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Supporting Information

The role of the solvent and the size of the nanotube in the non-covalent dispersion of carbon nanotubes with short organic oligomers - A DFT Study

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Table S1. Selected bond lengths (R) (in Å), bond angles (A), and dihedral angles ($|D_h|$) (in degrees) for the isolated FLU and for FLU interacting with (6,5) and (8,7) SWCNTs obtained using B97D with 6-31G(d) and 6-31++G(d,p) basis sets. The labeling of atoms is shown in Figure 1.

	B97D/6-31G(d)			B97D/6-31++G(d,p)		
Bond Length (R)	Isolated	With (6,5) SWCNT	With (8,7) SWCNT	Isolated	With (6,5) SWCNT	With (8,7) SWCNT
R_{1-2}	1.407	1.408	1.408	1.409	1.408	1.407
R_{2-3}	1.404	1.405	1.405	1.406	1.404	1.405
R_{3-4}	1.403	1.404	1.403	1.405	1.403	1.403
R_{4-5}	1.468	1.469	1.470	1.469	1.469	1.470
R_{5-6}	1.403	1.404	1.404	1.405	1.403	1.403
R_{6-7}	1.405	1.405	1.405	1.406	1.404	1.404
R_{7-8}	1.408	1.408	1.408	1.409	1.406	1.407
Bond Angle (A)						
A_{1-2-3}	120.7	120.7	120.7	120.7	120.8	120.7
A_{2-3-4}	118.7	118.8	118.8	118.7	118.9	118.9
A_{3-4-5}	131.1	131.2	131.1	131.1	131.1	131.2
A_{4-5-6}	131.1	131.2	131.4	131.1	131.3	131.3
A_{5-6-7}	118.7	118.7	118.7	118.7	118.8	118.7
A_{6-7-8}	120.7	120.7	120.7	120.6	120.8	120.7
Dihedral Angle (|Dh|)						
$D_{1-2-3-4}$	0.0	0.0	0.0	0.0	0.1	0.0
$D_{2-3-4-5}$	180.0	180.0	179.9	180.0	179.4	179.9
$D_{3-4-5-6}$	0.0	0.1	0.3	0.0	0.6	0.2
$D_{4-5-6-7}$	180.0	179.9	179.4	180.0	178.5	179.6
$D_{5-6-7-8}$	0.0	0.1	0.1	0.0	0.3	0.1

Table S2. Selected bond lengths (R) (in Å), bond angles (A), and dihedral angles ($|D_h|$) (in degrees) for the isolated DDTF and for DDTF interacting with (6,5) and (8,7) SWCNTs obtained using B97D with 6-31G(d) and 6-31++G(d,p) basis sets. The labeling of atoms is shown in Figure 1.

	B97D/6-31G(d)			B97D/6-31++G(d,p)		
Bond Length (R)	Isolated	With (6,5) SWCNT	With (8,7) SWCNT	Isolated	With (6,5) SWCNT	With (8,7) SWCNT
R_{1-2}	1.777	1.767	1.768	1.776	1.768	1.768
R_{2-3}	1.782	1.795	1.796	1.782	1.793	1.794
R_{3-4}	1.795	1.782	1.780	1.793	1.782	1.780
R_{4-5}	1.349	1.353	1.353	1.352	1.355	1.355
Bond Angle (A)						
A_{1-2-3}	116.7	118.7	118.8	116.8	118.8	118.9
A_{2-3-4}	97.0	96.1	95.5	97.0	96.3	95.7
A_{3-4-5}	123.9	124.1	124.2	123.9	123.8	124.1
Dihedral Angle (|Dh|)						
$D_{1-2-3-4}$	179.8	176.2	172.3	179.8	177.7	173.5
$D_{2-3-4-5}$	179.9	164.4	159.4	179.9	166.0	160.9

Table S3. Selected bond lengths (R) (in Å), bond angles (A), and dihedral angles ($|D_h|$) (in degrees) for the isolated BDOB and for BDOB interacting with (6,5) and (8,7) SWCNTs obtained using B97D with 6-31G(d) and 6-31++G(d,p) basis sets. The labeling of atoms is shown in Figure 1.

	B97D/6-31G(d)			B97D/6-31++G(d,p)		
Bond Length (R)	Isolated	With (6,5) SWCNT	With (8,7) SWCNT	Isolated	With (6,5) SWCNT	With (8,7) SWCNT
R_{1-2}	1.376	1.378	1.377	1.378	1.376	1.374
R_{2-3}	1.406	1.406	1.406	1.407	1.406	1.406
R_{3-4}	1.401	1.401	1.401	1.403	1.400	1.400
R_{4-5}	1.411	1.410	1.410	1.411	1.410	1.410
R_{5-6}	1.376	1.378	1.379	1.378	1.375	1.374
Bond Angle (A)						
A_{1-2-3}	116.0	116.4	116.2	116.0	116.7	116.1
A_{2-3-4}	120.8	120.6	120.6	120.9	120.6	120.8
A_{3-4-5}	120.0	120.1	120.1	120.0	120.1	120.0
A_{4-5-6}	124.9	124.3	124.3	124.7	124.4	124.8
Dihedral Angle (|Dh|)						
$D_{1-2-3-4}$	180.0	176.2	176.3	180.0	175.7	177.2
$D_{2-3-4-5}$	0.0	1.0	0.7	0.0	0.4	0.6
$D_{3-4-5-6}$	180.0	175.0	174.5	180.0	175.5	176.6

Table S4. Selected bond lengths (R) (in Å), bond angles (A), and dihedral angles (|D_h|) (in degrees) for the isolated FLU and for FLU interacting with (6,5) and (8,7) SWCNTs obtained using wB97XD and B3LYP-D3 with 6-31G(d) basis set. The labeling of atoms is shown in Figure 1.

	wB97XD			B3LYP-D3		
Bond Length (R)	Isolated	With (6,5) SWCNT	With (8,7) SWCNT	Isolated	With (6,5) SWCNT	With (8,7) SWCNT
R_{1-2}	1.395	1.395	1.395	1.399	1.400	1.399
R_{2-3}	1.393	1.393	1.393	1.397	1.398	1.398
R_{3-4}	1.391	1.391	1.391	1.395	1.396	1.396
R_{4-5}	1.470	1.471	1.471	1.468	1.469	1.468
R_{5-6}	1.391	1.391	1.391	1.395	1.396	1.396
R_{6-7}	1.393	1.393	1.393	1.397	1.397	1.397
R_{7-8}	1.395	1.395	1.395	1.399	1.400	1.399
Bond Angle (A)						
A_{1-2-3}	120.6	120.6	120.6	120.6	120.6	120.5
A_{2-3-4}	118.8	118.7	118.8	118.8	118.8	118.8
A_{3-4-5}	131.0	131.1	131.1	131.0	131.1	131.0
A_{4-5-6}	131.0	131.0	131.1	131.0	131.0	131.0
A_{5-6-7}	118.8	118.8	118.7	118.8	118.9	118.8
A_{6-7-8}	120.6	120.6	120.6	120.6	120.6	120.6
Dihedral Angle (|Dh|)						
$D_{1-2-3-4}$	0.0	0.1	0.0	0.0	0.0	0.2
$D_{2-3-4-5}$	180.0	179.9	180.0	180.0	180.0	179.5
$D_{3-4-5-6}$	0.0	0.0	0.1	0.0	0.2	0.1
$D_{4-5-6-7}$	180.0	180.0	179.9	180.0	179.9	179.5
$D_{5-6-7-8}$	0.0	0.0	0.0	0.0	0.0	0.0

Table S5. Selected bond lengths (R) (in Å), bond angles (A), and dihedral angles (|D_h|) (in degrees) for the isolated DDTF and for DDTF interacting with (6,5) and (8,7) SWCNTs obtained using wB97XD and B3LYP-D3 with 6-31G(d) basis set. The labeling of atoms is shown in Figure 1.

	wB97XD			B3LYP-D3		
Bond Length (R)	Isolated	With (6,5) SWCNT	With (8,7) SWCNT	Isolated	With (6,5) SWCNT	With (8,7) SWCNT
R_{1-2}	1.768	1.761	1.760	1.775	1.767	1.768
R_{2-3}	1.765	1.775	1.777	1.776	1.788	1.790
R_{3-4}	1.778	1.769	1.768	1.790	1.780	1.777
R_{4-5}	1.335	1.337	1.338	1.340	1.343	1.343
Bond Angle (A)						
A_{1-2-3}	116.6	118.9	119.1	116.4	118.8	118.9
A_{2-3-4}	96.5	95.6	94.9	96.7	95.9	95.2
A_{3-4-5}	123.7	123.9	124.0	123.8	123.8	124.1
Dihedral Angle (|Dh|)						
$D_{1-2-3-4}$	179.9	176.6	171.8	180.0	175.9	171.9
$D_{2-3-4-5}$	179.9	165.1	159.8	179.9	164.9	159.7

