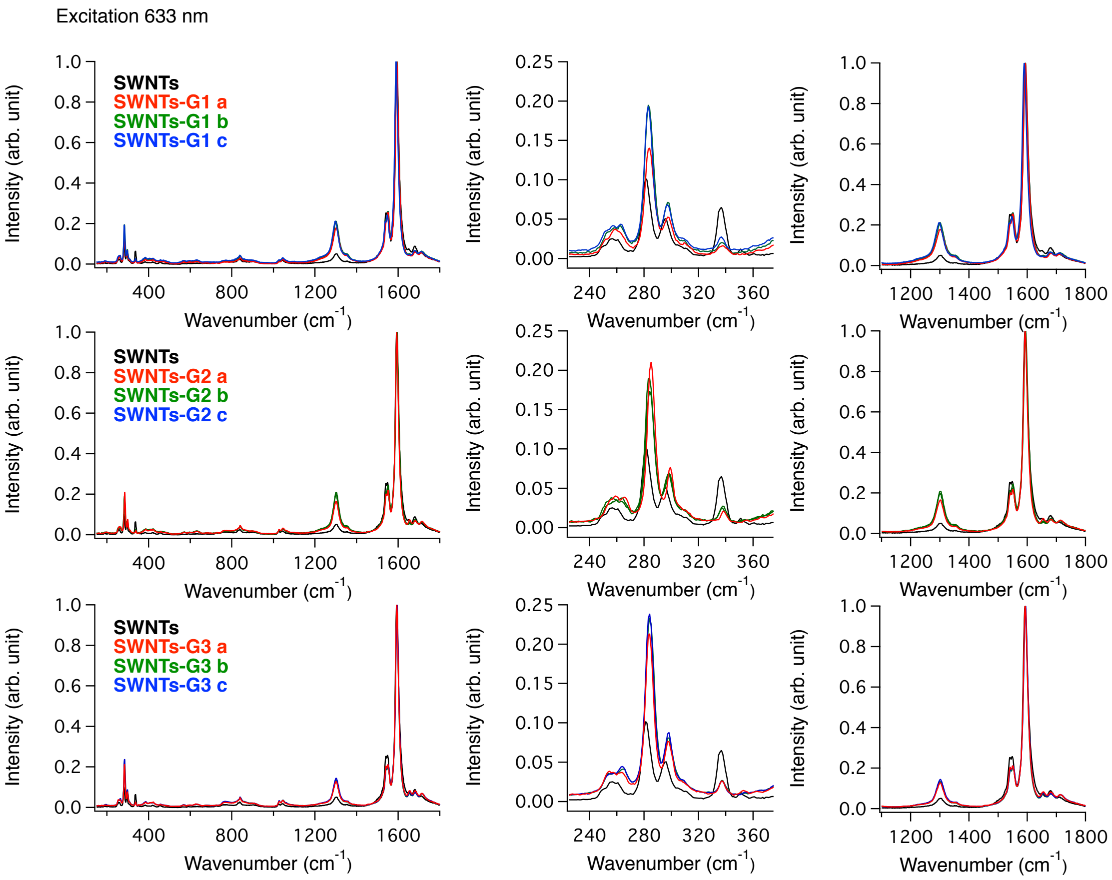


Fig. S3. Raman spectra of SWNTs derivatives at excitation wavelength of 633 nm. Each functionalized SWNTs-a, -b, and -c was prepared individually under the same reaction condition.

