Supporting Information

Molecular dynamics simulation study of Glycine tip-functionalization of single-walled carbon nanotubes as emerging nanovectors for the delivery of anticancer drugs

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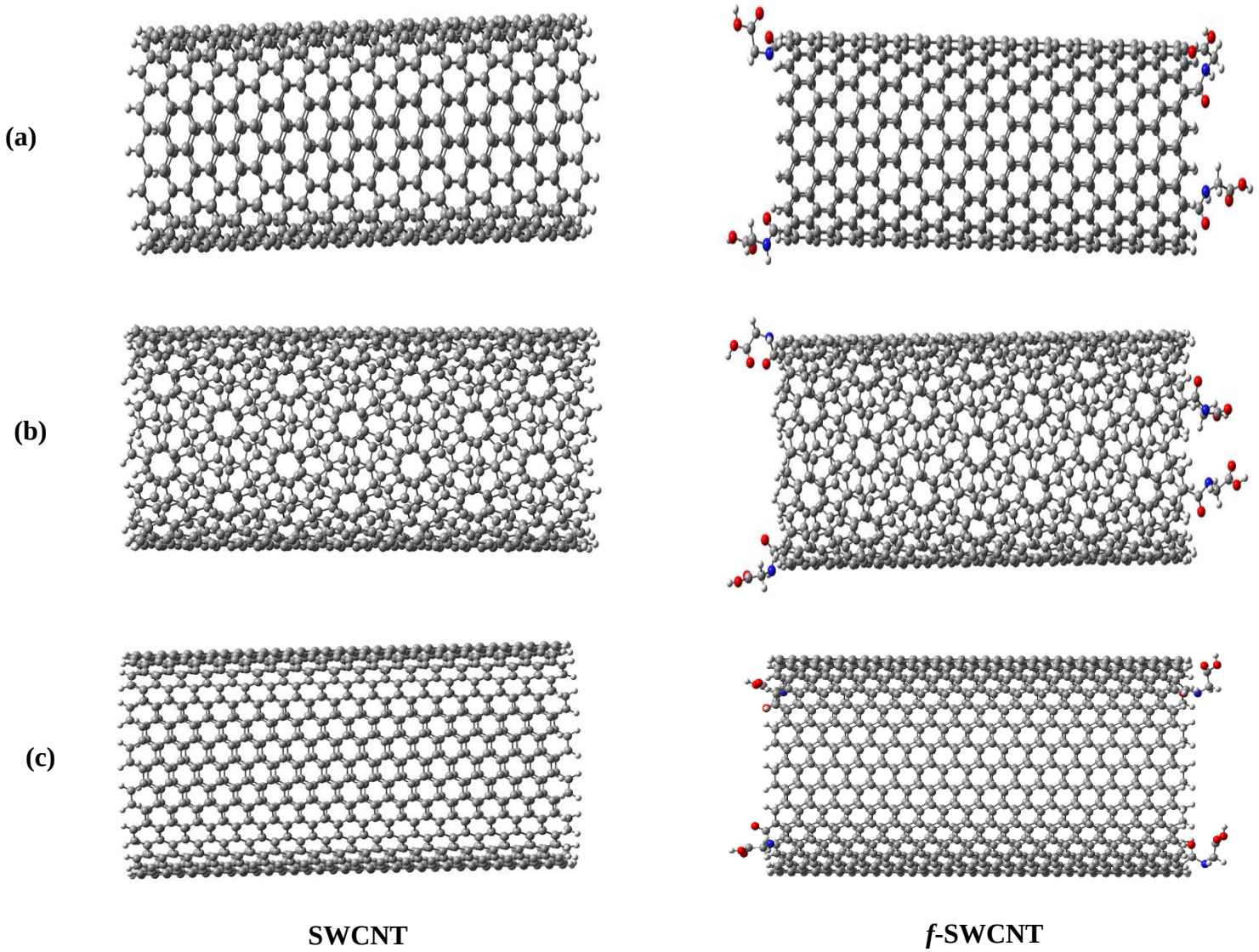


Figure SF1. The structures of (a) zigzag, (b) chiral and (c) armchiar pristine and functionalized carbon nanotubes.

