Electronic Supplementary Material (ESI) for RSC Advances.

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     1   120.000    527.184
  CJ    CJ    HJ     1   120.000    292.880
  HJ    CJ    HJ     1   117.000    292.880

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

List of Figures:

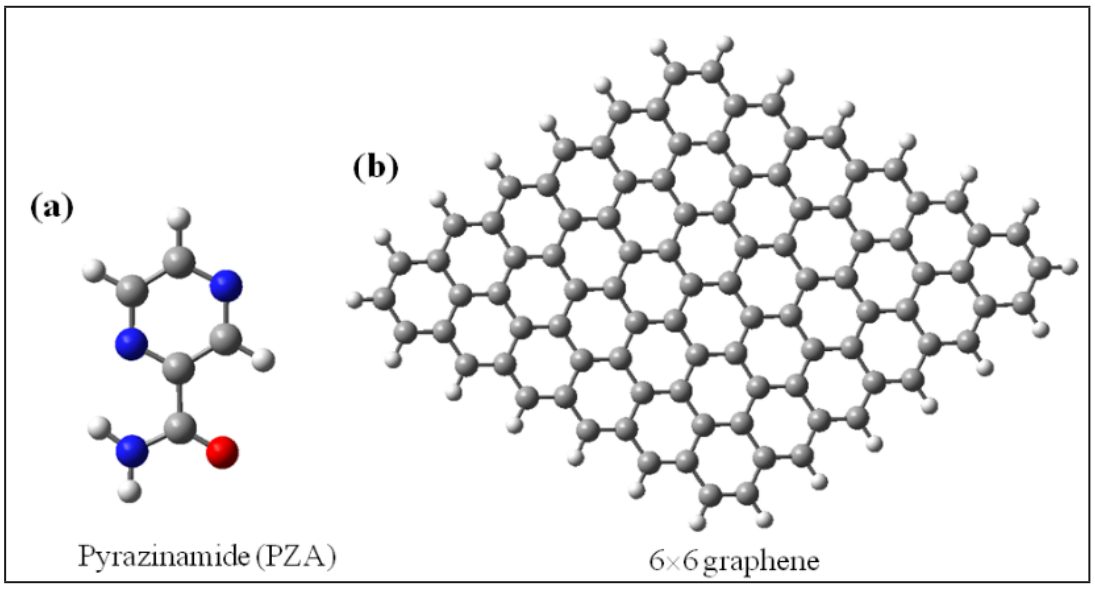

Fig. S1. The optimized geometries of (a) PZA, (b) 6×6 graphene.

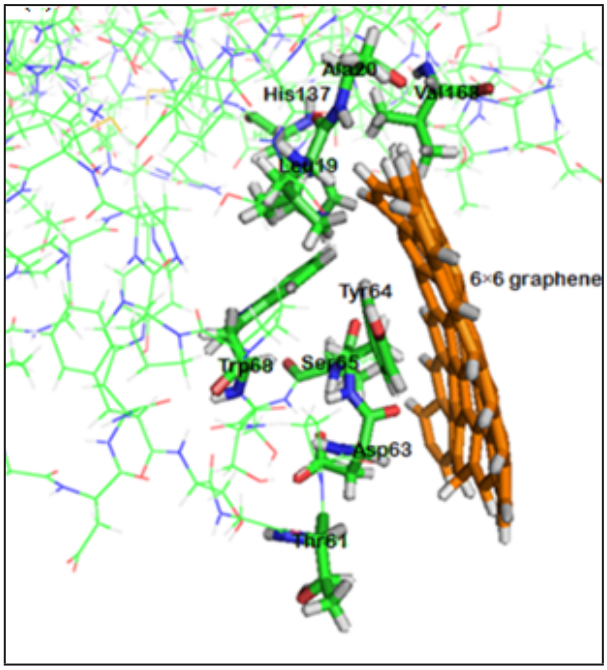

Fig. S2. Interaction of 6×6 graphene with some of the closely oriented ligand binding residues of pncA along the binding pathway.