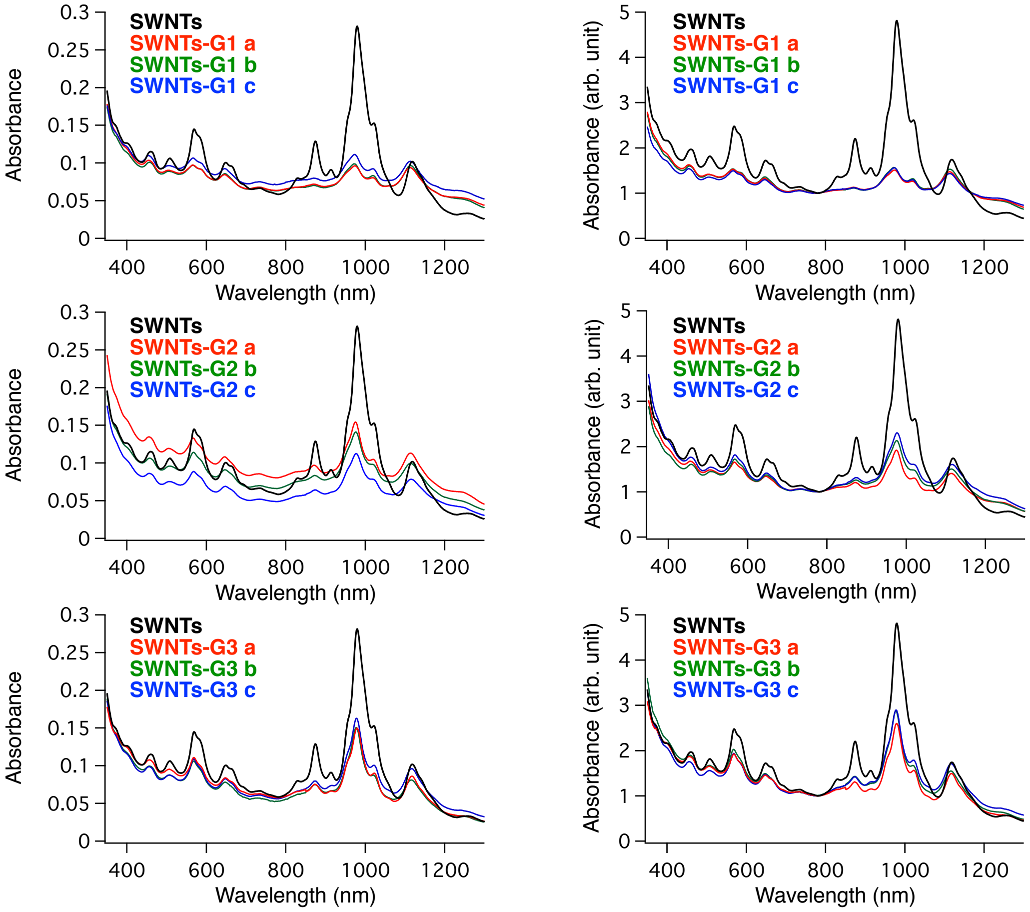
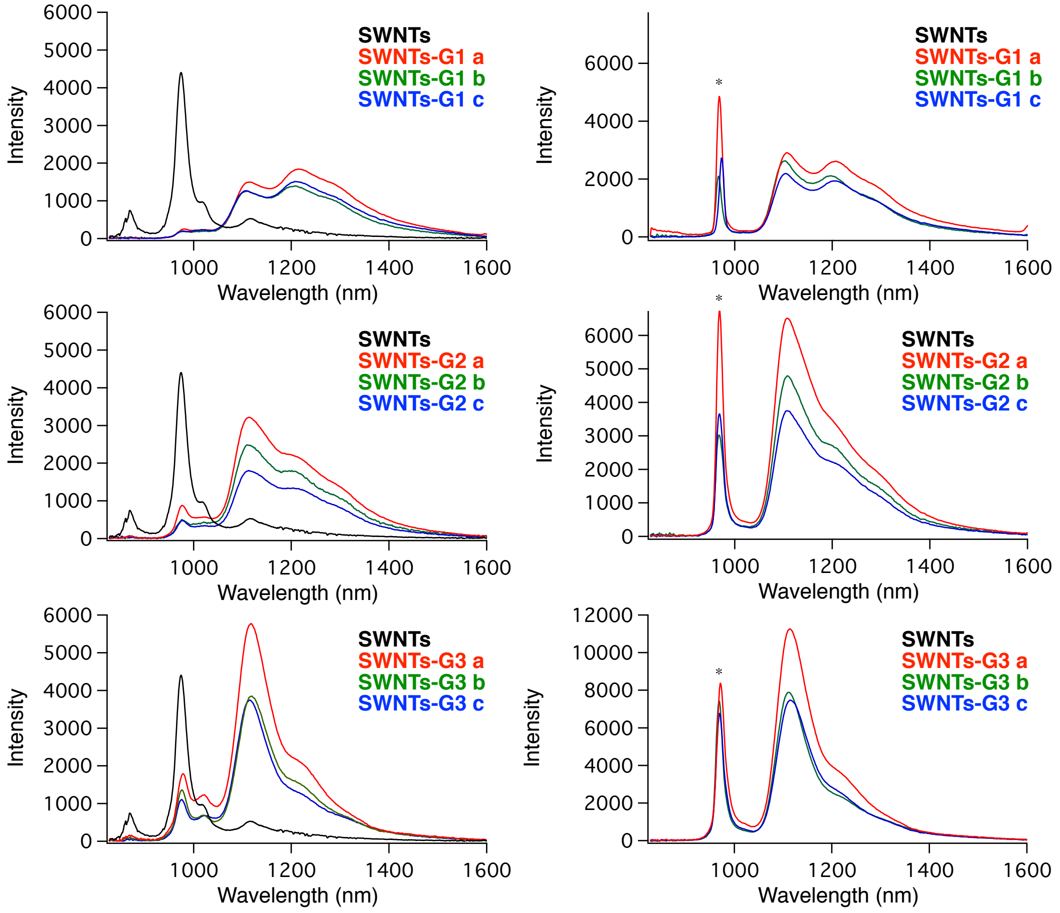


