Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Understanding Co-loading and Releasing of Doxorubicin and Paclitaxel using Chitosan Functionalized Single-Walled Carbon Nanotubes by Molecular Dynamics Simulations

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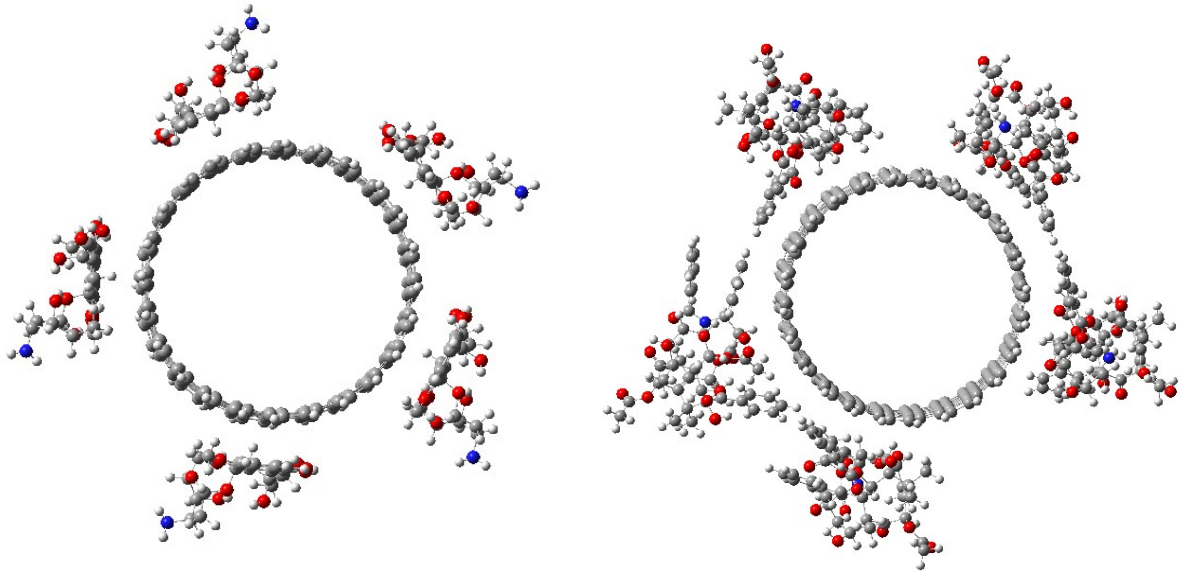

Figure S1. Five DOX (left) and PTX (right) were binding with the sidewall of SWCNT with PM6-DH2.