Table S6. Selected bond lengths (R) (in Å), bond angles (A), and dihedral angles (|D_h|) (in degrees) for the isolated BDOB and for BDOB interacting with (6,5) and (8,7) SWCNTs obtained using wB97XD and B3LYP-D3 with 6-31G(d) basis set. The labeling of atoms is shown in Figure 1.

	wB97XD			B3LYP-D3		
Bond Length (R)	Isolated	With (6,5) SWCNT	With (8,7) SWCNT	Isolated	With (6,5) SWCNT	With (8,7) SWCNT
R_{1-2}	1.362	1.363	1.362	1.370	1.371	1.369
R_{2-3}	1.394	1.394	1.394	1.400	1.398	1.398
R_{3-4}	1.390	1.390	1.390	1.394	1.394	1.393
R_{4-5}	1.397	1.397	1.397	1.402	1.402	1.402
R_{5-6}	1.362	1.363	1.362	1.370	1.370	1.369
Bond Angle (A)						
A_{1-2-3}	116.1	116.9	116.4	116.0	116.8	116.3
A_{2-3-4}	121.0	120.7	120.9	121.0	120.7	120.9
A_{3-4-5}	119.9	120.0	120.0	119.9	120.0	120.0
A_{4-5-6}	124.8	124.2	124.5	124.9	124.4	124.6
Dihedral Angle (|Dh|)						
$D_{1-2-3-4}$	180.0	176.9	177.8	180.0	177.3	177.8
$D_{2-3-4-5}$	0.0	0.6	0.6	0.0	0.7	0.7
$D_{3-4-5-6}$	180.0	176.6	177.2	180.0	176.7	177.1

Table S7. Differences between bond lengths (R) (in Å), bond angles (A), and dihedral angles (|Dh|) (in degrees) obtained using B97D/6-31G(d) and those using B97D/6-31++G(d,p) for the isolated FLU and for FLU interacting with (6,5) and (8,7) SWCNTs. The labeling of atoms is shown in Figure 1.

Bond Length (R)	Isolated	With (6,5) SWCNT	With (8,7) SWCNT
R_{1-2}	0.001	0.000	0.001
R_{2-3}	0.000	0.001	0.000
R_{3-4}	0.001	0.001	0.000
R_{4-5}	0.001	0.000	0.000
R_{5-6}	0.000	0.001	0.001
R_{6-7}	0.001	0.001	0.001
R_{7-8}	0.002	0.002	0.001
Bond Angle (A)			
A_{1-2-3}	0.0	0.1	0.0
A_{2-3-4}	0.0	0.1	0.1
A_{3-4-5}	0.0	0.1	0.1
A_{4-5-6}	0.0	0.1	0.1
A_{5-6-7}	0.0	0.1	0.0
A_{6-7-8}	0.1	0.1	0.0
Dihedral Angle (|Dh|)			
$D_{1-2-3-4}$	0.0	0.1	0.0
$D_{2-3-4-5}$	0.0	0.6	0.0
$D_{3-4-5-6}$	0.0	0.5	0.1
$D_{4-5-6-7}$	0.0	1.4	0.2
$D_{5-6-7-8}$	0.0	0.2	0.0

Table S8. Differences between bond lengths (R) (in Å), bond angles (A), and dihedral angles (|Dh|) (in degrees) obtained using B97D/6-31G(d) and those using B97D/6-31++G(d,p) for the isolated DDTF and for DDTF interacting with (6,5) and (8,7) SWCNTs. The labeling of atoms is shown in Figure 1.

Bond Length (R)	Isolated	With (6,5) SWCNT	With (8,7) SWCNT
R_{1-2}	0.000	0.000	0.001
R_{2-3}	0.000	0.001	0.001
R_{3-4}	0.002	0.000	0.001
R_{4-5}	0.002	0.001	0.001
Bond Angle (A)			
A_{1-2-3}	0.0	0.0	0.0
A_{2-3-4}	0.0	0.0	0.0
A_{3-4-5}	0.0	0.0	0.0
Dihedral Angle (|Dh|)			
$D_{1-2-3-4}$	0.4	0.6	0.2
$D_{2-3-4-5}$	1.3	0.2	0.4

Table S9. Differences between bond lengths (R) (in Å), bond angles (A), and dihedral angles (|Dh|) (in degrees) obtained using B97D/6-31G(d) and those using B97D/6-31++G(d,p) for the isolated BDOB and for BDOB interacting with (6,5) and (8,7) SWCNTs. The labeling of atoms is shown in Figure 1.

Bond Length (R)	Isolated	With (6,5) SWCNT	With (8,7) SWCNT
R_{1-2}	0.002	0.002	0.003
R_{2-3}	0.001	0.000	0.000
R_{3-4}	0.002	0.001	0.001
R_{4-5}	0.000	0.000	0.000
R_{5-6}	0.002	0.003	0.005
Bond Angle (A)			
A_{1-2-3}	0.0	0.3	0.1
A_{2-3-4}	0.1	0.0	0.2
A_{3-4-5}	0.0	0.0	0.1
A_{4-5-6}	0.2	0.1	0.5
Dihedral Angle (|Dh|)			
$D_{1-2-3-4}$	0.0	0.5	0.9
$D_{2-3-4-5}$	0.0	0.6	0.1
$D_{3-4-5-6}$	0.0	0.5	2.1

Table S10. Selected bond lengths (R) (in Å), bond angles (A), and dihedral angles (|D_h|) (in degrees) for the isolated FLU and for FLU interacting with (6,5) and (8,7) SWCNTs obtained using B97D/6-31G(d) in PCM with chloroform and hexane solvents. The labeling of atoms is shown in Figure 1.

	Chloroform			Hexane		
Bond Length (R)	Isolated	With (6,5) SWCNT	With (8,7) SWCNT	Isolated	With (6,5) SWCNT	With (8,7) SWCNT
R_{1-2}	1.408	1.409	1.408	1.408	1.408	1.408
R_{2-3}	1.405	1.405	1.405	1.405	1.405	1.405
R_{3-4}	1.404	1.404	1.404	1.404	1.404	1.404
R_{4-5}	1.469	1.470	1.470	1.469	1.469	1.469
R_{5-6}	1.404	1.404	1.404	1.404	1.404	1.404
R_{6-7}	1.405	1.405	1.405	1.405	1.405	1.405
R_{7-8}	1.408	1.408	1.408	1.408	1.408	1.408
Bond Angle (A)						
A_{1-2-3}	120.7	120.7	120.7	120.7	120.7	120.7
A_{2-3-4}	118.7	118.7	118.7	118.7	118.7	118.7
A_{3-4-5}	131.0	131.2	131.3	131.1	131.2	131.3
A_{4-5-6}	131.0	131.1	131.2	131.1	131.2	131.1
A_{5-6-7}	118.7	118.7	118.7	118.7	118.7	118.8
A_{6-7-8}	120.7	120.7	120.7	120.7	120.7	120.8
Dihedral Angle (|Dh|)						
$D_{1-2-3-4}$	0.0	0.1	0.1	0.0	0.1	0.3
$D_{2-3-4-5}$	180.0	179.9	179.7	180.0	180.0	179.0
$D_{3-4-5-6}$	0.0	0.1	0.3	0.0	0.0	0.5
$D_{4-5-6-7}$	180.0	180.0	180.0	180.0	180.0	179.6
$D_{5-6-7-8}$	0.0	0.0	0.0	0.0	0.0	0.0

Table S11. Selected bond lengths (R) (in Å), bond angles (A), and dihedral angles (|D_h|) (in degrees) for the isolated DDTF and for DDTF interacting with (6,5) and (8,7) SWCNTs obtained using B97D/6-31G(d) in PCM with chloroform and hexane solvents. The labeling of atoms is shown in Figure 1.