Fig. S4. Absorption spectra of SWNTs derivatives dispersed in D_2O solution containing 1wt% SDBS. Each functionalized SWNTs-a, -b, and -c was prepared individually under the same reaction condition.



*: excitation light

Fig. S5. PL spectra of SWNTs derivatives dispersed in D_2O solution containing 1wt% SDBS. Each functionalized SWNTs-a, -b, and -c was prepared individually under the same reaction condition. Left: Excitation at the E_{22} energy. Right: Excitation at the E_{11} energy.

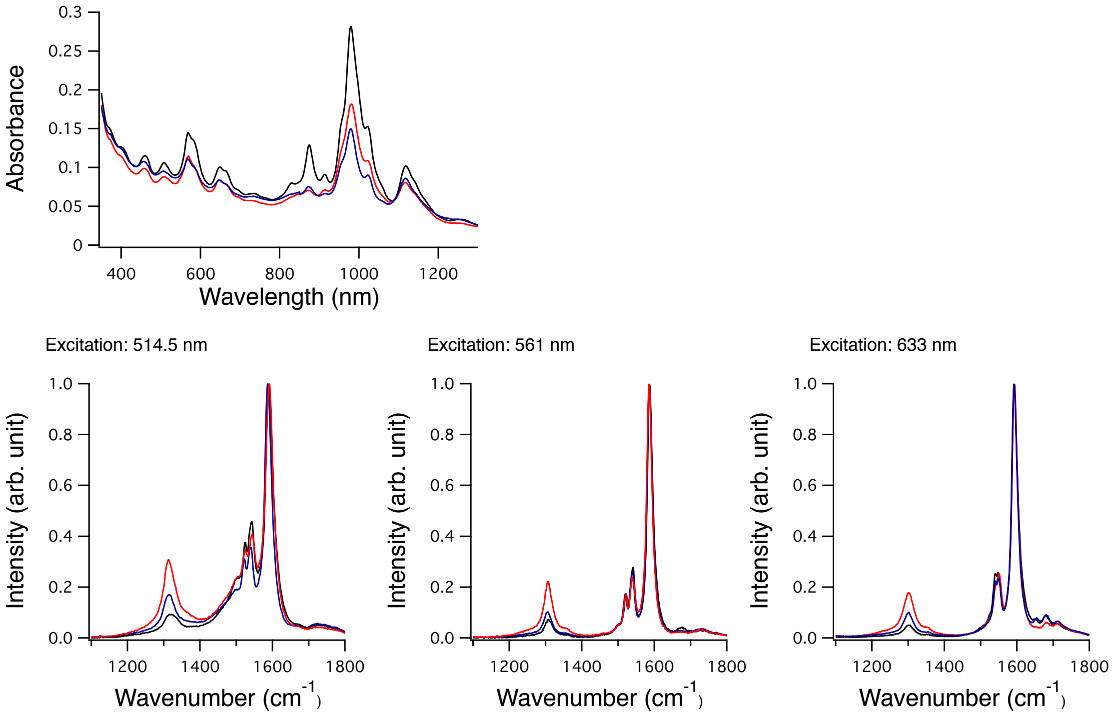
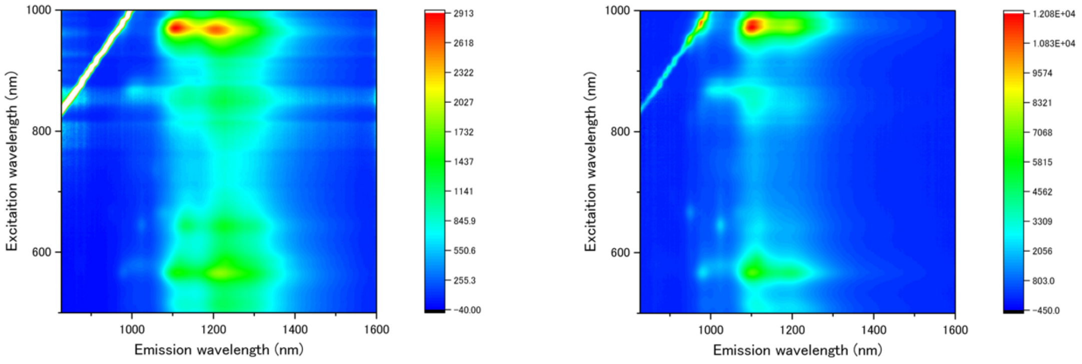
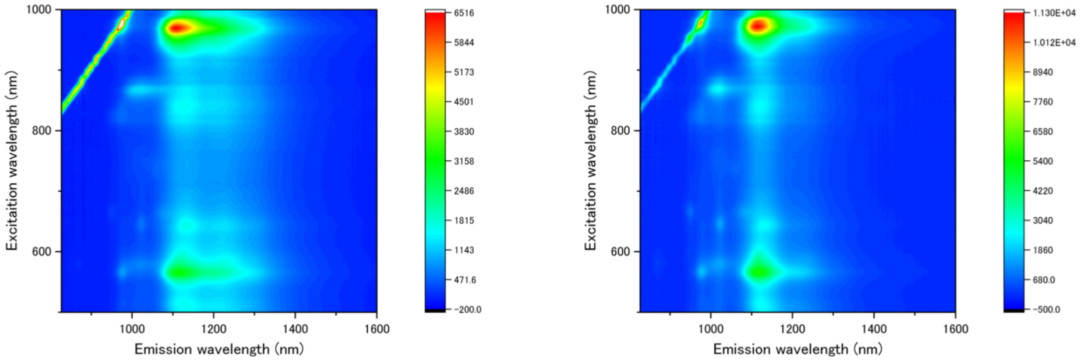


