Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Si doped single-wall carbon nanotubes interacting with isoniazid–a density functional and molecular docking study

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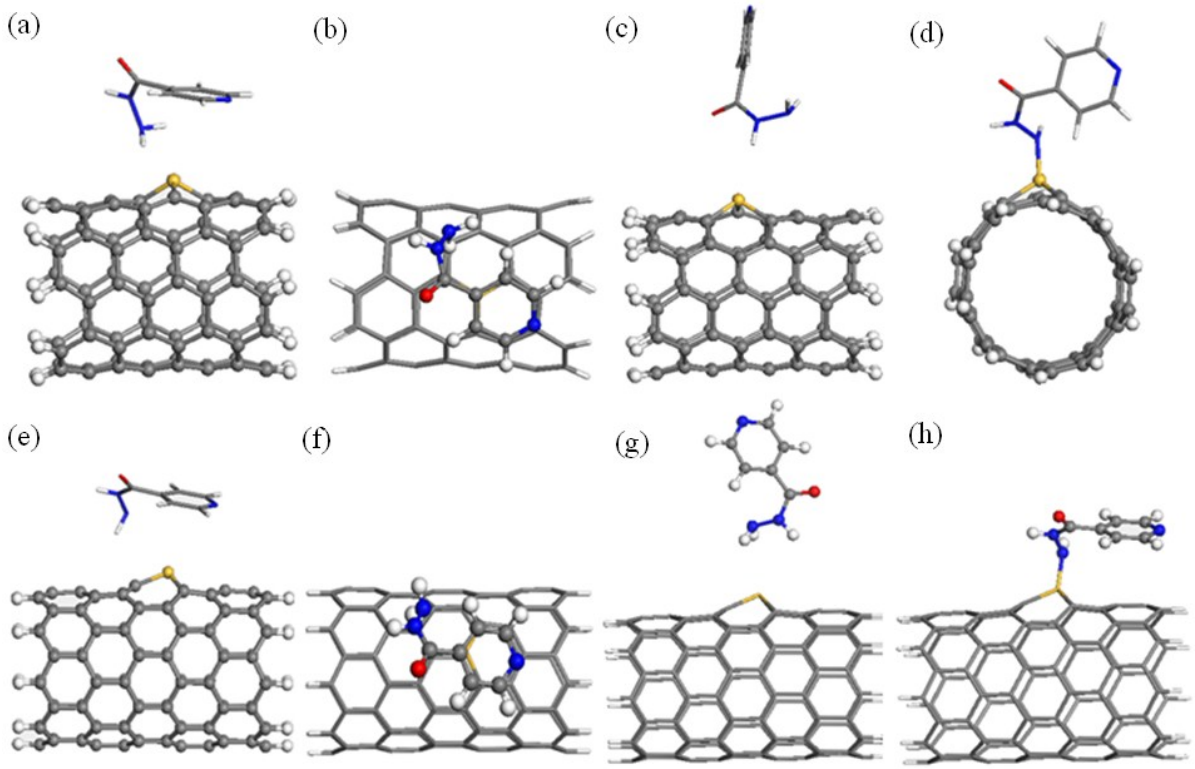

Fig. S1. Noncovalent adsorption of INH onto (5,5) and (9,0) SWNTs; (a) side view of INH adsorbed onto Si–doped (5,5) SWNT at hollow site (parallel orientation), (b) corresponding front view, (c) side view of INH adsorbed onto (5,5) SWNT at slipped hollow site (perpendicular orientation), (d) the covalent adsorption of INH onto Si–doped (5,5) SWNT, (e) side view of INH adsorbed onto Si–doped (9,0) SWNT at hollow site (parallel orientation), (f) corresponding front view, (g) perpendicular adsorption of INH onto (9,0) SWNT, (h) the covalent adsorption of INH onto Si–doped (9,0) SWNT.

Table S1. Optimum distance of interaction (Å), adsorption energy (eV), HOMO – LUMO energy gap (eV) and global reactivity descriptors of INH, pristine and Si-doped (9,0) SWNTs along with their functionalization with INH drug (cluster models).

System	Optimum distance	E_{ads}	HOMO – LUMO gap	η	μ	ω
INH	–	–	3.476	1.738	-4.117	4.876
(9,0) SWNT	–	–	0.617	0.308	-4.269	29.544
Si–doped (9,0) SWNT	–	–	0.566	0.283	-4.489	35.603
INH/(9,0) SWNT (parallel)	3.067	0.073	0.620	0.310	-4.327	30.198
INH/(9,0) SWNT (perpendicular)	3.038	0.064	0.614	0.307	-4.306	30.198
INH/ Si–doped (9,0) SWNT (parallel)	3.428	0.299	0.563	0.281	-4.505	36.056
INH/Si–doped (9,0) SWNT (perpendicular)	2.978	0.290	0.575	0.287	-4.632	37.322
INH/Si–doped (9,0) SWNT (covalent functionalization)	1.751 (N–Si bond length)	2.782	0.307	0.153	-4.425	63.795