	Chloroform			Hexane		
Bond Length (R)	Isolated	With (6,5) SWCNT	With (8,7) SWCNT	Isolated	With (6,5) SWCNT	With (8,7) SWCNT
R_{1-2}	1.776	1.769	1.769	1.776	1.768	1.768
R_{2-3}	1.784	1.795	1.796	1.783	1.795	1.796
R_{3-4}	1.796	1.785	1.783	1.796	1.784	1.782
R_{4-5}	1.349	1.351	1.351	1.349	1.352	1.352
Bond Angle (A)						
A_{1-2-3}	116.8	118.5	118.7	116.7	118.6	118.8
A_{2-3-4}	97.1	96.0	95.3	97.0	96.0	95.4
A_{3-4-5}	124.0	124.1	124.2	123.9	124.1	124.2
Dihedral Angle (|Dh|)						
$D_{1-2-3-4}$	179.9	175.4	171.8	179.8	175.8	172.1
$D_{2-3-4-5}$	179.9	163.9	159.0	179.9	164.2	159.4

Table S12. Selected bond lengths (R) (in Å), bond angles (A), and dihedral angles ($|D_h|$) (in degrees) for the isolated BDOB and for BDOB interacting with (6,5) and (8,7) SWCNTs obtained using B97D/6-31G(d) in PCM with chloroform and hexane solvents. The labeling of atoms is shown in Figure 1.

	Chloroform			Hexane		
Bond Length (R)	Isolated	With (6,5) SWCNT	With (8,7) SWCNT	Isolated	With (6,5) SWCNT	With (8,7) SWCNT
R_{1-2}	1.375	1.377	1.375	1.376	1.377	1.375
R_{2-3}	1.408	1.406	1.407	1.407	1.406	1.406
R_{3-4}	1.402	1.400	1.400	1.401	1.400	1.400
R_{4-5}	1.411	1.410	1.410	1.411	1.410	1.410
R_{5-6}	1.375	1.376	1.375	1.376	1.376	1.375
Bond Angle (A)						
A_{1-2-3}	116.0	116.8	116.2	116.0	116.7	116.2
A_{2-3-4}	120.9	120.5	120.8	120.9	120.5	120.8
A_{3-4-5}	120.0	120.1	120.0	120.0	120.1	120.0
A_{4-5-6}	124.9	124.3	124.6	124.9	124.4	124.7
Dihedral Angle (|Dh|)						
$D_{1-2-3-4}$	180.0	176.0	177.5	180.0	175.9	177.4
$D_{2-3-4-5}$	0.0	0.4	0.6	0.0	0.4	0.6
$D_{3-4-5-6}$	180.0	175.7	176.9	180.0	175.6	176.8

Table S13. Differences between bond lengths (R) (in Å), bond angles (A), and dihedral angles (|Dh|) (in degrees) obtained using B97D/6-31G(d) without a solvent and those obtained using B97D/6-31G(d) in PCM/chloroform and in PCM/hexane respectively for the isolated FLU and for FLU interacting with (6,5) and (8,7) SWCNTs. The labeling of atoms is shown in Figure 1.

	Chloroform			Hexane		
Bond Length (R)	Isolated	With (6,5) SWCNT	With (8,7) SWCNT	Isolated	With (6,5) SWCNT	With (8,7) SWCNT
R_{1-2}	0.001	0.001	0.000	0.001	0.000	0.000
R_{2-3}	0.001	0.000	0.000	0.001	0.000	0.000
R_{3-4}	0.001	0.000	0.001	0.001	0.000	0.001
R_{4-5}	0.001	0.001	0.000	0.001	0.000	0.001
R_{5-6}	0.001	0.000	0.000	0.001	0.000	0.000
R_{6-7}	0.000	0.000	0.000	0.000	0.000	0.000
R_{7-8}	0.000	0.000	0.000	0.000	0.000	0.000
Bond Angle (A)						
A_{1-2-3}	0.0	0.0	0.0	0.0	0.0	0.0
A_{2-3-4}	0.0	0.1	0.1	0.0	0.1	0.1
A_{3-4-5}	0.1	0.0	0.2	0.0	0.0	0.2
A_{4-5-6}	0.1	0.1	0.2	0.0	0.0	0.3
A_{5-6-7}	0.0	0.0	0.0	0.0	0.0	0.1
A_{6-7-8}	0.0	0.0	0.0	0.0	0.0	0.1
Dihedral Angle (|Dh|)						
$D_{1-2-3-4}$	0.0	0.1	0.1	0.0	0.1	0.3
$D_{2-3-4-5}$	0.0	0.1	0.2	0.0	0.0	0.9
$D_{3-4-5-6}$	0.0	0.0	0.0	0.0	0.1	0.2
$D_{4-5-6-7}$	0.0	0.1	0.6	0.0	0.1	0.2
$D_{5-6-7-8}$	0.0	0.1	0.1	0.0	0.1	0.1

Table S14. Differences between bond lengths (R) (in Å), bond angles (A), and dihedral angles (|Dh|) (in degrees) obtained using B97D/6-31G(d) without a solvent and those obtained using B97D/6-31G(d) in PCM/chloroform and in PCM/hexane respectively for the isolated DDTF and for DDTF interacting with (6,5) and (8,7) SWCNTs. The labeling of atoms is shown in Figure 1.

	Chloroform			Hexane		
Bond Length (R)	Isolated	With (6,5) SWCNT	With (8,7) SWCNT	Isolated	With (6,5) SWCNT	With (8,7) SWCNT
R_{1-2}	0.001	0.002	0.001	0.001	0.001	0.000
R_{2-3}	0.002	0.000	0.000	0.001	0.000	0.000
R_{3-4}	0.001	0.003	0.003	0.001	0.002	0.002
R_{4-5}	0.000	0.002	0.002	0.000	0.001	0.001
Bond Angle (A)						
A_{1-2-3}	0.1	0.2	0.1	0.0	0.1	0.0
A_{2-3-4}	0.1	0.1	0.2	0.0	0.1	0.1
A_{3-4-5}	0.1	0.0	0.0	0.0	0.0	0.0
Dihedral Angle (|Dh|)						
$D_{1-2-3-4}$	0.1	0.8	0.5	0.0	0.4	0.2
$D_{2-3-4-5}$	0.0	0.5	0.4	0.0	0.2	0.0

Table S15. Differences between bond lengths (R) (in Å), bond angles (A), and dihedral angles (|Dh|) (in degrees) obtained using B97D/6-31G(d) without a solvent and those obtained using B97D/6-31G(d) in PCM/chloroform and in PCM/hexane respectively for the isolated BDOB and for BDOB interacting with (6,5) and (8,7) SWCNTs. The labeling of atoms is shown in Figure 1.

	Chloroform			Hexane		
Bond Length (R)	Isolated	With (6,5) SWCNT	With (8,7) SWCNT	Isolated	With (6,5) SWCNT	With (8,7) SWCNT
R_{1-2}	0.001	0.001	0.002	0.000	0.001	0.002
R_{2-3}	0.002	0.000	0.001	0.001	0.000	0.000
R_{3-4}	0.001	0.001	0.001	0.000	0.001	0.001
R_{4-5}	0.000	0.000	0.000	0.000	0.000	0.000
R_{5-6}	0.001	0.002	0.004	0.000	0.002	0.004
Bond Angle (A)						
A_{1-2-3}	0.0	0.4	0.0	0.0	0.3	0.0
A_{2-3-4}	0.1	0.1	0.2	0.1	0.1	0.2
A_{3-4-5}	0.0	0.0	0.1	0.0	0.0	0.1
A_{4-5-6}	0.0	0.0	0.3	0.0	0.1	0.4
Dihedral Angle (|Dh|)						
$D_{1-2-3-4}$	0.0	0.2	1.2	0.0	0.3	1.1
$D_{2-3-4-5}$	0.0	0.6	0.1	0.0	0.6	0.1
$D_{3-4-5-6}$	0.0	0.7	2.4	0.0	0.6	2.3

Table S16. HOMO and LUMO energies (in eV) for isolated FLU, DDTF, BDOB, and SWCNTs obtained using B3LYP/6-31G(d) without a solvent and with chloroform and hexane solvents.

	Isolated molecules			SWCNT	
No solvent	FLU	DDTF	BDOB	(6,5)	(8,7)
E_{HOMO}	-5.72	-5.19	-5.18	-4.41	-4.70
E_{LUMO}	-0.77	-0.95	0.15	-2.55	-2.28
Chloroform					
E_{HOMO}	-5.80	-5.36	-5.36	-4.48	-4.78
E_{LUMO}	-0.84	-1.07	-0.05	-2.62	-2.36
Hexane					
E_{HOMO}	-5.76	-5.28	-5.27	-4.43	-4.72
E_{LUMO}	-0.80	-1.01	0.05	-2.58	-2.31

Table S17. HOMO and LUMO energies (in eV) for interacting FLU, DDTF, and BDOB with (6,5) and (8,7) SWCNTs obtained using B3LYP/6-31G(d)//B3LYP-D3/6-31G(d) without a solvent.