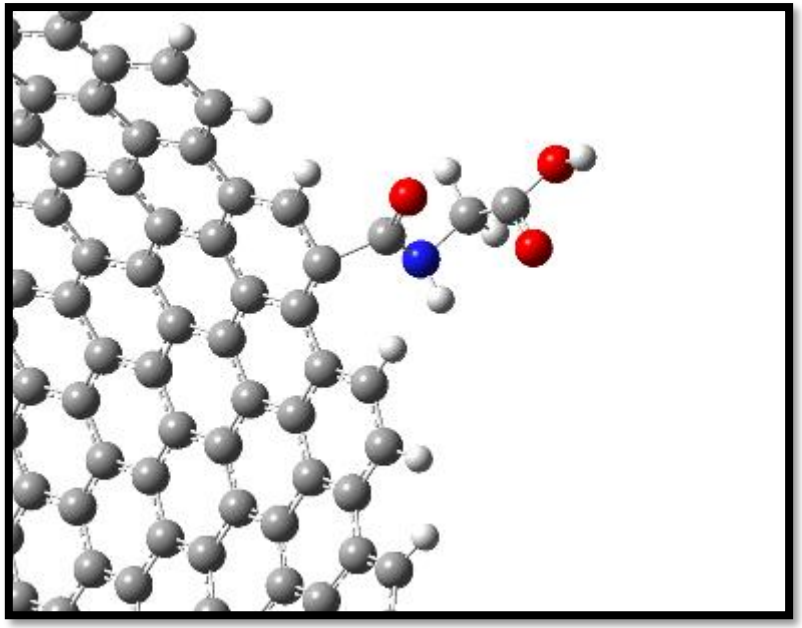
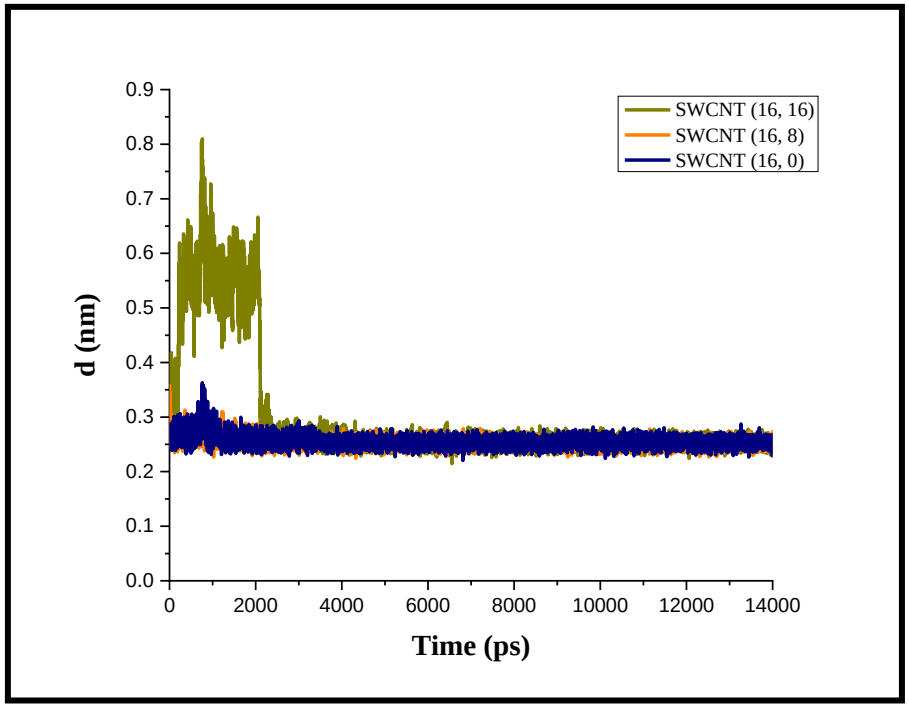
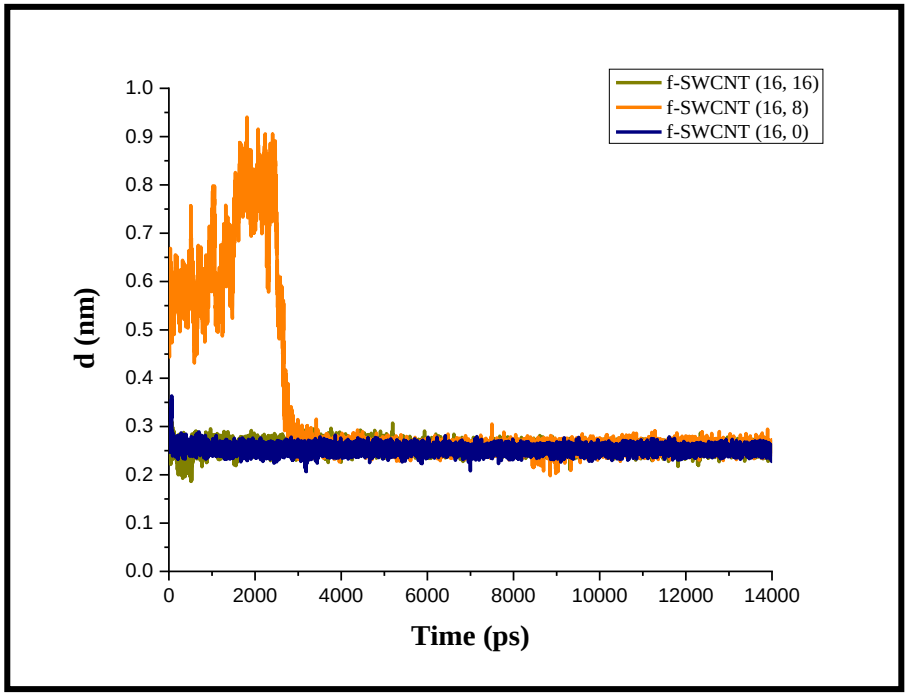


