Supplementary information to:

Theoretical encapsulation of Fluorouracil (5-FU) anti-cancer chemotherapy drug into carbon nanotubes (CNT) and boron nitride nanotubes (BNNT)

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Details on Computations

The potential energy of the molecule 5-FU (E) is defined as below [1]:

$$E = E_{val} + E_{nb} \tag{S1}$$

where E_{val} is valence or bonded interactions, and E_{nb} refers to non-bonded interactions which are the superposition of the van der Waals energy (E_{vdW}) and Coulombic energy (E_Q) (as shown in Eq. S2) [1]:

$$E_{nb} = E_{vdW} + E_Q \tag{S2}$$

E_{vdW} depends on the two parameters of D_0 and R_0, which are van der Waals well depth (kcal.mol^{-1}), and van der Waals bond length (as defined in Eq. S3) [1]. The obtained values of the D_0 and R_0 for each atom type of the drug 5-FU are tabulated in Table S1.

$$E_{vdW} = D_0 \left(\left(\frac{R}{R_0}\right)^{-12} - 2\left(\frac{R}{R_0}\right)^{-6} \right) \tag{S3}$$

Table S1. Van der Waals parameters of 5-FU atoms.

Atom Type	R_0 (Å)	D_0 (Kcal.mol^{-1})
C_R	3.458	0.0950
N_R	3.293	0.1450
F_	2.928	0.3050
O_2	3.128	0.2150
H___A	2.852	0.0100
H_	2.852	0.0100

The valence interaction comprises of the bonding stretch (E_B), bond-angle bend (E_A), dihedral angle torsion (E_T), and inversion terms (E_I) as represented in Eq. S4 [1]:

$$E_{val} = E_B + E_A + E_T + E_I \tag{S4}$$

The Bond stretch interaction is described as below [1]:

$$E_B = K_e (R - R_e)^2 \tag{S5}$$

The force constant (K_e) and anharmonic terms near equilibrium (R_e) for bond types of the drug 5-FU are reported in Table S2.

Table S2. K_e and R_e constants for bond types of drug 5-FU

Bond Type	K_e (Kcal.mol^{-1}. Å^{-2})	R_e (Å)
C_R-N_R	350	1.340
C_R-C_R	525	1.390
C_R-O_2	700	0.970
N_R-H___A	350	1.020
C_R-H_	350	1.020
C_R-F_	350	1.301

The bond-angle bend interaction energy (E_A) between is defined in Eq. S6 [1]. The values of equilibrium angle (θ_J°) and force constant (K_{IJK}) for angle types of the drug 5-FU are summarized in Table S3.

$$E_A = E_{IJK} = K_{IJK}(\theta_{IJK} - \theta_J^{\circ})^2 \tag{S6}$$

Table S3. Quantities of θ_J° and K_{IJK} for angle types of the drug 5-FU

Angle Type	K_{IJK} (kcal.mol^{-1}.rad^{-2})	θ_J° (rad)
C_R-C_R-N_R	50	120.00
N_R-C_R-O_2	50	120.00
C_R-C_R-O_2	50	120.00
C_R-N_R-C_R	50	120.00
C_R-N_R-H___A	50	120.00
N_R-C_R-N_R	50	120.00
N_R-C_R-H_	50	120.00
C_R-C_R-H_	50	120.00
C_R-C_R-C_R	50	120.00
C_R-C_R-F_	50	120.00

The torsion or dihedral interaction energy (E_D) for two bonds IJ and KL connected with bond is defined as below [1]:

$$E_D = E_{IJKL} = V_{JK}(1 - \cos(n_{IL}(\varphi - \varphi_{JK}^{\circ}))) \tag{S7}$$

where V_{JK}, n_{IL}, and φ_{JK}° correspond to the barrier to rotation, the periodicity, and the equilibrium angle constants. The values of these constants for dihedral types of the drug 5-FU are summarized in Table S4.

Table S4. The values of V_{JK}, n_{IL}, and φ_{JK}° for dihedral types of the drug 5-FU

Dihedral Type	V_{JK} (Kcal.mol^{-1})	n_{IL}	φ_{JK}°
C_R-C_R-N_R-C_R	5	2	0
C_R-C_R-N_R-H___A	5	2	0
O_2-C_R-N_R-C_R	5	2	0
O_2-C_R-N_R-H___A	5	2	0
C_R-C_R-C_R-N_R	5	2	0
N_R-C_R-C_R-F_	5	2	0
C_R-C_R-C_R-O_2	5	2	0
F_-C_R-C_R-O_2	5	2	0
N_R-C_R-N_R-C_R	5	2	0
N_R-C_R-N_R-H___A	5	2	0
H_-C_R-N_R-C_R	5	2	0
H_-C_R-N_R-H___A	5	2	0
C_R-C_R-C_R-H_	5	2	0
F_-C_R-C_R-H_	5	2	0

The improper (inversion) interaction energy (E_I) for drug 5-FU with planar equilibrium geometry is considered in Eq. S8 [1].

$$E_I = E_{IJKL} = K_I(1 - cos\Psi_I) \tag{S8}$$

where Ψ_I is an angle between the *IL* bond and *JIK* plane. The values of force constant K_I for improper types of the drug 5-FU are listed in Table S5.

Table S5. values of K_I for improper types of the drug 5-FU

Improper Type	K_I (kcal.mol-^{1}.rad^{-2})
C_R-C_R-N_R-O_2	40.00
C_R-N_R-C_R-H___A	40.00
N_R-C_R-N_R-O_2	40.00
C_R-C_R-N_R-H_	40.00
C_R-C_R-C_R-F_	40.00

The partial charges of atoms in drug 5-FU are reported in Table S6.

Table S6. Atomic charges of elements in drug 5-FU

Atom	Charge
C_R	0.495100
N_R	-0.494500
C_R	0.590000
N_R	-0.526200
C_R	-0.001900
C_R	0.487600
F_	-0.550500
O_2	-0.390100

O_2	-0.370200
H___A	0.289100
H___A	0.287200
H_	0.184300

Reference

1. Mayo, S.L., B.D. Olafson, and W.A. Goddard, *DREIDING: a generic force field for molecular simulations.* Journal of Physical chemistry, 1990. **94**(26): p. 8897-8909.