Fig. S6. Absorption and Raman spectra of SWNTs derivatives. Black: SWNTs. Red: SWNTs-G1. Blue: SWNTs-G1(200˚C). Green: SWNTs-G3.



SWNTs-G1

SWNTs-G1(200˚C)



SWNTs-G2

SWNTs-G3

Fig. S7. Contour plots of SWNTs-G1, SWNTs-G1(200˚C), SWNTs-G2, and SWNTs-G3.

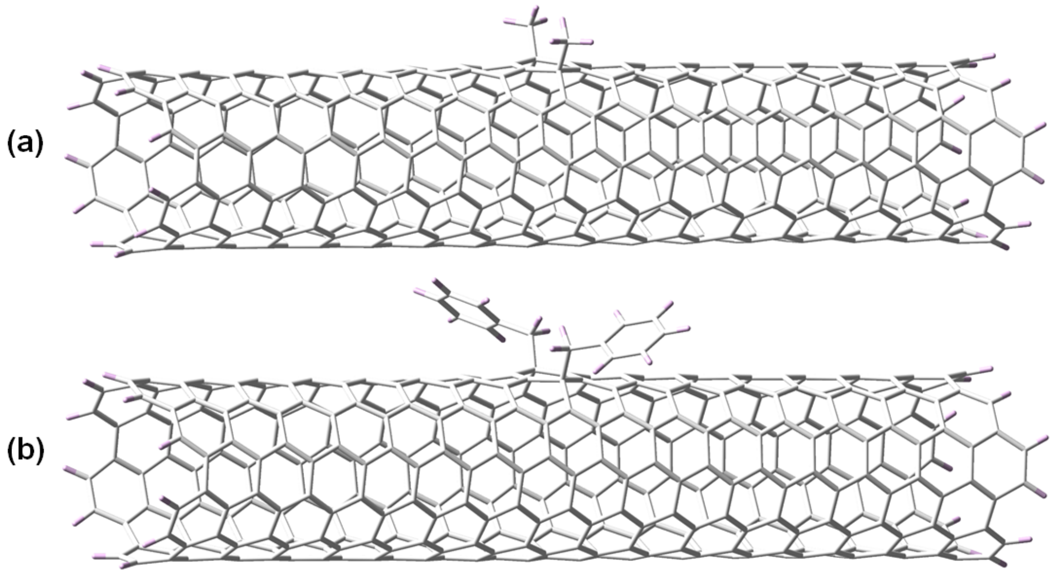


Fig. S8. The optimized structures of 1,4-adduct (L_{87}) of (a) Me-SWNT-Me and (b) Bn-SWNT-Bn (Grey: C; pink: H).