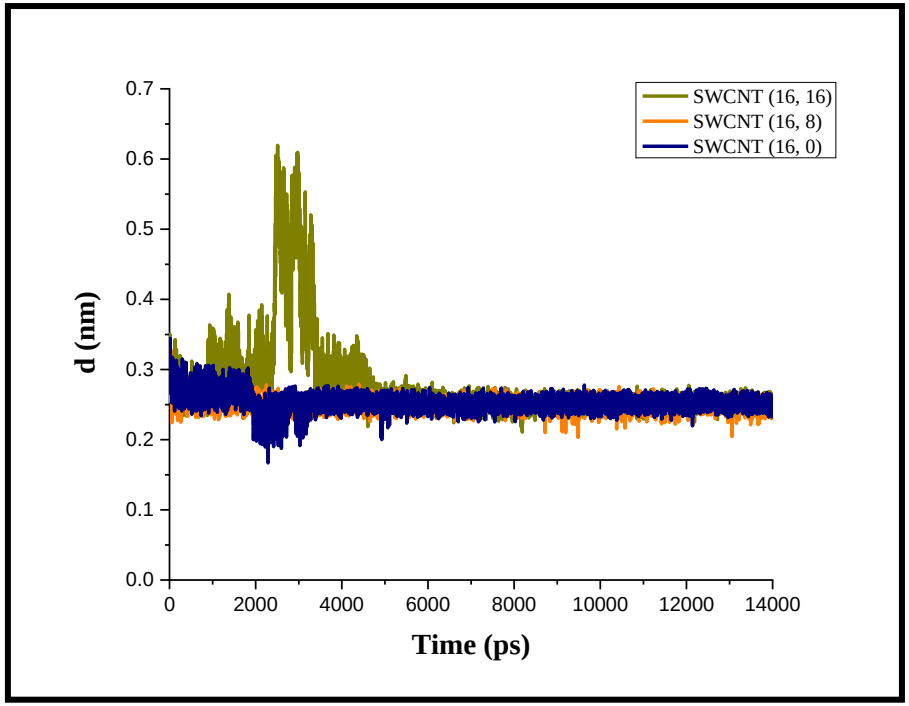
Figure SF2. The graphical representation of Glycine linkage in the tip of the SWCNT.

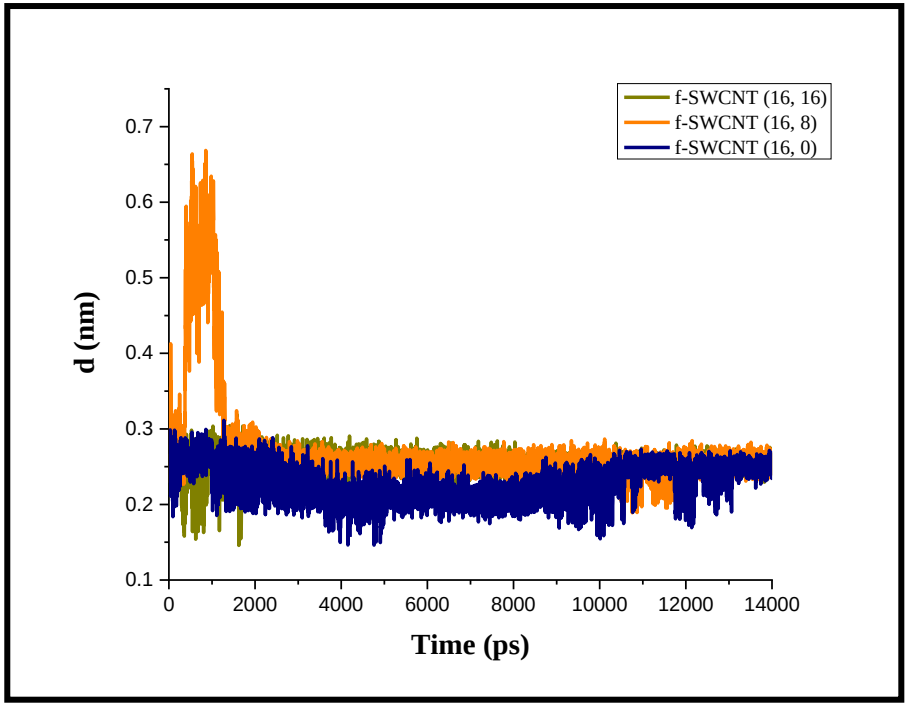
(a)