	With (6,5) SWCNT			With (8,7) SWCNT		
No solvent	FLU	DDTF	BDOB	FLU	DDTF	BDOB
E_{HOMO}	-5.73	-4.97	-5.27	-5.72	-4.90	-5.21
E_{LUMO}	-0.77	-0.52	0.12	-0.75	-0.58	0.13

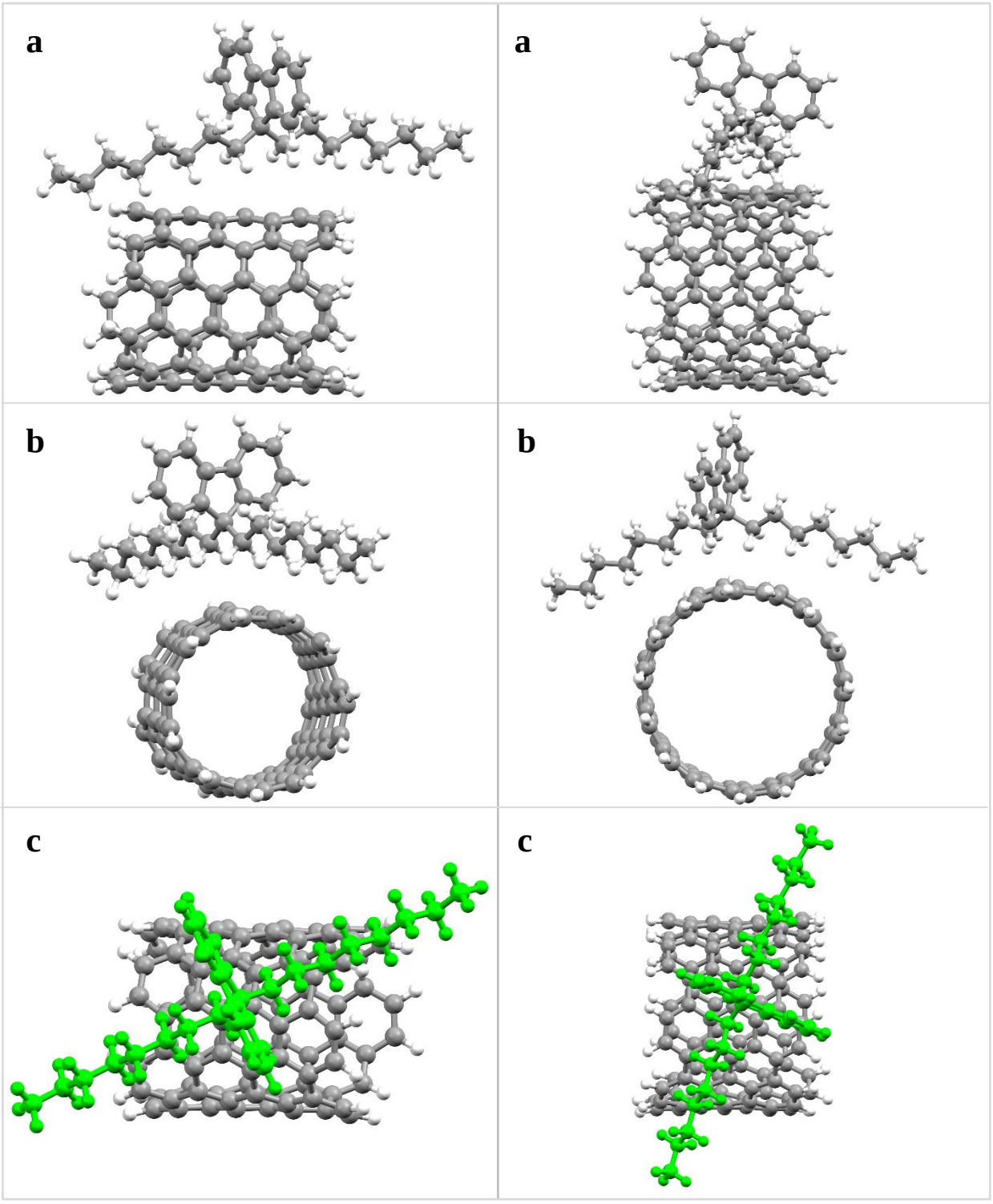


Figure S1. Representative (partially) optimized structures of FLU molecule interacting with (6,5) SWCNT (left) and (8,7) SWCNT (right) obtained using B97D/6-31G(d); (a) side view, (b) front view, and (c) top view with the oligomers highlighted (similar results are obtained with B97D/6-31++G(d,p) and other D-DFT methods with 6-31G(d) basis set).

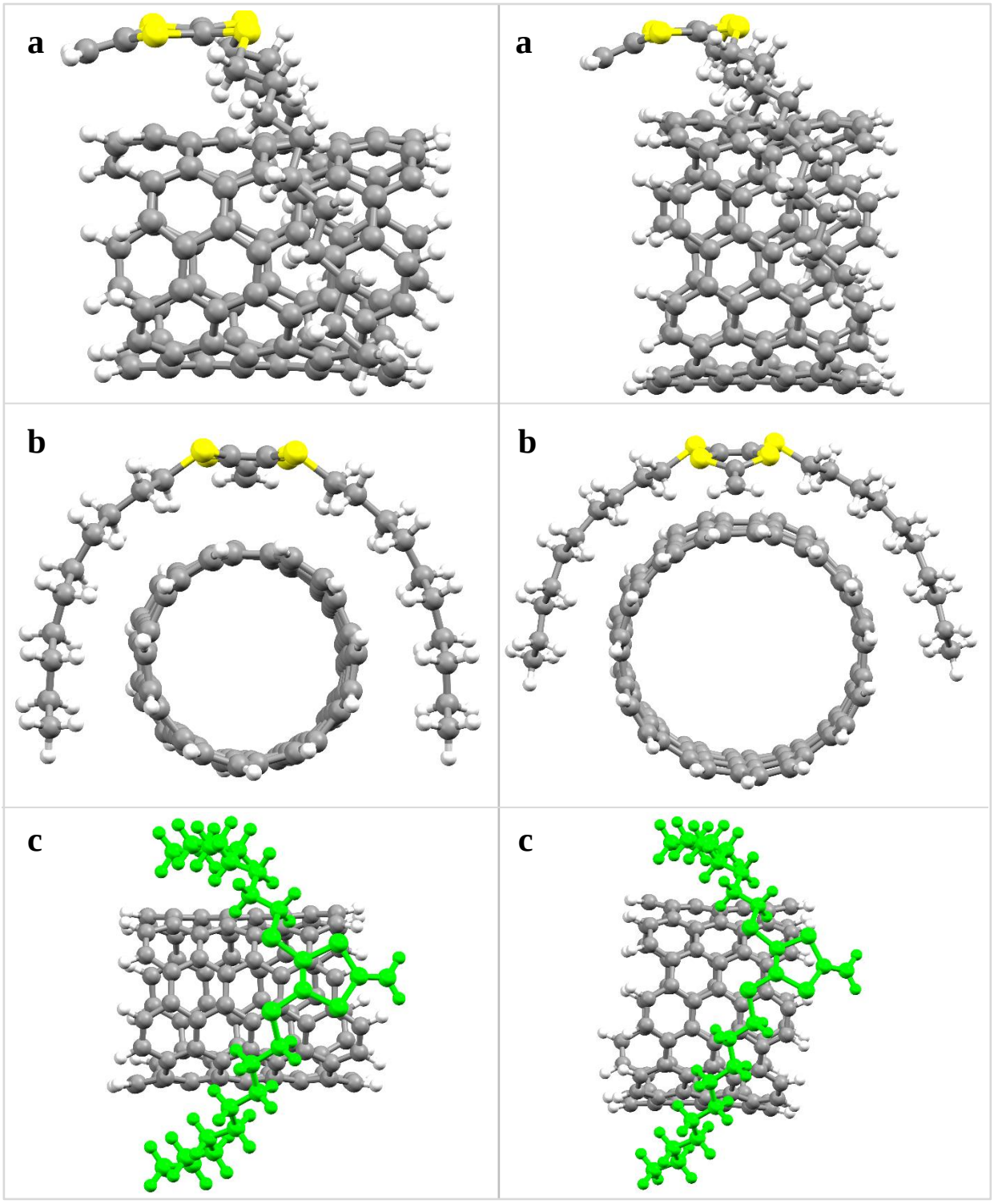


Figure S2. Representative (partially) optimized structures of DDTF molecule interacting with (6,5) SWCNT (left) and (8,7) SWCNT (right) obtained using B97D/6-31G(d); (a) side view, (b) front view, and (c) top view with the oligomers highlighted (similar results are obtained with B97D/6-31++G(d,p) and other D-DFT methods with 6-31G(d) basis set).