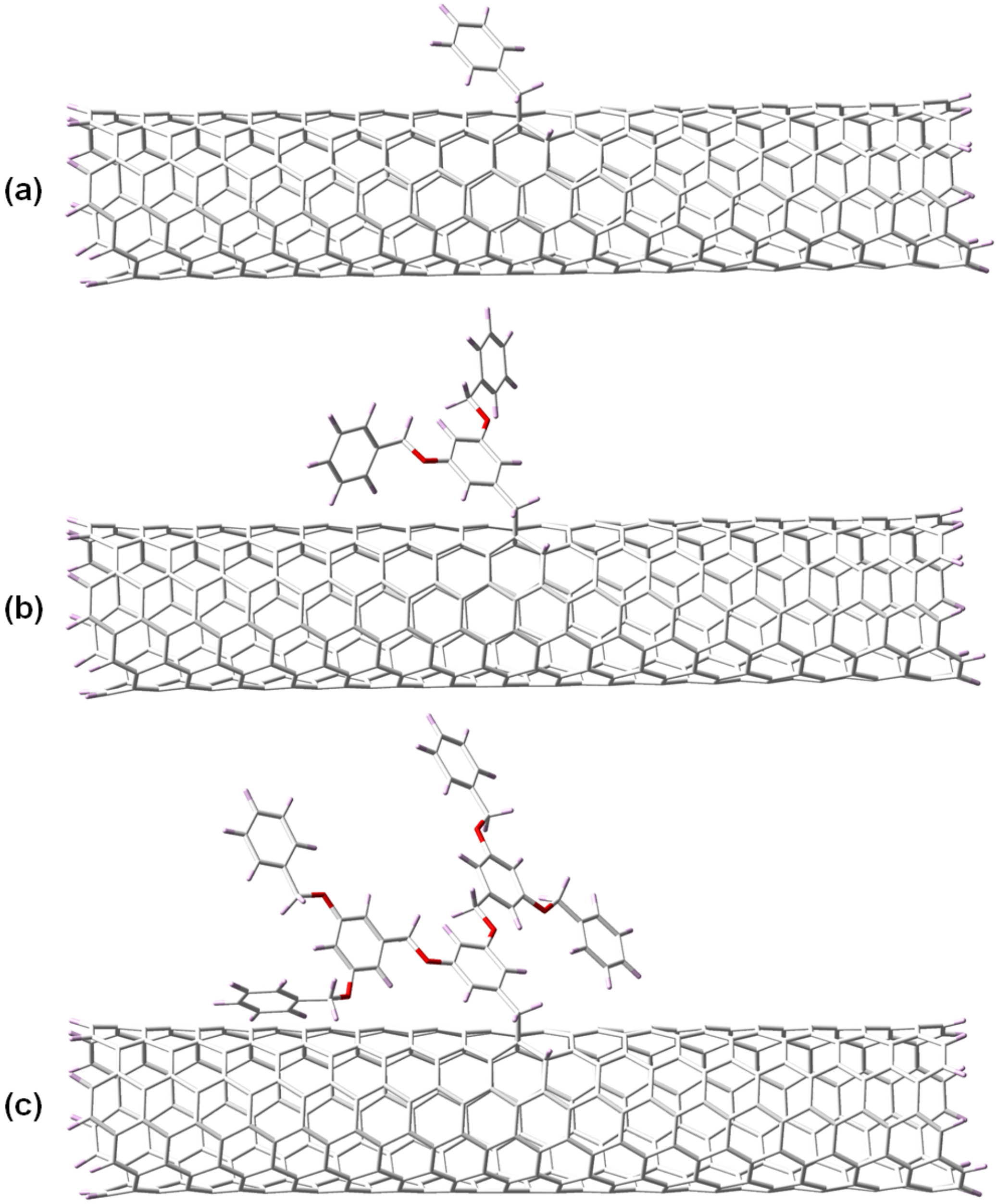


Fig. S9. The optimized structures of 1,2-adduct (L_{-33}) of (a) Bn-SWNT-H, (b) G2-SWNT-H, and (c) G3-SWNT-H (Grey: C; pink: H; red: O).