SWCNT (16, 16)
SWCNT (16, 8)
SWCNT (16, 0)
d (nm)
Time (ps)

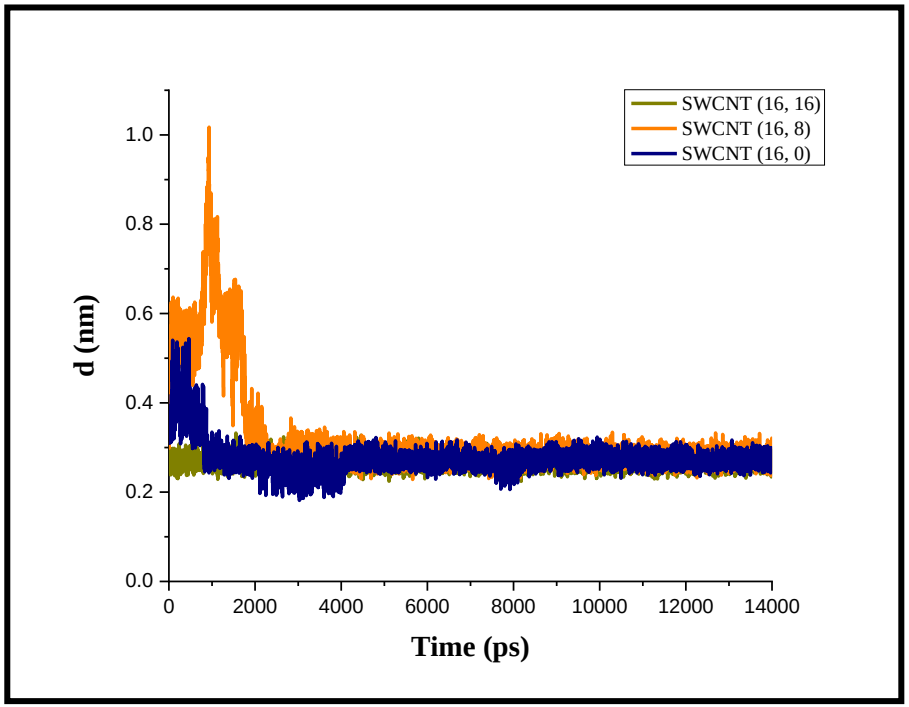

f-SWCNT (16, 16)
f-SWCNT (16, 8)
f-SWCNT (16, 0)
d (nm)
Time (ps)

(b)


SWCNT (16, 16)
SWCNT (16, 8)
SWCNT (16, 0)
d (nm)
Time (ps)


f-SWCNT (16, 16)
f-SWCNT (16, 8)
f-SWCNT (16, 0)
d (nm)
Time (ps)

(c)



