Supporting Information

Dynamics study on graphene mediated pyrazinamide drug delivery onto pncA protein

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Table S1. The force field parameters for carbon and hydrogen atoms used for describing graphene.

[ atomtypes ]
; name     mass     charge   ptype     sigma     eps
CJ  6 12.01100  0.000   A  3.55000e-01  2.92880e-01
HJ  1  1.00800  0.000   A  2.42000e-01  1.25520e-01

[bondtypes]
; i    j    func    b0    kb
CJ  CJ  1  0.14000  392459.2
CJ  HJ  1  0.10800  307105.6

[ angletypes ]
CJ  CJ  CJ  CJ  1  120.000  527.184
CJ  CJ  HJ  CJ  1  120.000  292.880
HJ  CJ  HJ  HJ  1  117.000  292.880

[ dihedraltypes ]
CJ  CJ  CJ  CJ  C  3  30.33400  0.00000 -30.33400  0.00000  0.00000  0.00000 ; aromatic ring
HJ  CJ  CJ  HJ  C  3  30.33400  0.00000 -30.33400  0.00000  0.00000  0.00000 ; aromatic ring
HJ  CJ  CJ  CJ  C  3  30.33400  0.00000 -30.33400  0.00000  0.00000  0.00000 ; aromatic ring

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![Pyrazinamide (PZA) and 6×6 graphene](image)

Fig. S1. The optimized geometries of (a) PZA, (b) 6×6 graphene.
**Fig. S2.** Interaction of 6×6 graphene with some of the closely oriented ligand binding residues of pncA along the binding pathway.

**Fig. S3.** (a) COM distance between the selected ligand binding residues of pncA (described in Fig. S2) and 6×6 graphene, (b) RMSF of non H atoms of pncA with respect to atom number of pncA atoms.
Fig. S4. (a) The RMSD vs. time (ns) plot for PZA, pncA and PZA/pncA combined with PZA placed along the entering pathway of pncA, (b) variation in COM distance between PZA and selected amino acid residues oriented in close proximity.

Fig. S5. The snapshots corresponding to simulation of PZA/pncA protein with PZA docked within the binding pocket of pncA for 40 ns time frame.
Fig. S6. The RMSD vs. time (ns) plot for PZA, pncA and PZA/pncA combined with PZA docked within the binding pocket of pncA.

Fig. S7. (a) Interaction of PZA and graphene with some of the ligand binding residues of pncA, (b) RMSF of non H atoms of pncA with respect to the residue number of the protein atoms.