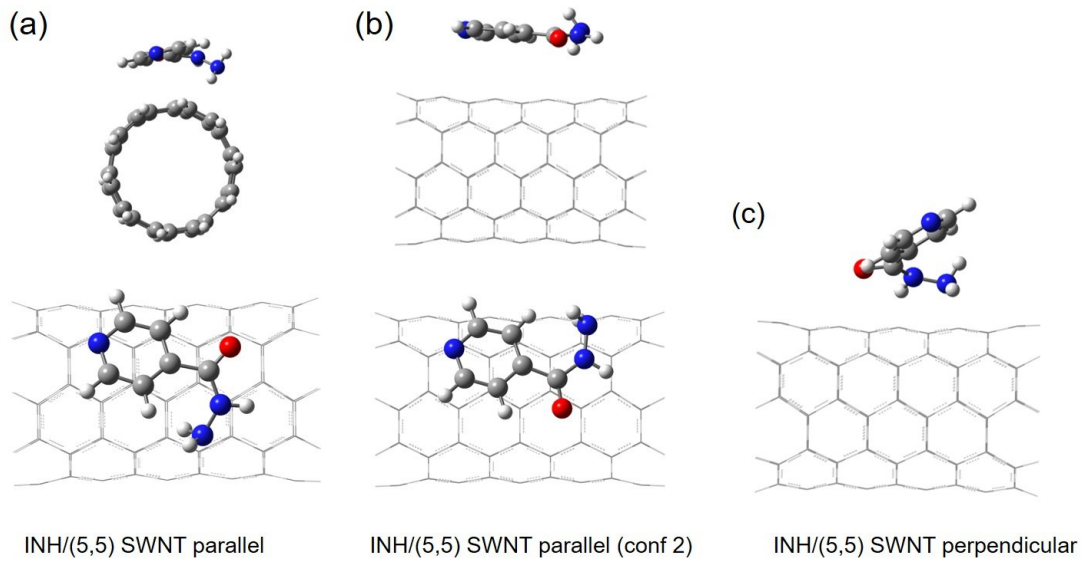

Fig. S2. Noncovalent adsorption of INH onto (5,5) SWNT with vdW dispersion correction; (a) INH/(5,5) SWNT at top site (parallel orientation), (b) INH/(5,5) SWNT at top site (configuration 2), (c) perpendicular adsorption of INH onto (5,5) SWNT.

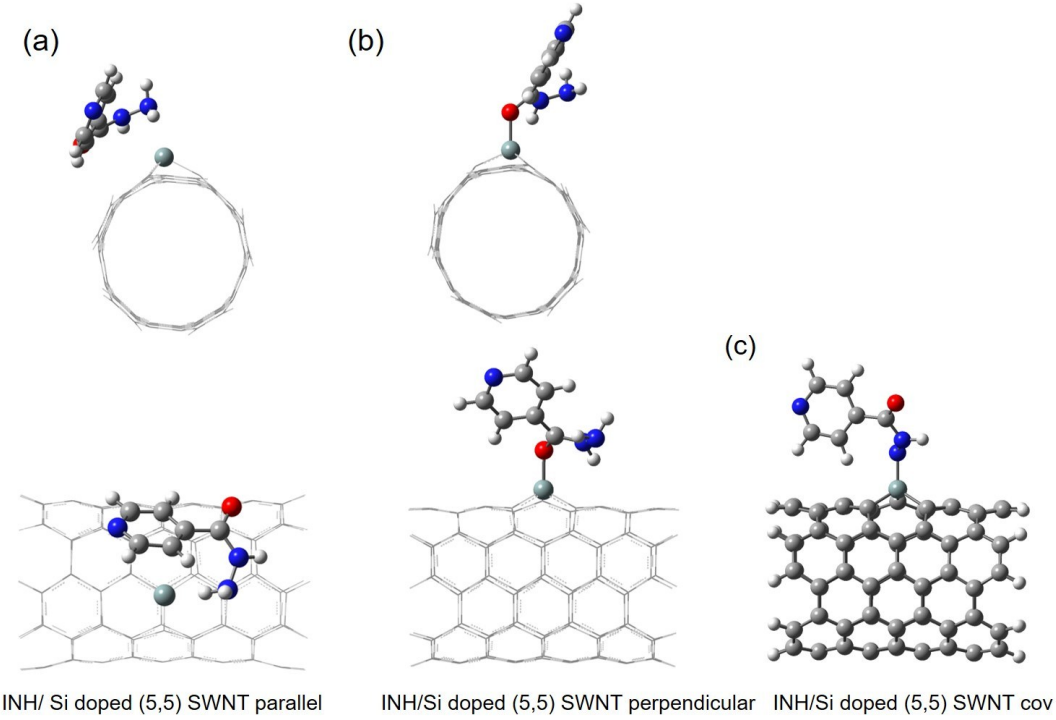

Fig. S3. Noncovalent adsorption of INH onto Si doped (5,5) SWNTs with vdW dispersion correction; (a) INH/Si–doped (5,5) SWNT (parallel orientation), (b) INH/Si doped (5,5) SWNT at perpendicular conformation, (c) covalent adsorption of INH onto Si doped (5,5) SWNT.

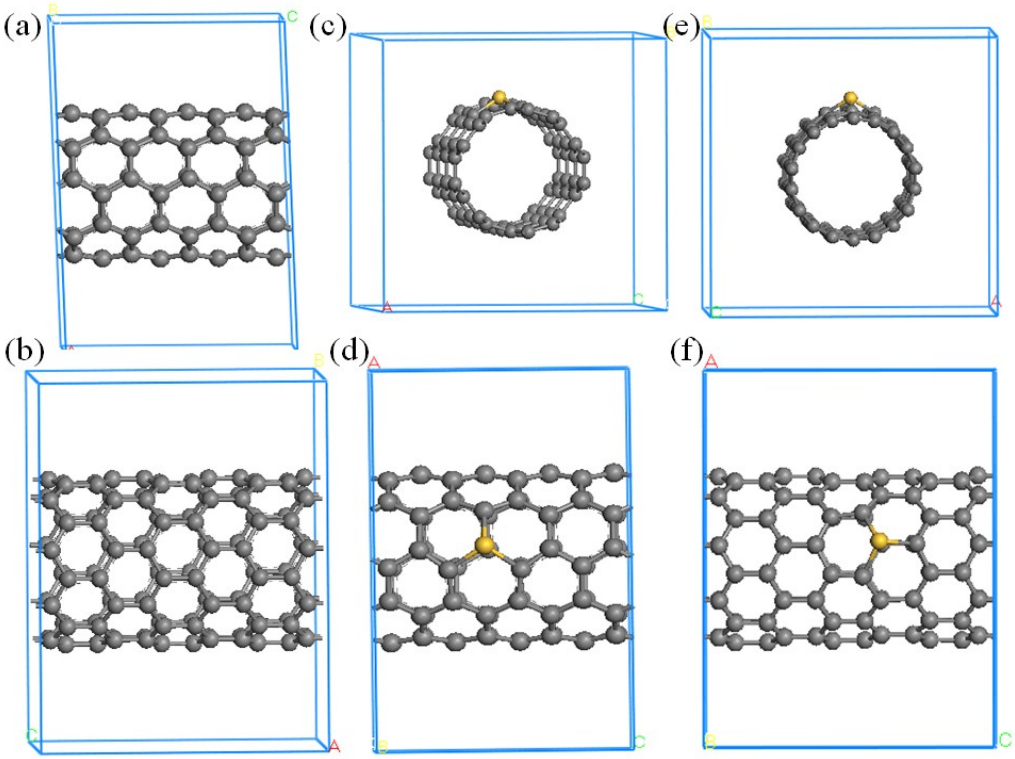

Fig. S4. The optimized geometries of the periodic models of (a) (5,5) SWNT comprising of 4 unit cells, (b) (9,0) SWNT consisting of three unit cells, (c) front view depiction of Si doped (5,5) SWNT, (d) corresponding side view, (e) front view depiction of Si doped (9,0) SWNT, (f) corresponding side view.