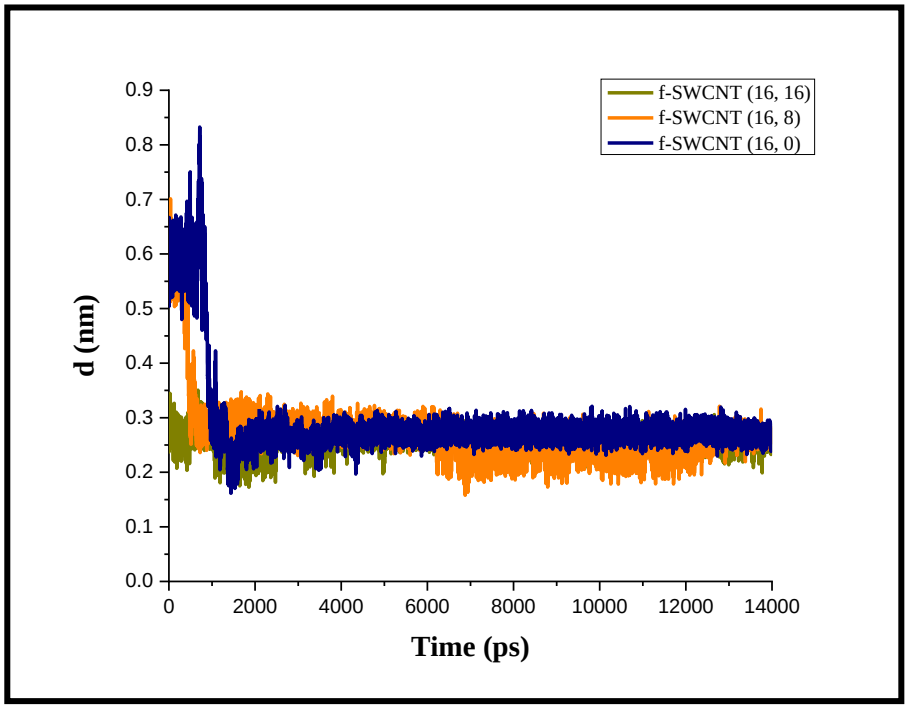
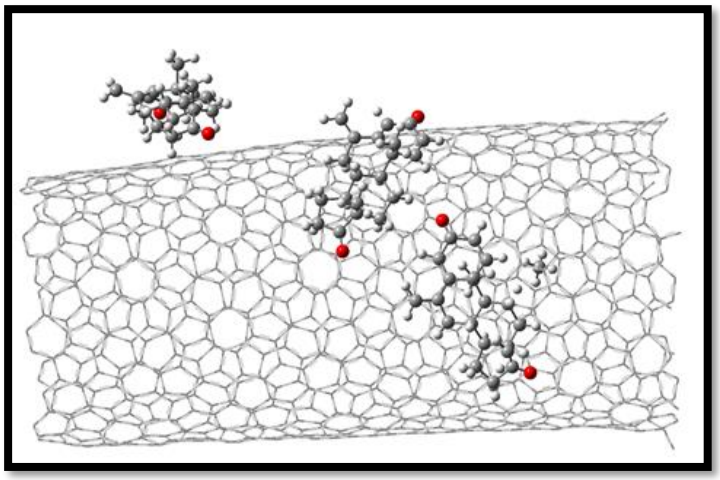
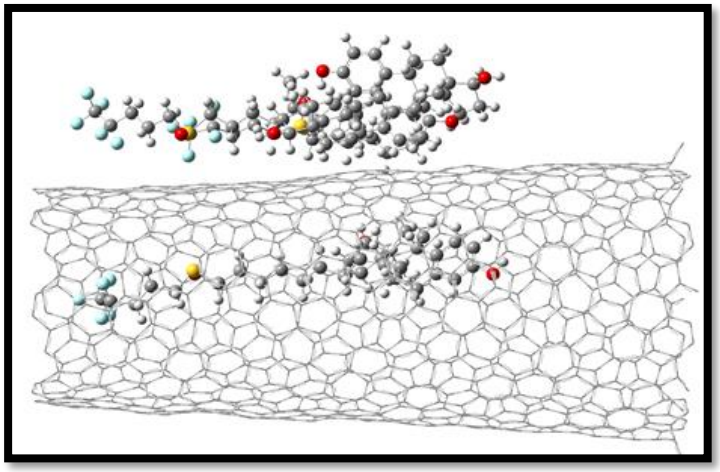


Figure SF3. The center of mass of distance of (a) EXE, (b) FLV and (c) LTZ drug molecules with pristine and functionalized carbon nanotubes.

(16, 8) SWCNT-EXE



(16, 8) SWCNT-FLV



(16, 0) SWCNT-LTZ

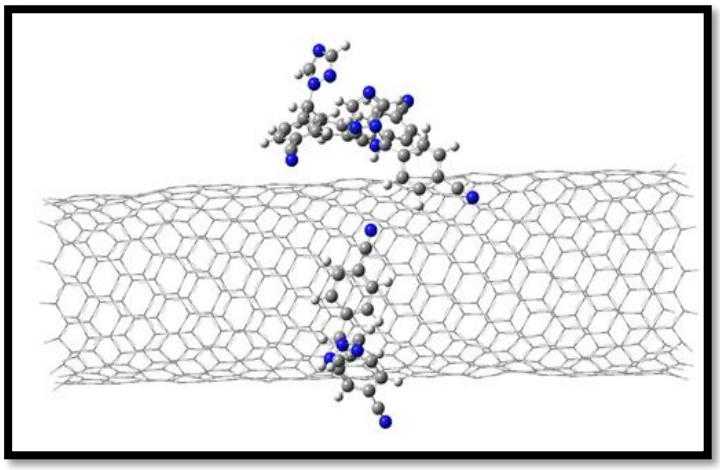


Figure SF4. The snapshots corresponding to MD simulations of the most stable systems for SWCNTs with studied drug molecules. Water and ions molecules are not displayed for clarity.