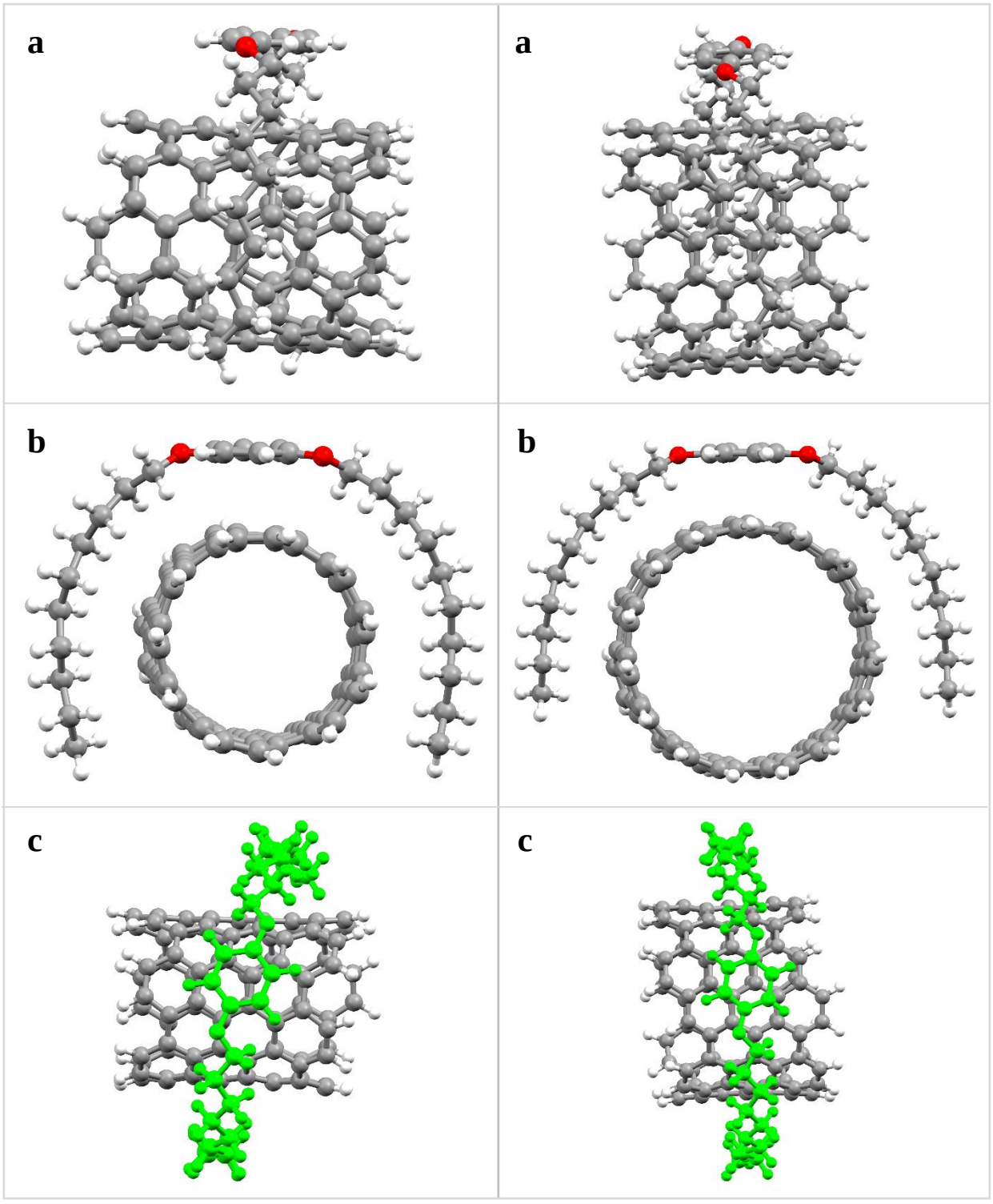
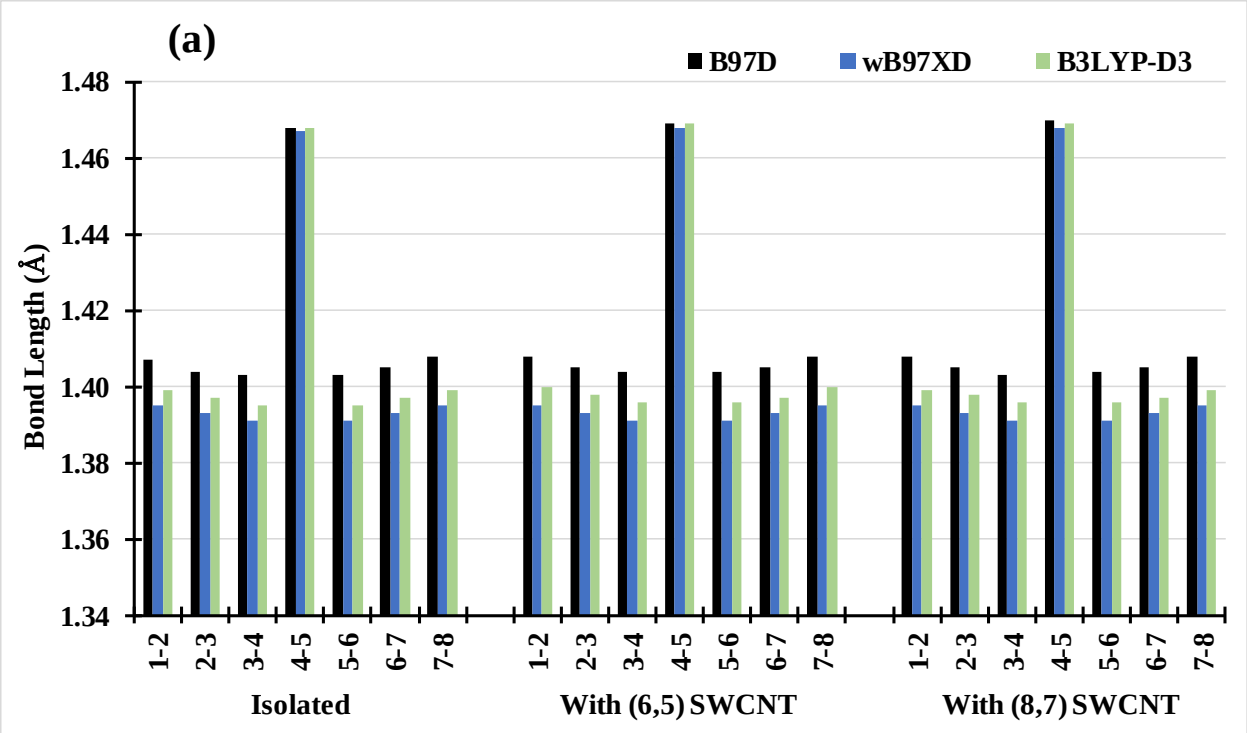
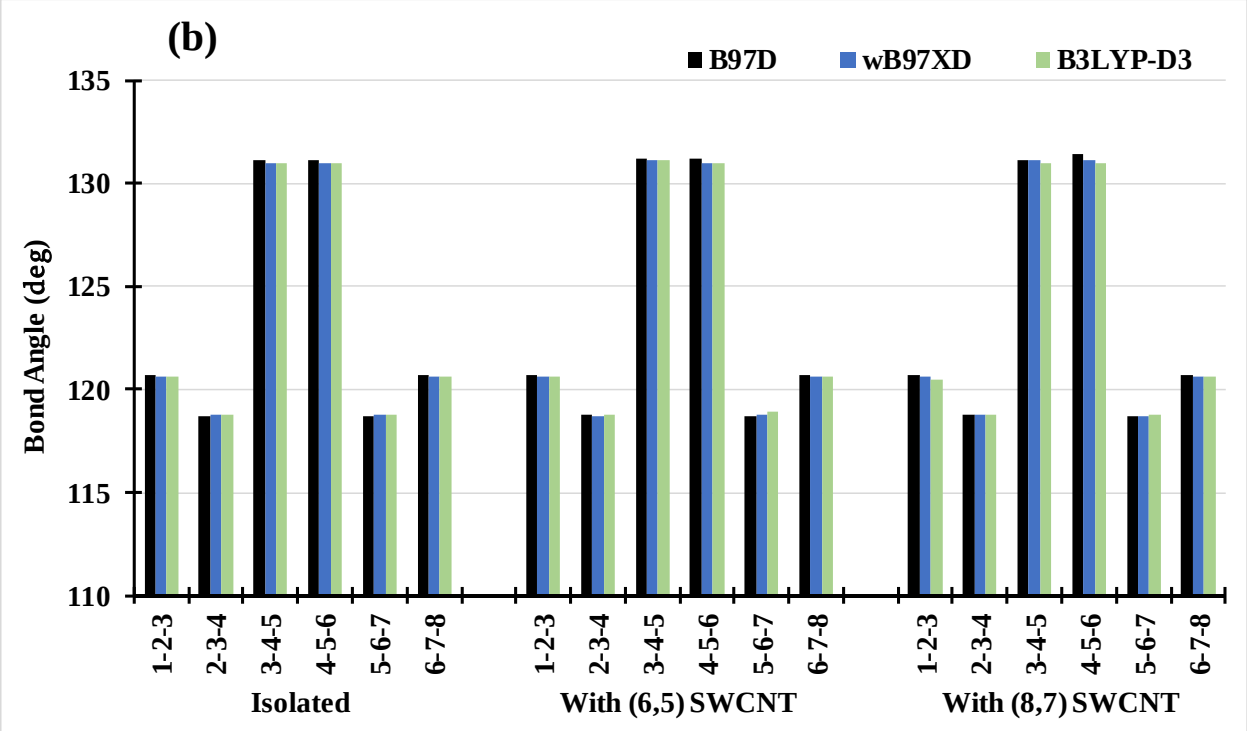