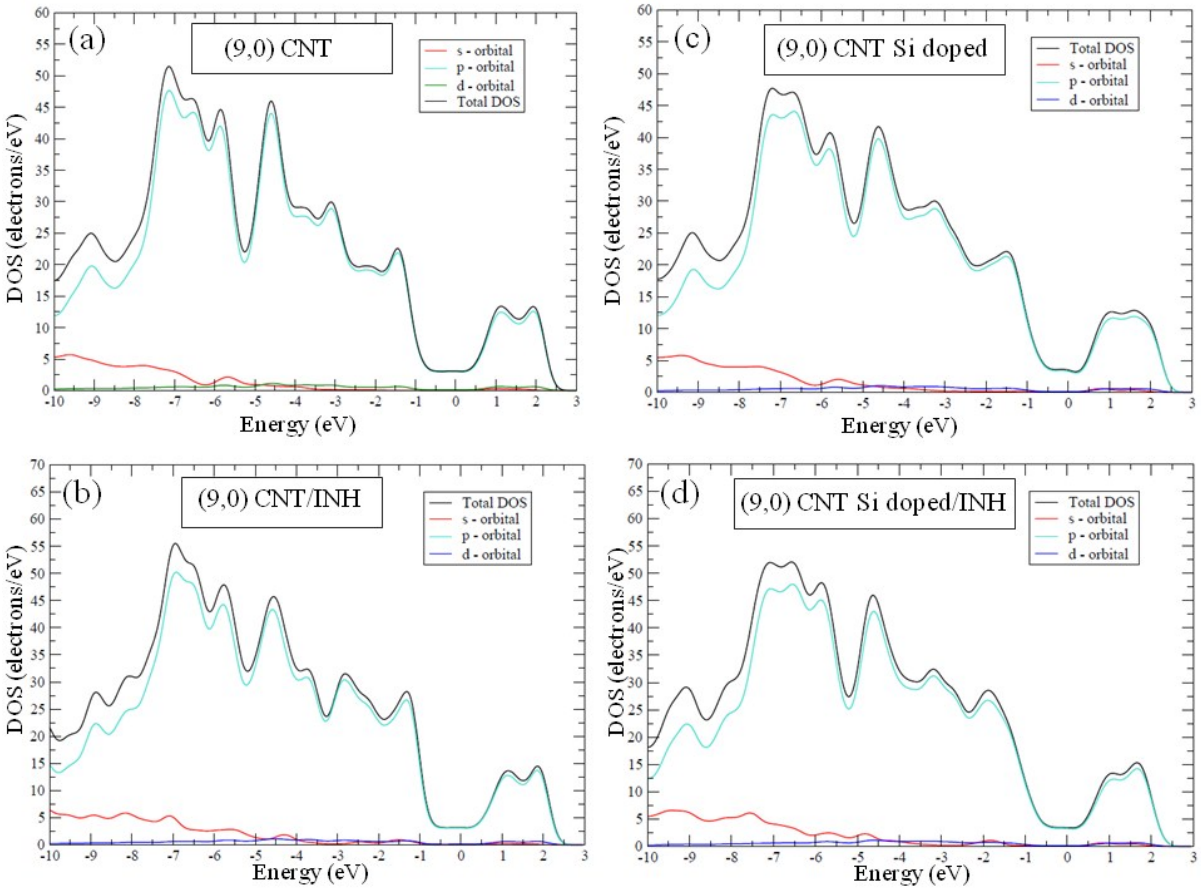

Fig. S5. The total DOS and PDOS corresponding to s, p and d orbitals for (a) perfect (9,0) SWNT, (b) INH adsorbed onto (9,0) SWNT, (c) Si doped (9,0) SWNT, and (d) INH adsorbed onto Si doped (9,0) SWNT.