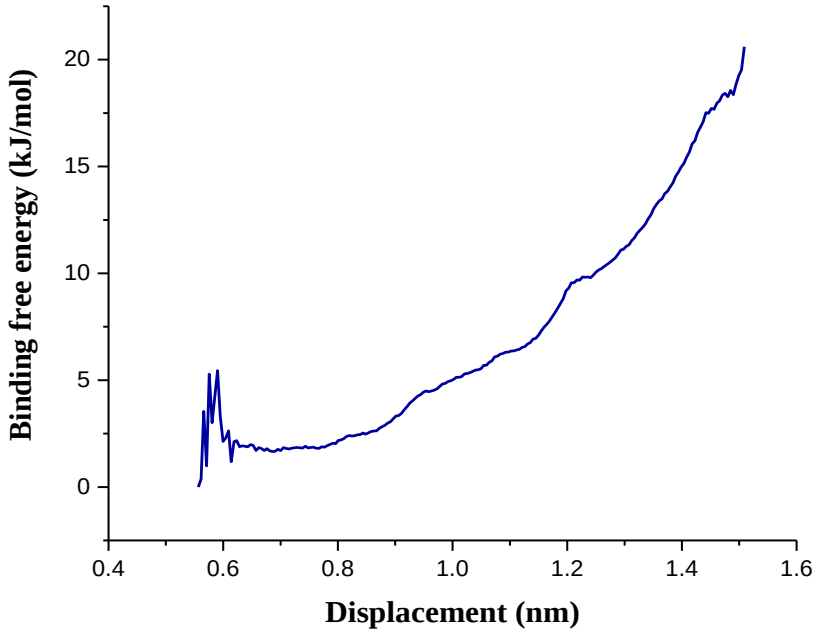


Figure SF5. PMF profile as a function of FLV's displacement at the FLV-(16, 0) *f*-SWCNT

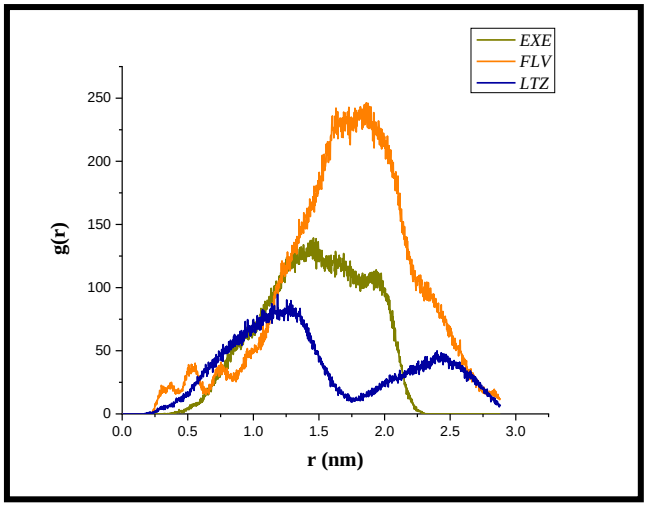


Figure SF6. Comparison of the radial distribution functions of various drug molecules around the Glycine functional groups of SWCNT (16, 0) versus distance.

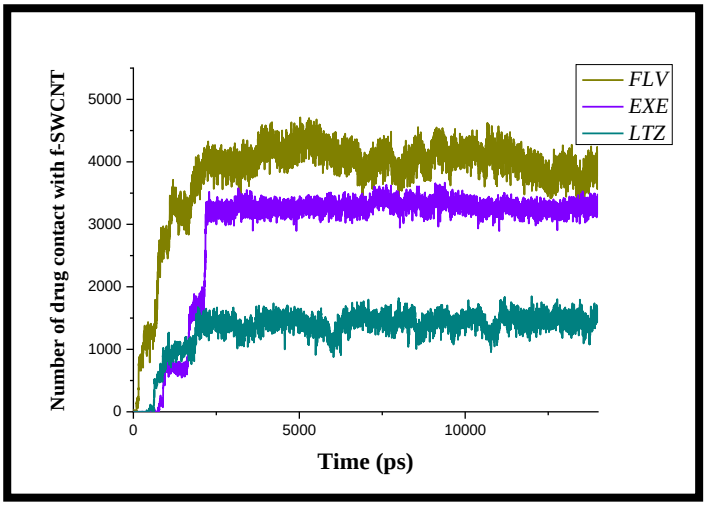


Figure SF7. The number of atomic contacts between the anticancer drugs and the nanotubes as a function of simulation time.