Figure S3. Representative (partially) optimized structures of BDOB molecule interacting with (6,5) SWCNT (left) and (8,7) SWCNT (right) obtained using B97D/6-31G(d); (a) side view, (b) front view, and (c) top view with the oligomers highlighted (similar results are obtained with B97D/6-31++G(d,p) and other D-DFT methods with 6-31G(d) basis set).


(a)
B97D
wB97XD
B3LYP-D3
Bond Length (Å)
1.48
1.46
1.44
1.42
1.40
1.38
1.36
1.34
1-2
2-3
3-4
4-5
5-6
6-7
7-8
Isolated
With (6,5) SWCNT
With (8,7) SWCNT


(b)
B97D
wB97XD
B3LYP-D3
Bond Angle (deg)
135
130
125
120
115
110
1-2-3
2-3-4
3-4-5
4-5-6
5-6-7
6-7-8
Isolated
With (6,5) SWCNT
With (8,7) SWCNT

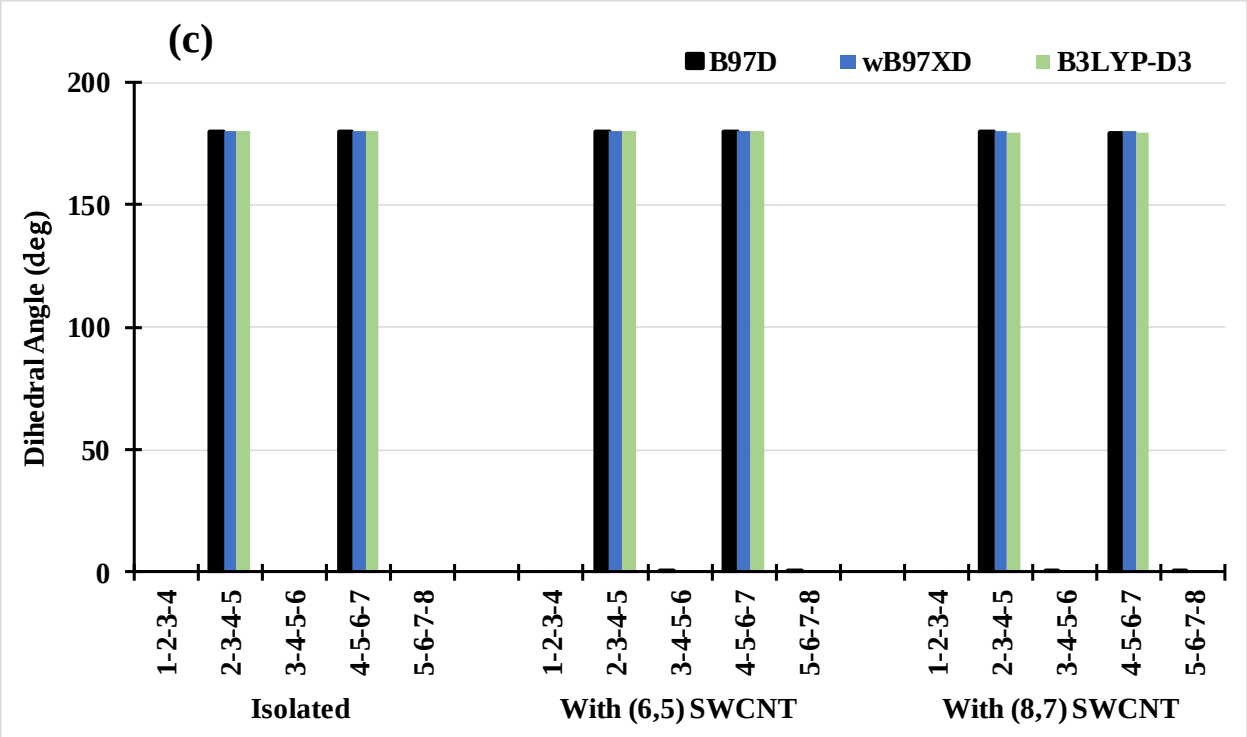
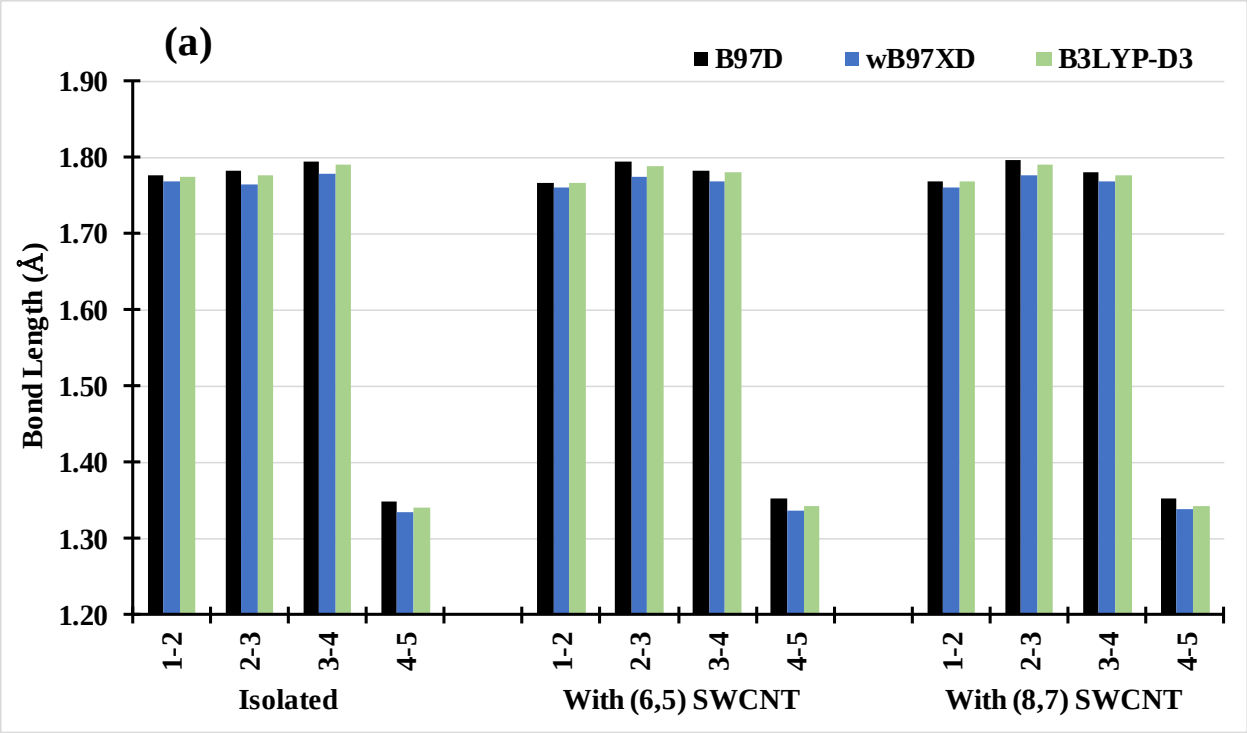
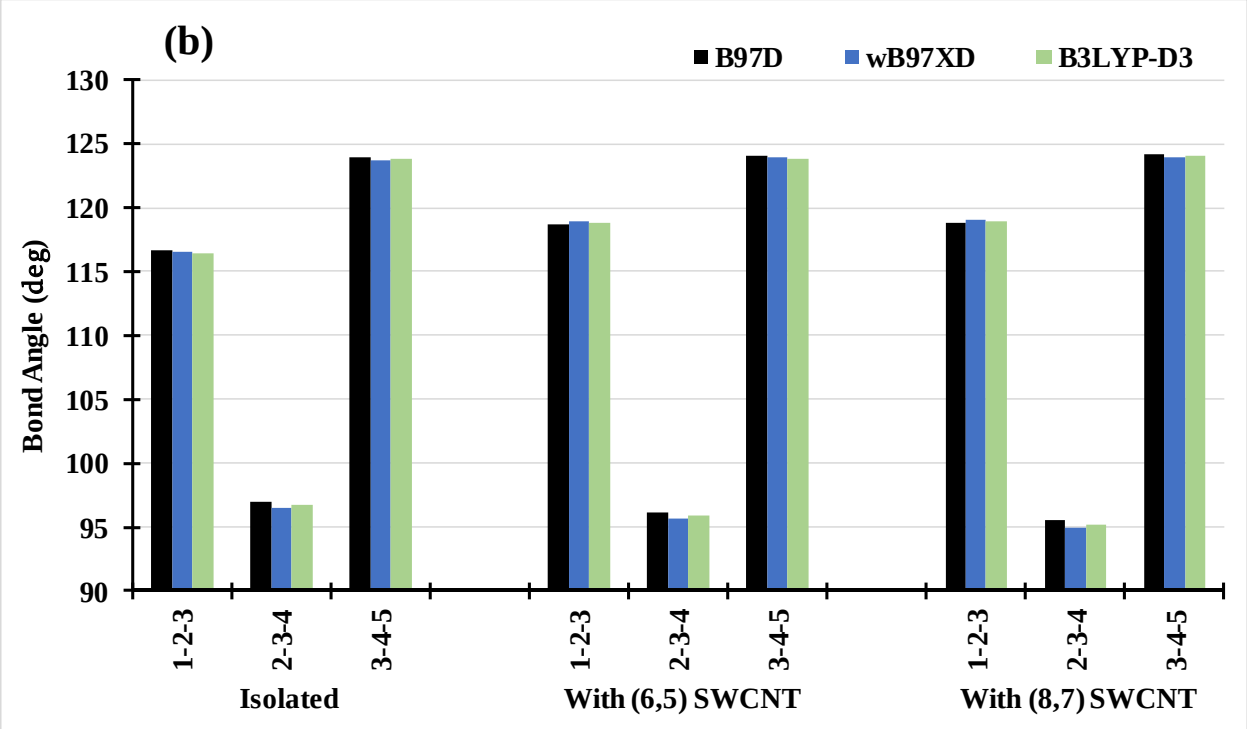