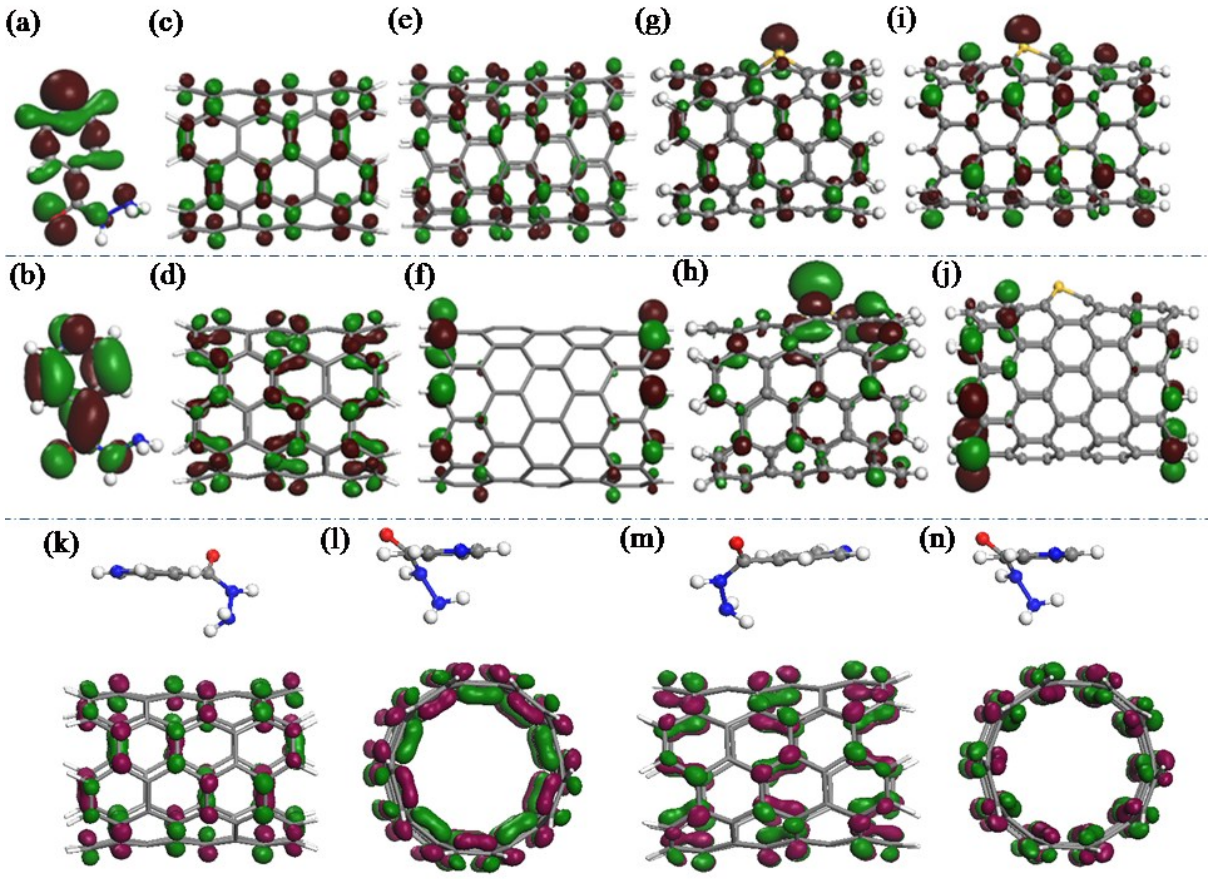

Fig. S6. (a) The HOMO of INH, (b) LUMO of INH, (c) the side view depiction of HOMO in pristine (5,5) SWNT, (d) LUMO in pristine (5,5) SWNT, (e) the side view depiction of HOMO in pristine (9,0) SWNT, (f) LUMO in pristine (9,0) SWNT, (g) the side view depiction of HOMO in Si–doped (5,5) SWNT, (h) side view depiction of LUMO in Si–doped (5,5) SWNT, (i) the side view depiction of HOMO in Si–doped (9,0) SWNT, (j) side view depiction of LUMO in Si–doped (9,0) SWNT, (k) side view of the HOMO in parallel adsorption of INH onto (5,5) SWNT, (l) the corresponding front view, (m) side view of the LUMO in parallel stacking noncovalent adsorption of INH onto (5,5) SWNT, (n) the corresponding front view.

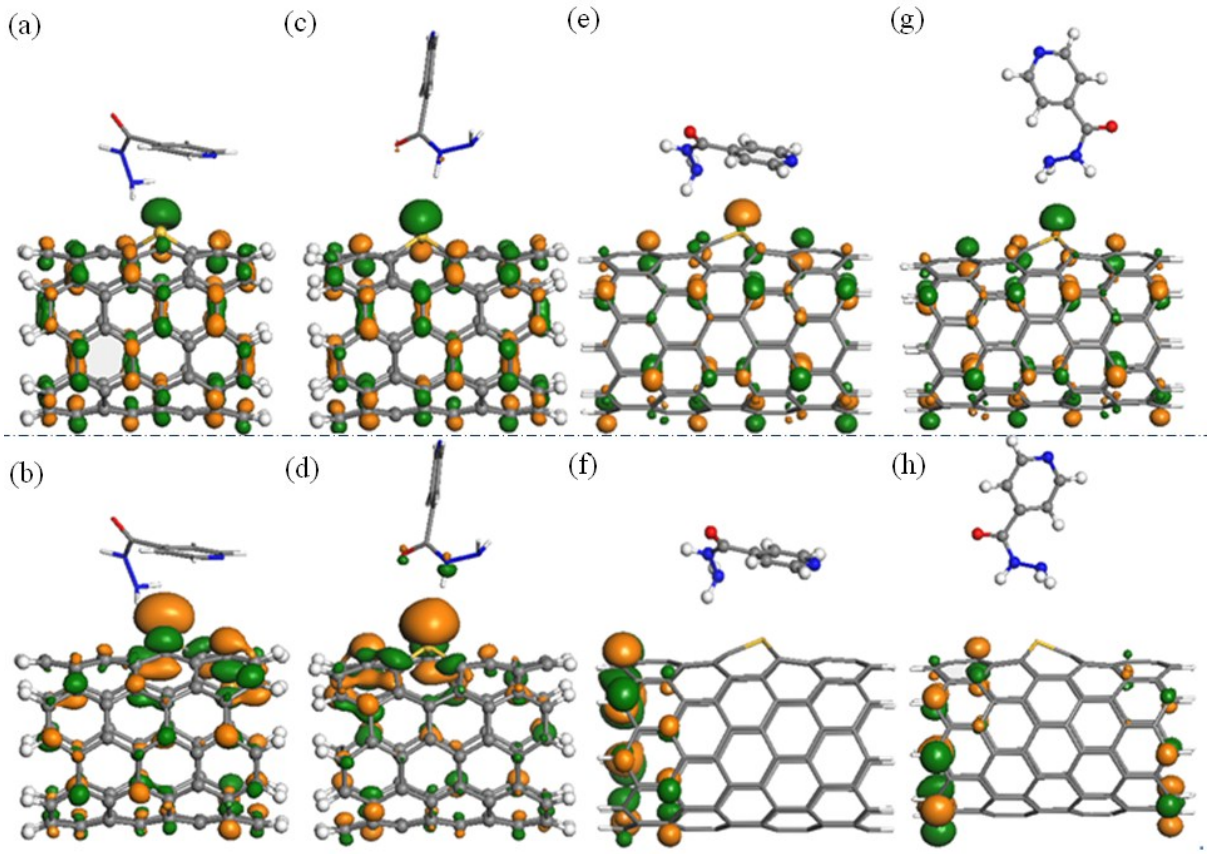

Fig. S7. (a) The side view of the HOMO in parallel adsorption of INH onto Si–doped (5,5) SWNT, (b) the corresponding LUMO plot, (c) perpendicular adsorption of INH onto Si–doped (5,5) SWNT, (d) corresponding LUMO plot, (e) side view of the HOMO in parallel adsorption of INH onto Si–doped (9,0) SWNT, (f) the corresponding LUMO plot, (g) perpendicular adsorption of INH onto Si–doped (5,5) SWNT, (h) corresponding LUMO plot.