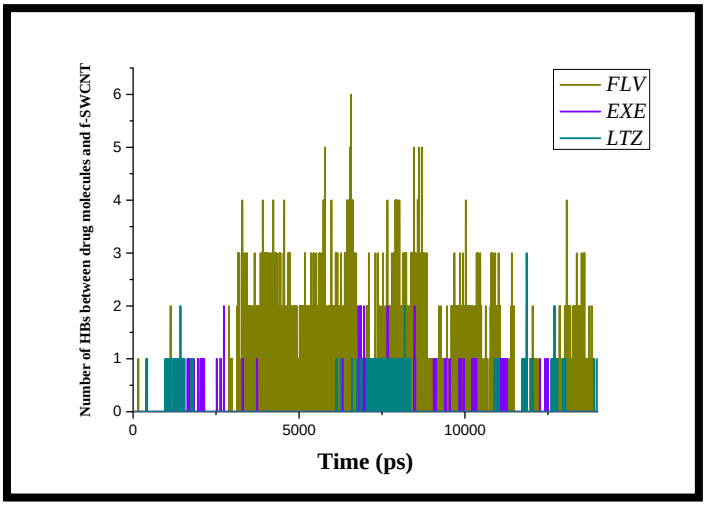


Figure SF8. The number of hydrogen bonds between *f*-SWCNT-drug molecules in the simulation system with (16, 0) chirality.

Table ST1. The force field parameters used for describing all atoms of the studied drug molecules and Glycine functional groups.

EXE

[atomtypes]

; name at.num mass charge ptype sigma epsilon

O=C 8 15.9994 0.0 A 0.302905 0.502080

CR 6 12.0110 0.0 A 0.387541 0.230120

C=O 6 12.0110 0.0 A 0.356359 0.460240

C=C 6 12.0110 0.0 A 0.372396 0.284512

HCMM 1 1.0079 0.0 A 0.235197 0.092048

[pairtypes]

; i j func sigma1-4 epsilon1-4 ; THESE ARE 1-4 INTERACTIONS

O=C O=C 1 0.249452 0.502080

O=C CR 1 0.293997 0.144938

O=C C=O 1 0.302905 0.480705

O=C C=C 1 0.310924 0.377952

O=C HCMM 1 0.242324 0.214978

CR CR 1 0.338541 0.041840

CR C=O 1 0.347450 0.138768

CR C=C 1 0.355469 0.109105

CR HCMM 1 0.286869 0.062059

FLV

[atomtypes]

; name at.num mass charge ptype sigma epsilon

CB 6 12.0110 0.0 A 0.355005 0.292880

S=O 16 32.0660 0.0 A 0.374177 1.966480

F 9 18.9984 0.0 A 0.290433 0.564840

OR 8 15.9994 0.0 A 0.315378 0.636386

O=C 8 15.9994 0.0 A 0.302905 0.502080

CR 6 12.0110 0.0 A 0.387541 0.230120

HCMM 1 1.0079 0.0 A 0.235197 0.092048

HOR 1 1.0079 0.0 A 0.040001 0.192464

HOCC 1 1.0079 0.0 A 0.040001 0.192464

[pairtypes]

; i j func sigma1-4 epsilon1-4 ; THESE ARE 1-4 INTERACTIONS

O=C CB 1 0.302228 0.383470

O=C S=O 1 0.311814 0.993645

O=C F 1 0.269942 0.532536

O=C OR 1 0.282415 0.565258

O=C O=C 1 0.249452 0.502080

O=C CR 1 0.293997 0.144938

O=C HCMM 1 0.242324 0.214978

O=C HOR 1 0.144726 0.310857

O=C HOCC 1 0.144726 0.310857

CR CB 1 0.346773 0.110698

CR S=O 1 0.356359 0.286841

CR F 1 0.314487 0.153730

CR OR 1 0.326960 0.163176

CR CR 1 0.338541 0.041840

CR HCMM 1 0.286869 0.062059

CR HOR 1 0.189271 0.089737

CR HOCC 1 0.189271 0.089737

LTZ

[atomtypes]