Figure S4. (**a**) bond lengths (in Å), (**b**) bond angles, and (**c**) dihedral angles (in degrees) for the isolated FLU and for FLU interacting with (6,5) and (8,7) SWCNTs obtained using B97D, wB97XD, and B3LYP-D3 with 6-31G(d) basis set.


(a)
B97D
wB97XD
B3LYP-D3
Bond Length (Å)
1.90
1.80
1.70
1.60
1.50
1.40
1.30
1.20
1-2
2-3
3-4
4-5
Isolated
With (6,5) SWCNT
With (8,7) SWCNT


(b)
B97D
wB97XD
B3LYP-D3
Bond Angle (deg)
130
125
120
115
110
105
100
95
90
1-2-3
2-3-4
3-4-5
Isolated
With (6,5) SWCNT
With (8,7) SWCNT

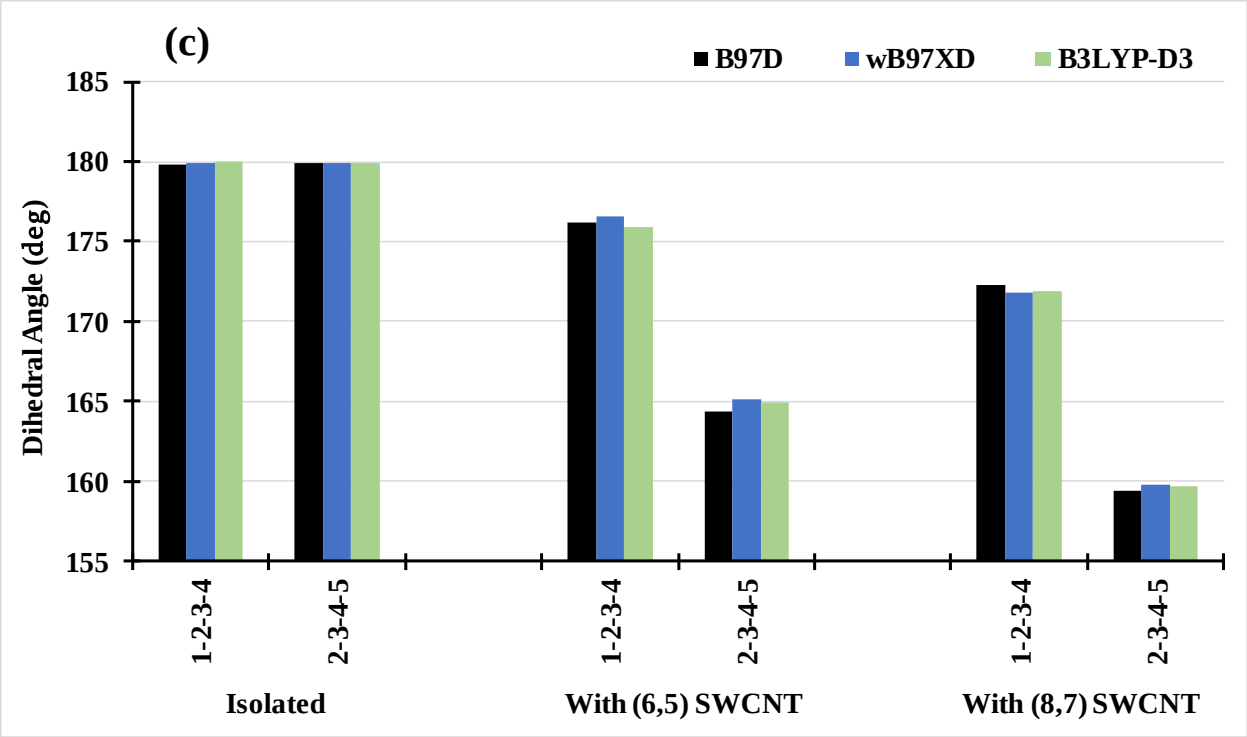
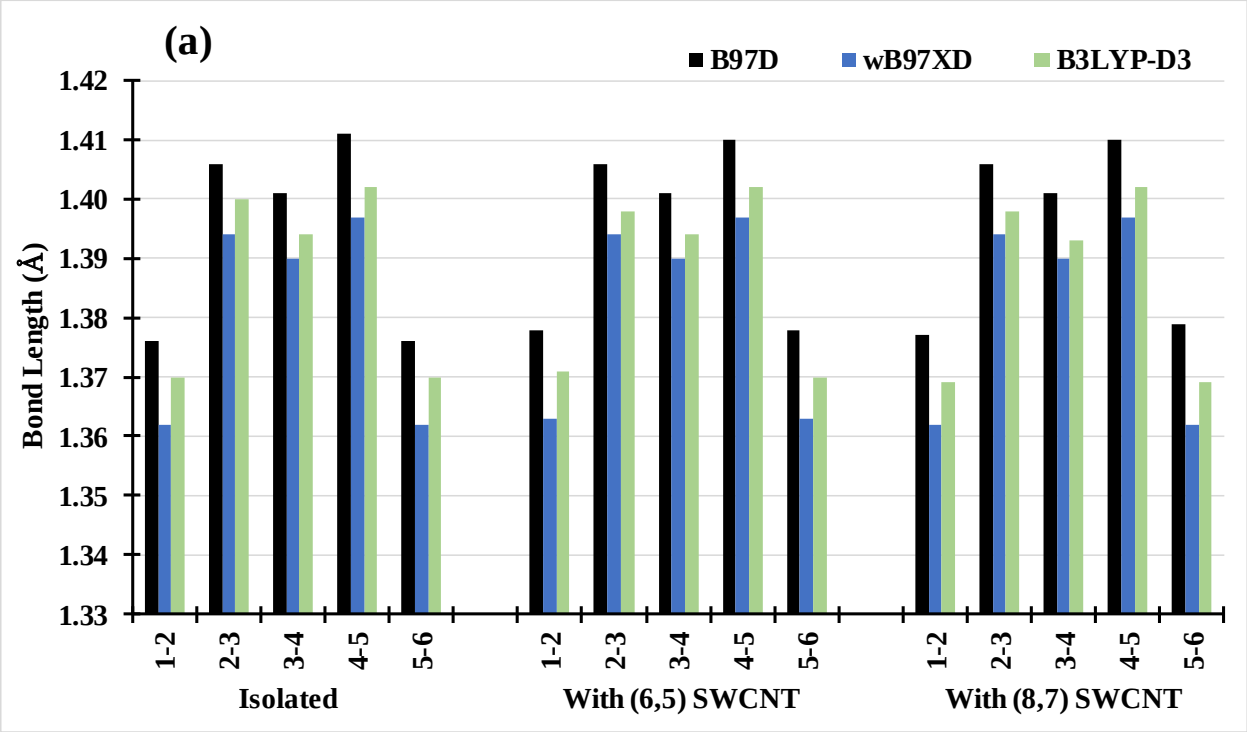
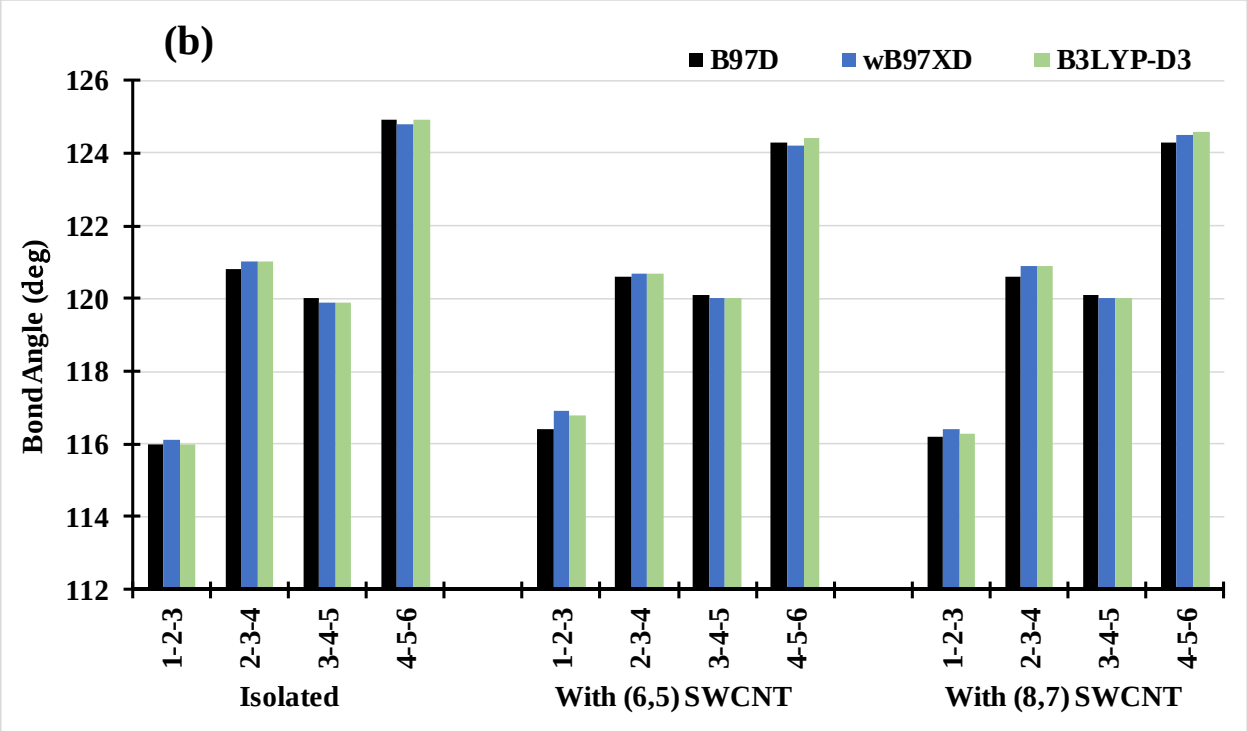