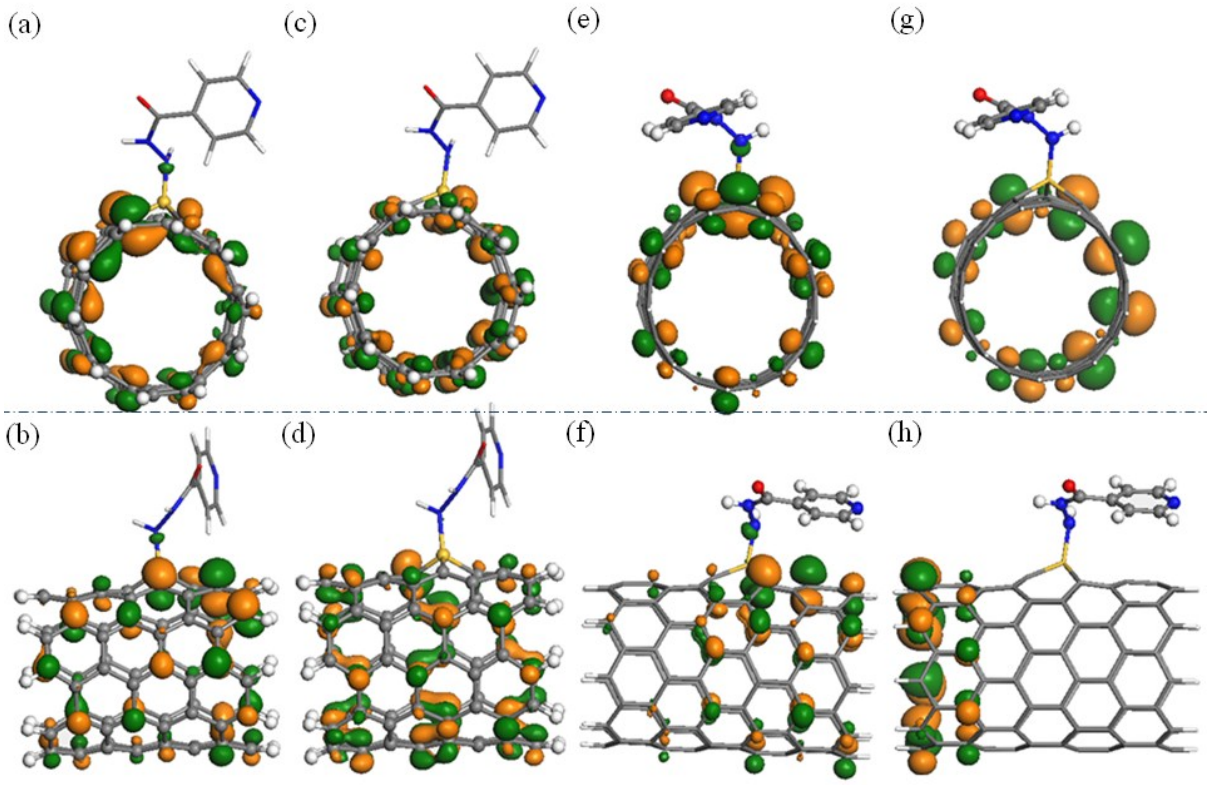

Fig. S8. Covalent functionalization of INH onto Si–doped (5,5) and (9,0) SWNTs; (a) The front view depiction of HOMO in INH adsorbed onto Si–doped (5,5) SWNT, (b) the corresponding LUMO plot depicting the same (c) front and side view depiction of LUMO of INH functionalized onto Si–doped (5,5) SWNT, (d) corresponding LUMO plot depicting the side view, (e) front view depiction of HOMO in INH adsorbed onto Si–doped (9,0) SWNT, (f) the corresponding HOMO plot depicting the side view, (g) front view depiction of LUMO in INH adsorbed onto Si–doped (9,0) SWNT, (h) corresponding LUMO plot depicting the side view.