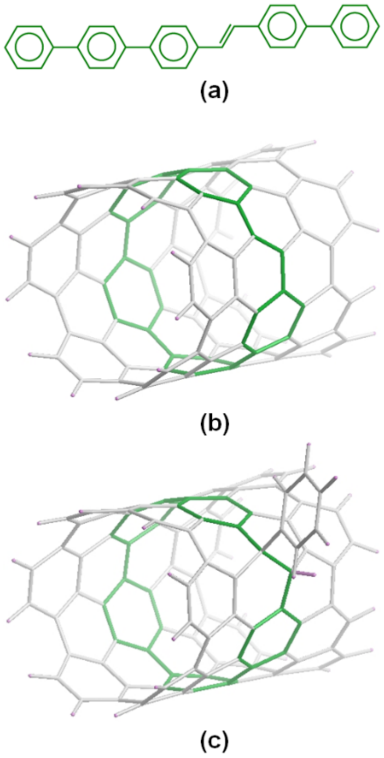


Figure S10. Finite length Clar cell (FLCC) model of (6,5) SWNT: (a) the planar representation of the unit cell, (b) the structure of pristine (6,5) SWNT consisting of three unit cells, and (c) the structure of Benzene-SWNT-H (Grey: C; pink: H). The Clar cell and the corresponding planar representation are shown in green.

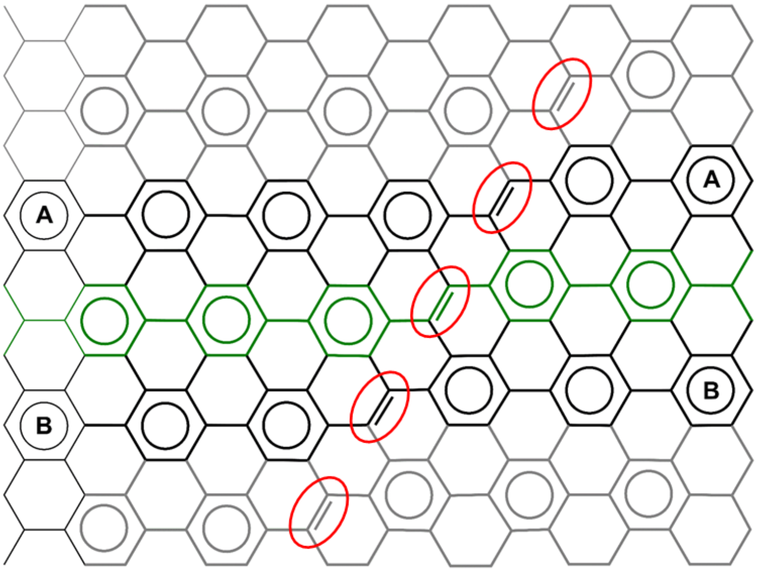


Figure S11. Schematic planar representation of FLCC model of (6,5) SWNT.