; name at.num mass charge ptype sigma epsilon

NPYL 7 14.0067 0.0 A 0.306469 0.376560

N5A 7 14.0067 0.0 A 0.329632 0.836800

N5B 7 14.0067 0.0 A 0.329632 0.836800

CB 6 12.0110 0.0 A 0.355005 0.292880

C5A 6 12.0110 0.0 A 0.363487 0.209200

C5B 6 12.0110 0.0 A 0.363487 0.209200

NSP 7 14.0067 0.0 A 0.329632 0.836800

CR 6 12.0110 0.0 A 0.387541 0.230120

CSP 6 12.0110 0.0 A 0.370614 0.284512

HCMM 1 1.0079 0.0 A 0.235197 0.092048

[pairtypes]

; i j func sigma1-4 epsilon1-4 ; THESE ARE 1-4 INTERACTIONS

CR NPYL 1 0.322505 0.125520

CR N5A 1 0.334087 0.187114

CR N5B 1 0.334087 0.187114

CR CB 1 0.346773 0.110698

CR C5A 1 0.351014 0.093557

CR C5B 1 0.351014 0.093557

CR NSP 1 0.334087 0.187114

CR CR 1 0.338541 0.041840

CR CSP 1 0.354578 0.109105

CR HCMM 1 0.286869 0.062059

Glycine functional group

[atomtypes]

; name at.num mass charge ptype sigma epsilon

C 6 12.01100 0.51 A 0.356359487256 0.46024

CT2 6 12.01100 -0.18 A 0.387540942391 0.23012

CT 6 12.01100 0.000 A 0.405358916754 0.08368 ; partial charge def not found

H 1 1.008000 0.31 A 0.0400013524445 0.192464

HP 1 1.008000 0.115 A 0.242003727796 0.12552

NH1 7 14.00700 -0.47 A 0.329632525712 0.8368

O	8	15.999400	-0.51	A	0.302905564168	0.50208
OH1	8	15.999400	-0.54	A	0.315378146222	0.6363864

[bondtypes]

CT1	C	1	0.149	209200.0
CT2	C	1	0.149	209200.0
NH1	C	1	0.1345	309616.0
NH1	CT2	1	0.143	267776.0
NH1	H	1	0.0997	368192.0
O	C	1	0.123	518816.0
OH1	H	1	0.096	456056.0

[angletypes]

; i	**j**	**k**	**func**	**th0**	**cth**	**ub0**	**cub**
CT2	NH1	C	5	120.0000	418.4	0.0	0.0
H	NH1	C	5	123.0000	284.512	0.0	0.0
H	NH1	CT2	5	117.0000	292.88	0.0	0.0
H	OH1	CA	5	108.0000	543.92	0.0	0.0
NH1	CT2	C	5	107.0000	418.4	0.0	0.0
O	C	CT2	5	121.0000	669.44	0.0	0.0
O	C	NH1	5	122.5000	669.44	0.0	0.0
O	C	CT1	5	121.0000	669.44	0.0	0.0
O	C	NH1	5	122.5000	669.44	0.0	0.0

[dihedraltypes]

; i	j	k	l	func	phi0	cp	mult	
C	CT2	NH1	C	9	180.00		0.8368	1
CT2	C	NH1	CT2	9	0.00	6.6944	1	
CT2	NH1	C	CT1	9	180.00		10.46	2
H	NH1	C	CT1	9	180.00		10.46	2
H	NH1	CT2	C	9	0.00	0.0	1	
NH1	C	CT1	CT1	9	0.00	0.0	1	
NH1	C	CT1	CT2	9	0.00	0.0	1	
NH1	C	CT1	CT3	9	0.00	0.0	1	
O	C	CT2	NH1	9	0.00	0.0	1	

Table ST2. Lenard Jones parameters applied for the studied SWCNTs in this study.

	Atom	Sigma (A˚)	Epsilon (kJ/mol)
SWCNT	CA	0.355	0.29288
	HA	0.242	0.12552

Table ST3. Calculated HOMA aromaticity indices index for the central six-membered rings of the pristine SWCNTs.

	(16, 0) SWCNT	(16, 16) SWCNT	(16, 8) SWCNT
HOMA index	0.727	0.766	**0.706**

Table ST4. The van der Waals and electrostatic energy calculations between FLV, EXE, LTZ and (16, 0) *f*-SWCNT in water solution.

Model	E_{LJ} (kJ/mol)	E_{elec} (kJ/mol)
EXE-*f*-SWCNT (16, 0)	-144.086	7.372
FLV-*f*-SWCNT (16, 0)	-237.781	-17.081
LTZ-*f*-SWCNT (16, 0)	-86.082	-8.801