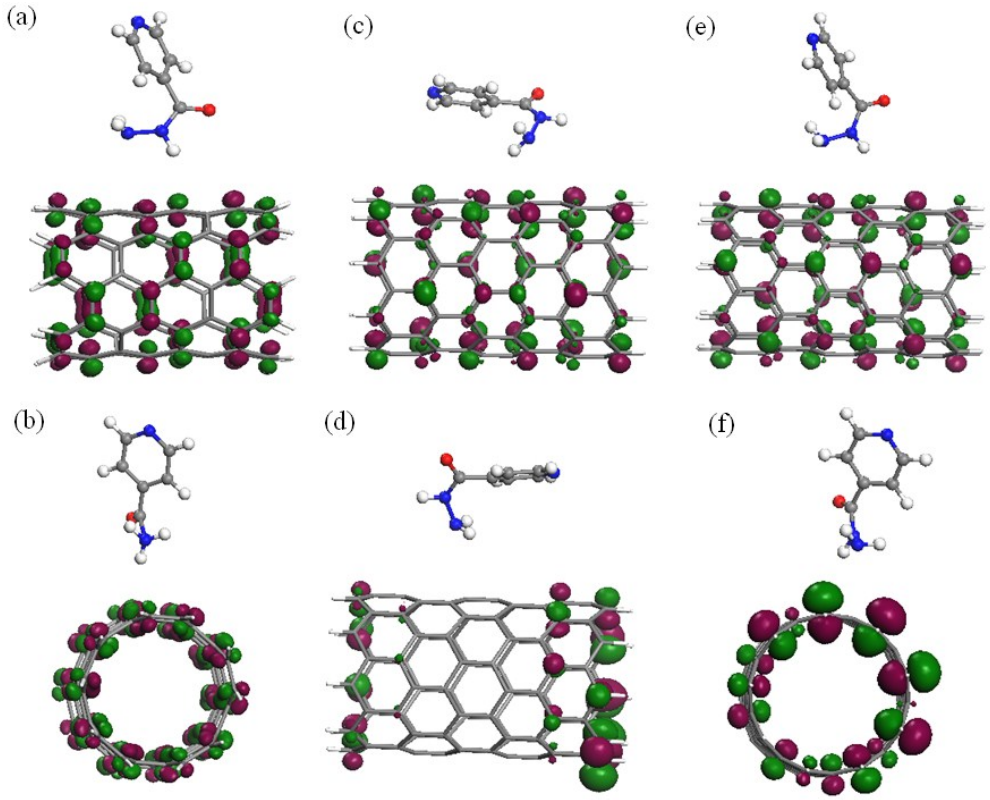

Fig. S9. (a) The side view of the HOMO in perpendicular adsorption of INH onto (5,5) SWNT, (b) the corresponding LUMO plot, (c) side view of HOMO in parallel adsorption of INH onto (9,0) SWNT, (d) the corresponding LUMO plot, (e) side view of the HOMO in perpendicular adsorption of INH onto (9,0) SWNT, (f) the corresponding LUMO plot.

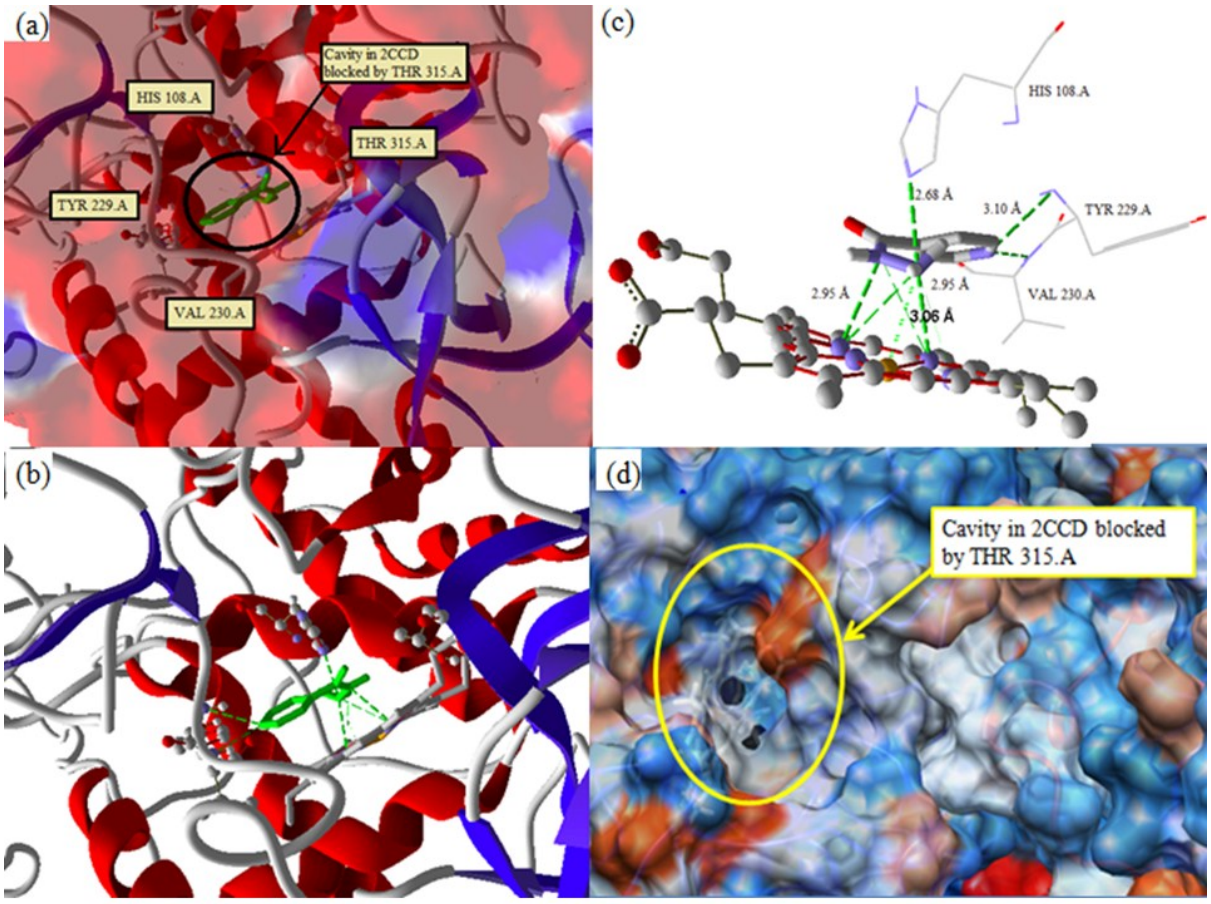

Fig. S10. (a) The secondary structure of INH docked onto mutant type *mtCP* (2CCD) protein, (b) closer view of the probable interactions of INH (shown in green color) with Tyr229, His108, Thr315 and Val230 residues, (c) the H-bonded interactions of INH with porphyrin ring, Tyr229, His108, Thr315 and Val230 residues, (d) the docked surface of INH within mutant type *mtCP* protein at the best docked conformation with the entering cavity blocked due to the mutation.

Table S2. The H–bonding distance between INH and protoporphyrin ring of Wild Type (PDB: 1SJ2) and Mutant type (PDB: 2CCD) *mtCP*.