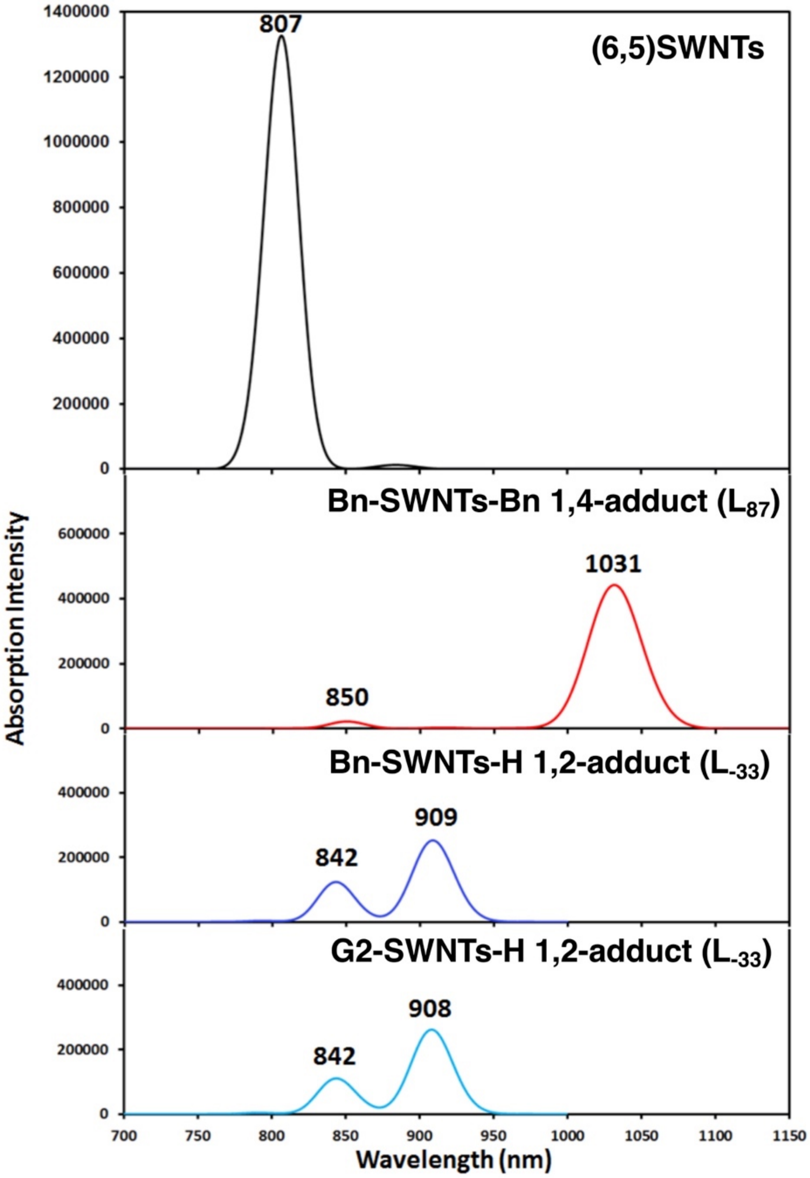


Fig. S12. Absorption spectra of the pristine (6,5) SWNT and its derivatives calculated at the level of B3LYP/6-31G*.

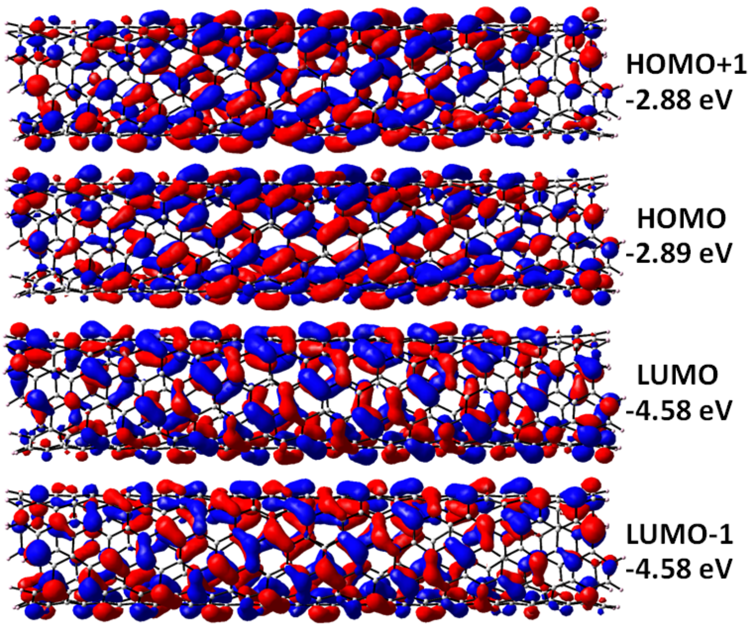


Fig. S13. Molecular orbitals of the pristine (6,5) SWNT at the level of B3LYP/6-31G* (isovalue=0.01).