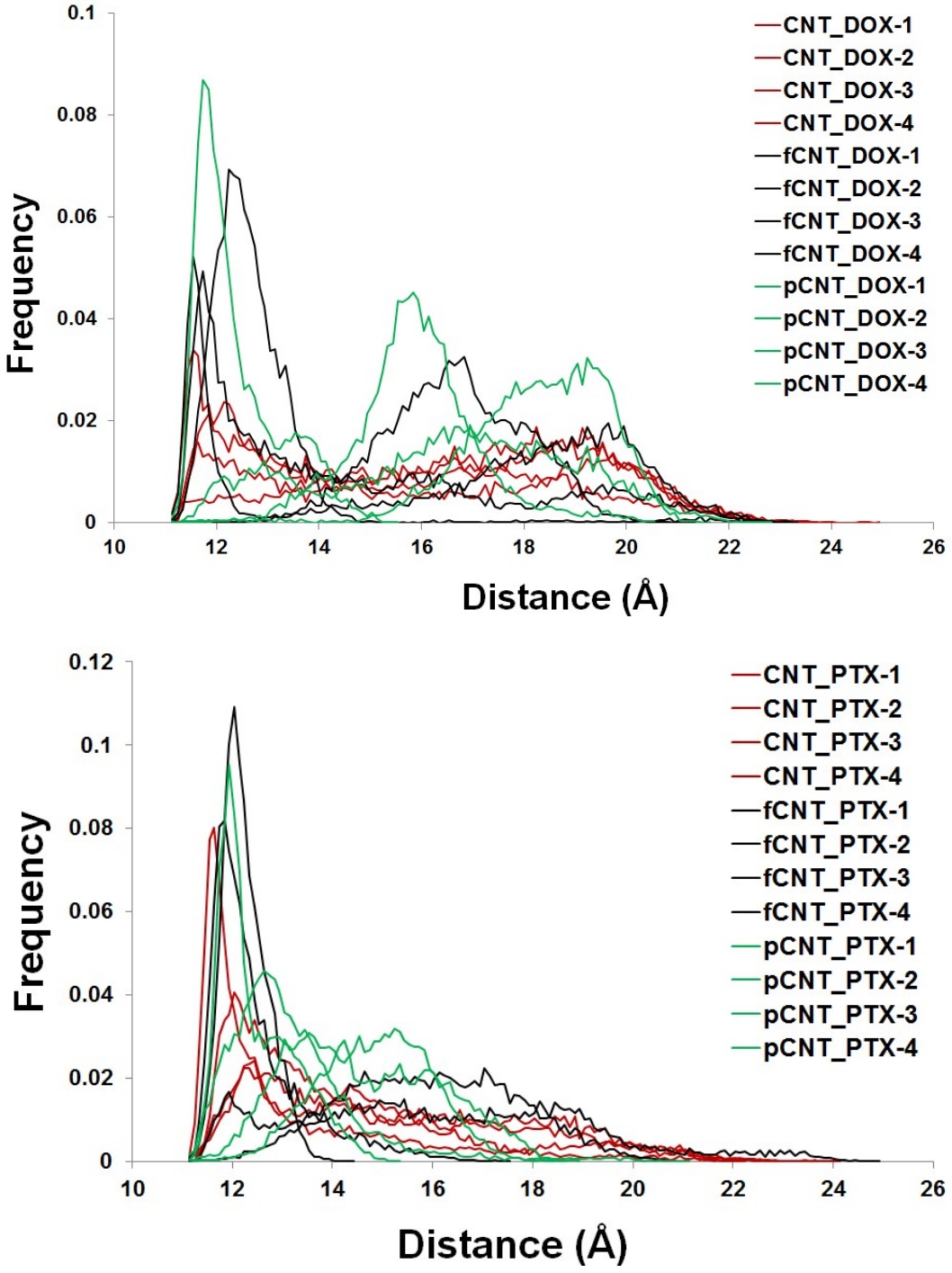

Figure S2. Distance frequencies of DOX (top) and PTX (bottom) binding with different CNT systems.

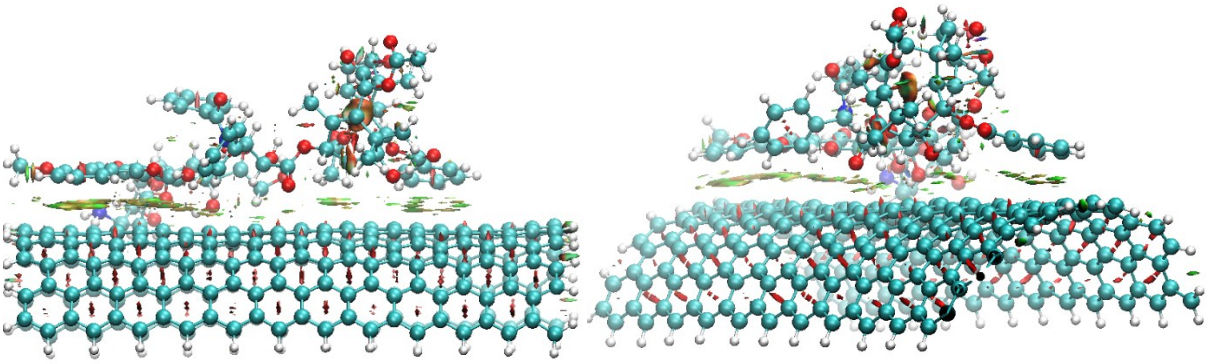

Figure S3. Reduced density gradient isosurface (0.5 au) for pristine CNT and DOX/PTX . Green and yellow indicates vdW interaction and red strong nonbonded overlap.

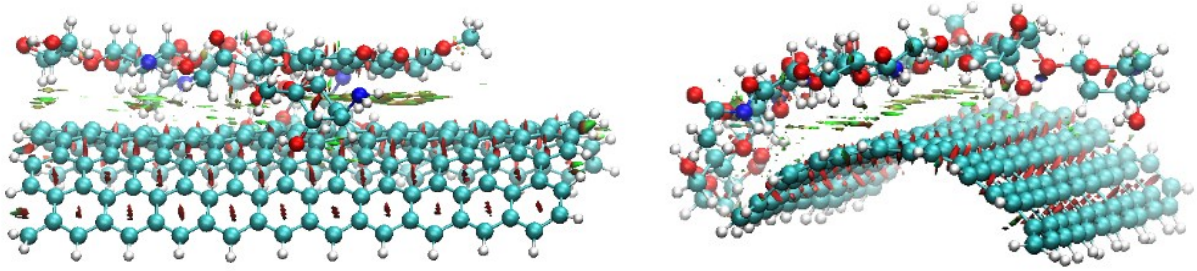

Figure S4. Reduced density gradient isosurface (0.5 au) for functionalized CNT and DOX . Green and yellow indicates vdW interaction and red strong nonbonded overlap.

Table S1. ΔH, -TΔS, ΔG (Kcal/mol) for the binding of *f*-SWCNT with DOX and PTX molecules.

	ΔH	**-TΔS**	**ΔG**
DOX-1	-36.03	44.75	8.71
DOX-2	-36.59	42.48	5.94
DOX-3	-35.73	43.22	7.49
DOX-4	-36.80	46.59	9.79
PTX-1	-42.83	67.83	25.0
PTX-2	-35.58	64.43	28.84
PTX-3	-46.01	65.93	19.92
PTX-4	-38.87	63.10	24.22

Table S2. ΔH, -TΔS, ΔG (Kcal/mol) for the binding of P-*f*-SWCNT with DOX and PTX molecules.

	ΔH	**-TΔS**	**ΔG**
DOX-1	-37.53	45.14	1.52
DOX-2	-31.40	45.49	14.09
DOX-3	-30.35	44.82	14.47
DOX-4	-29.99	44.41	14.41
PTX-1	-35.67	66.31	30.64
PTX-2	-31.01	63.93	32.92
PTX-3	-38.72	65.18	26.46
PTX-4	-33.11	70.32	37.21

Table S3. ΔH, -TΔS, ΔG (Kcal/mol) for the binding *f*-SWCNT with two encapsulated DOX (DOX-1 and DOX-2), two DOX and four PTX molecules on surface of SWCNT.

	ΔH	**-TΔS**	**ΔG**
DOX-1	-64.01	36.68	-27.34
DOX-2	-54.38	35.27	-19.11
DOX-3	-38.07	46.54	8.47
DOX-4	-37.61	41.13	3.52
PTX-1	-45.88	62.68	16.79
PTX-2	-40.88	63.96	23.08
PTX-3	-35.94	67.16	31.22
PTX-4	-40.55	65.99	25.45