System	H–bond distance between INH and protoporphyrin ring of Wild Type mtCP (1SJ2) (in Å)	H– bond distance between INH and protoporphyrin ring of Mutant Type mtCP (2CCD) (in Å)
Bare INH drug	2.83	3.06
INH/(5, 5) SWCNT (parallel)	2.52	2.39
INH/Si-doped (5, 5) SWCNT (parallel)	2.67	2.87

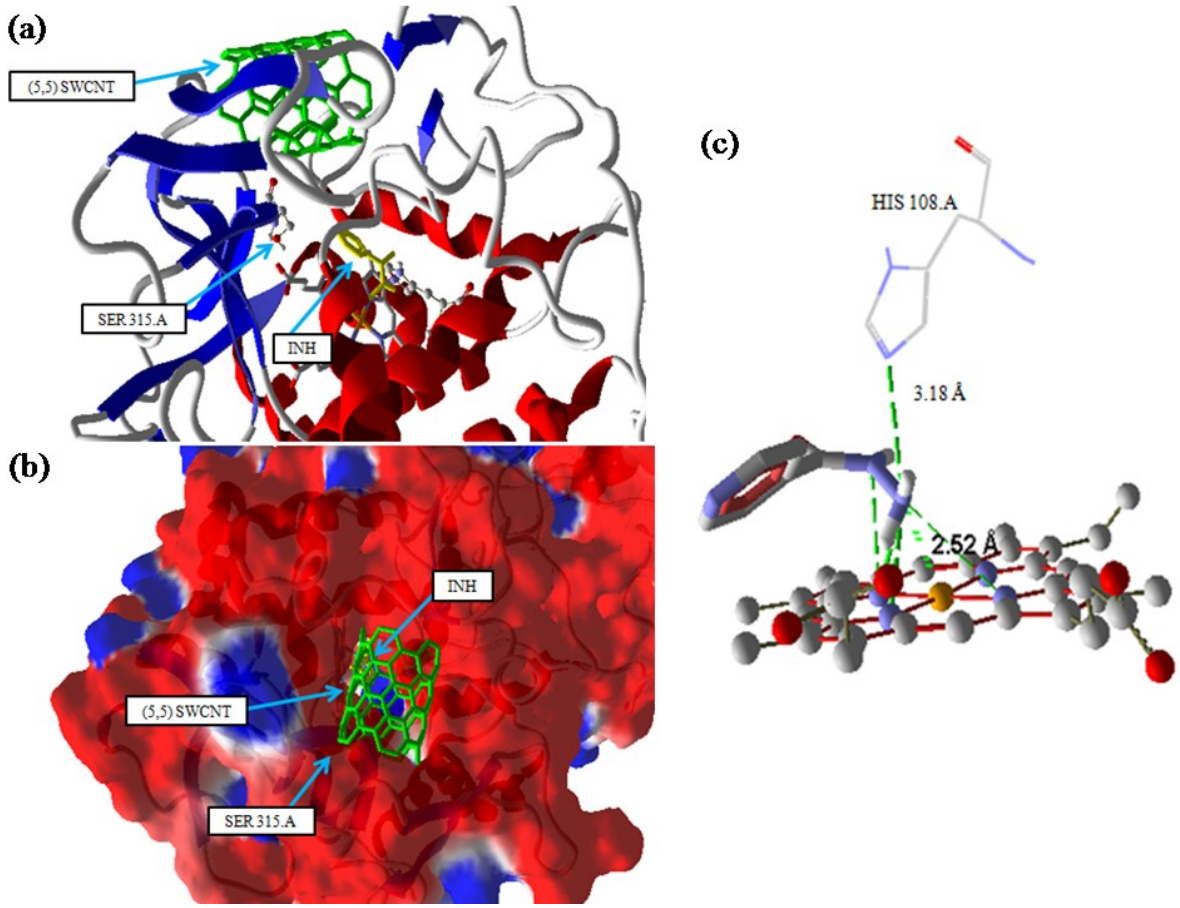

Fig. S11. (a) The secondary structure of INH noncovalently functionalized onto (5,5) SWNT docked onto wild type *mtCP* (1SJ2) protein, (b) hydrophobic surface depiction corresponding to the same, (c) the H–bonded distance between INH and the porphyrin ring along with His108 residues. The INH drug is shown in yellow and (5,5) SWNT is shown in green. For clarity we have omitted the Hydrogen atoms for the protein and the ligand structures.