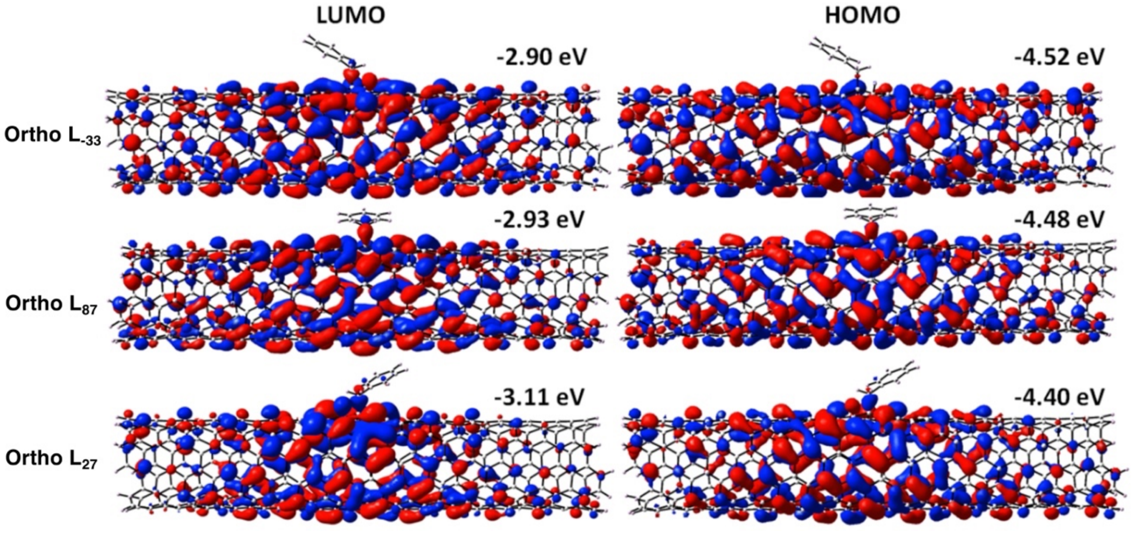


Fig. S14. Molecular orbitals of 1,2-adducts of Bn-SWNT-H at the level of B3LYP/6-31G* (isovalue=0.01).

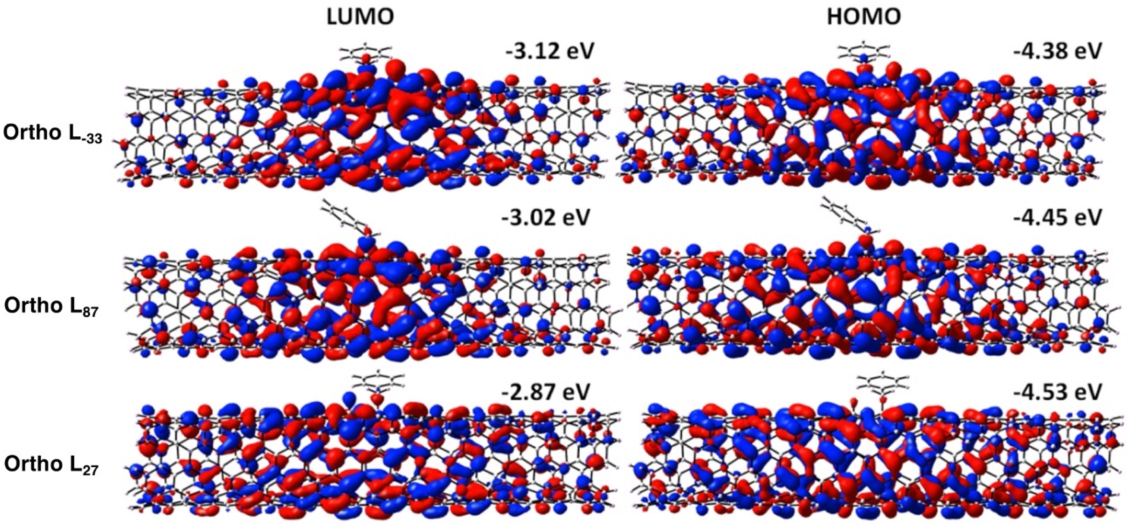


Fig. S15. Molecular orbitals of 1,4-adducts of Bn-SWNT-H at the level of B3LYP/6-31G* (isovalue=0.01).

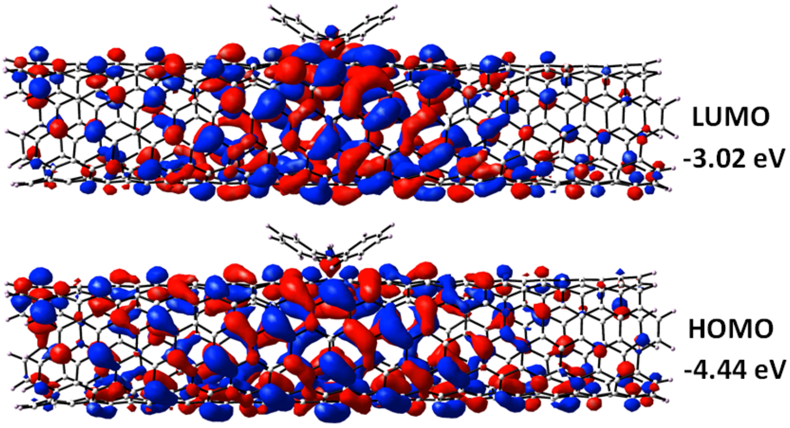


Fig. S16. Molecular orbitals of 1,4-adduct (L_{87}) of Bn-SWNT-Bn at the level of B3LYP/6-31G* (isovalue=0.01).