Figure S5. (**a**) bond lengths (in Å), (**b**) bond angles, and (**c**) dihedral angles (in degrees) for the isolated DDTF and for DDTF interacting with (6,5) and (8,7) SWCNTs obtained using B97D, wB97XD, and B3LYP-D3 with 6-31G(d) basis set.


(a)
B97D
wB97XD
B3LYP-D3
Bond Length (Å)
1.42
1.41
1.40
1.39
1.38
1.37
1.36
1.35
1.34
1.33
1-2
2-3
3-4
4-5
5-6
Isolated
With (6,5) SWCNT
With (8,7) SWCNT


(b)
B97D
wB97XD
B3LYP-D3
Bond Angle (deg)
126
124
122
120
118
116
114
112
1-2-3
2-3-4
3-4-5
4-5-6
Isolated
With (6,5) SWCNT
With (8,7) SWCNT

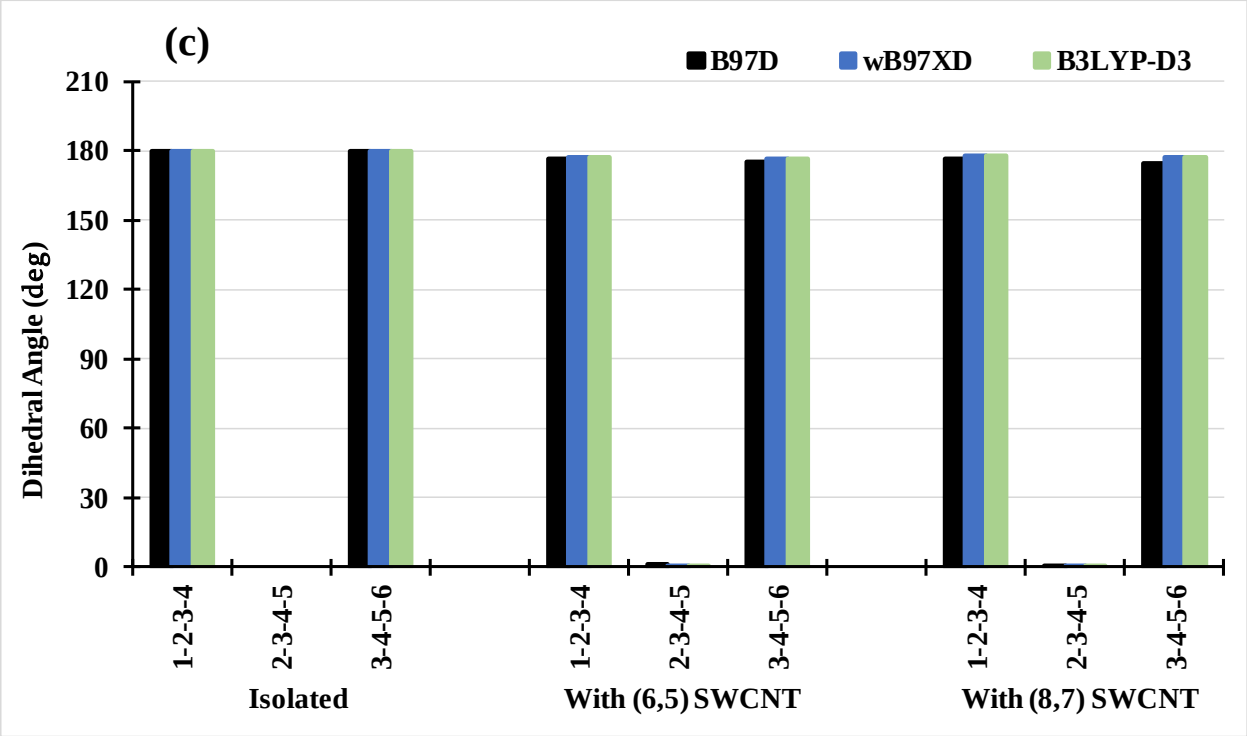


Figure S6. (**a**) bond lengths (in Å), (**b**) bond angles, and (**c**) dihedral angles (in degrees) for the isolated BDOB and for BDOB interacting with (6,5) and (8,7) SWCNTs obtained using B97D, wB97XD, and B3LYP-D3 with 6-31G(d) basis set.