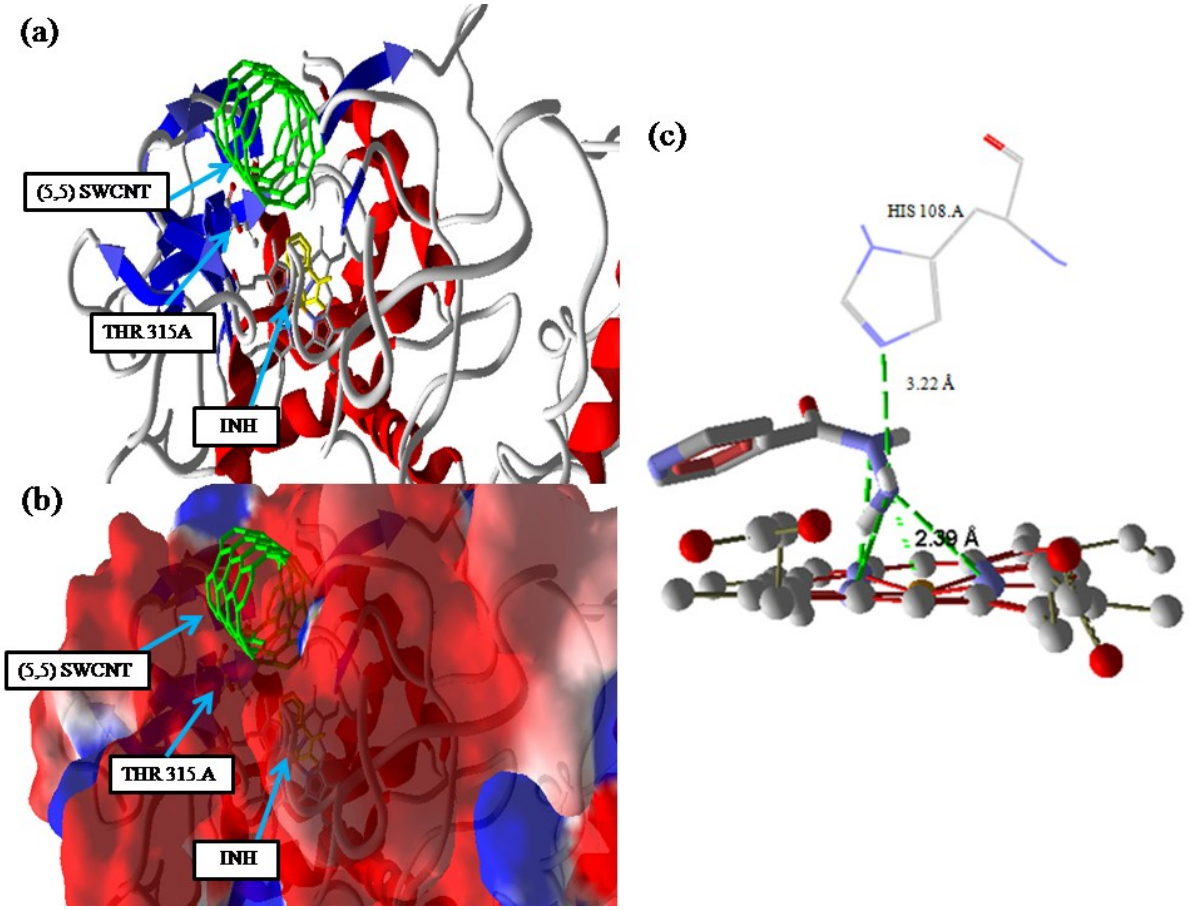

Fig. S12. (a) The secondary structure of INH noncovalently functionalized onto (5,5) SWNT docked onto mutant type *mtCP* (2CCD) protein, (b) hydrophobic surface depiction corresponding to the same, (c) the H–bonded distance between INH and the porphyrin ring along with His108 residues. The INH drug is shown in yellow and (5,5) SWNT is shown in green.

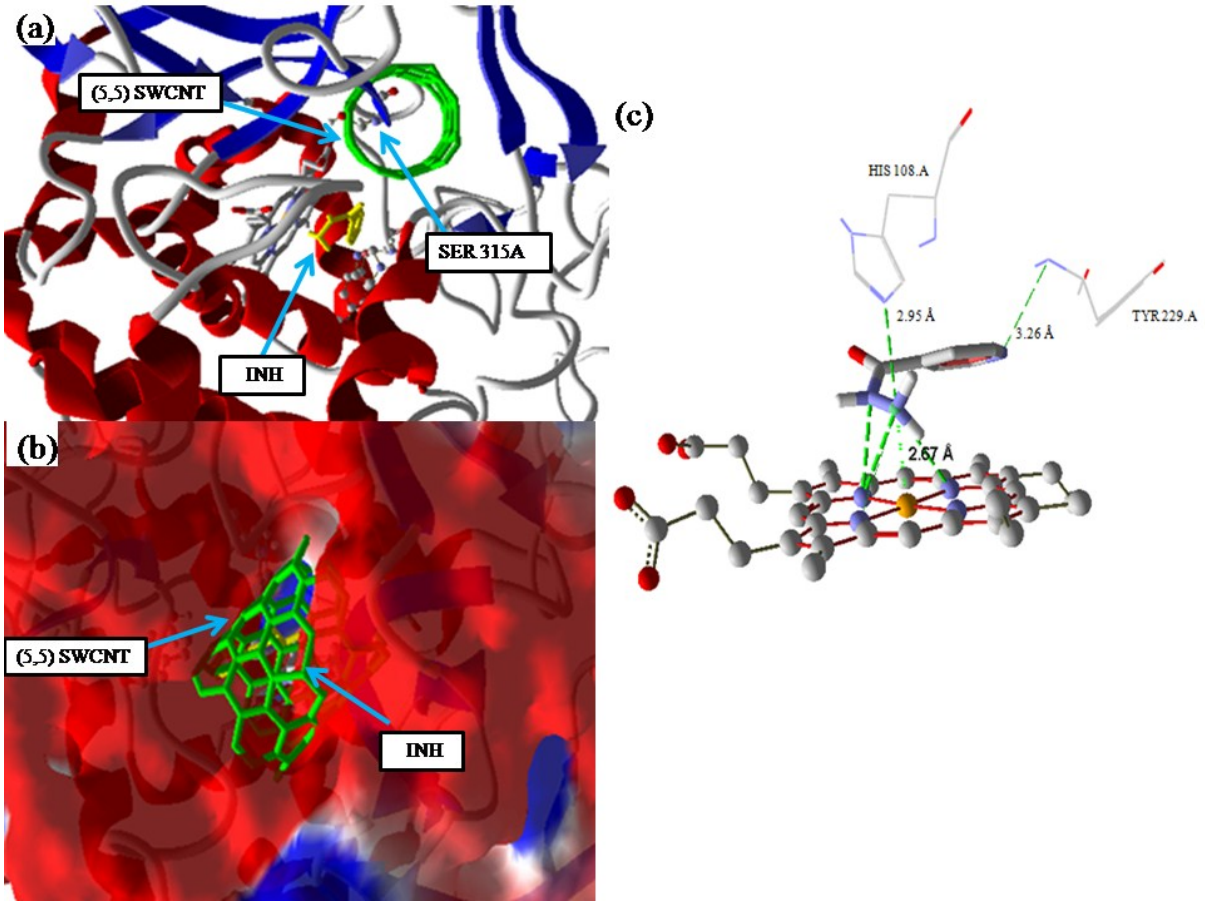

Fig. S13. (a) The secondary structure of INH noncovalently functionalized onto Si–doped (5,5) SWNT docked onto wild type *mtCP* (1SJ2) protein, (b) hydrophobic surface depiction corresponding to the same with the nanotube docked at the entering cavity of the protein, (c) the H–bonded distance between INH and the porphyrin ring along with His108 and Tyr229 residues. The INH drug is shown in yellow and (5,5) SWNT is shown in green.