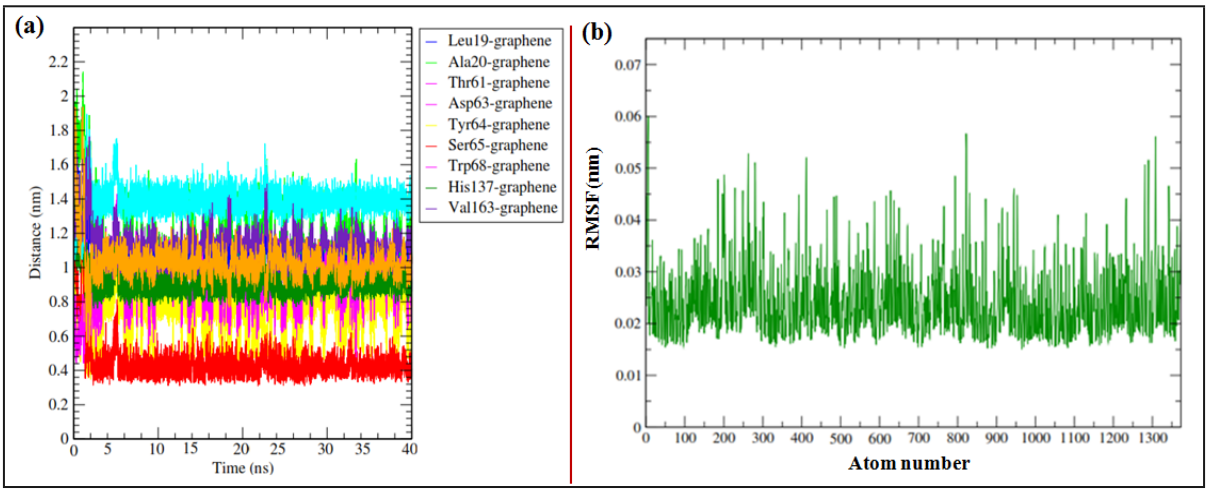

Fig. S3. (a) COM distance between the selected ligand binding residues of pncA (described in Fig. S2) and 6×6 graphene, (b) RMSF of non H atoms of pncA with respect to atom number of pncA atoms.

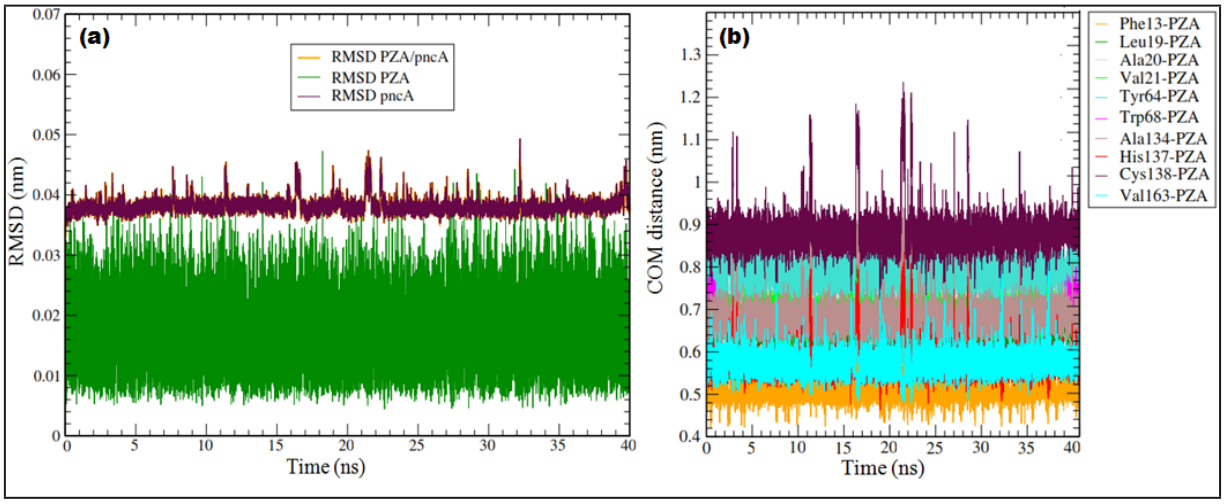

Fig. S4. (a) The RMSD vs. time (ns) plot for PZA, pncA and PZA/pncA combined with PZA placed along the entering pathway of pncA, (b) variation in COM distance between PZA and selected amino acid residues oriented in close proximity.

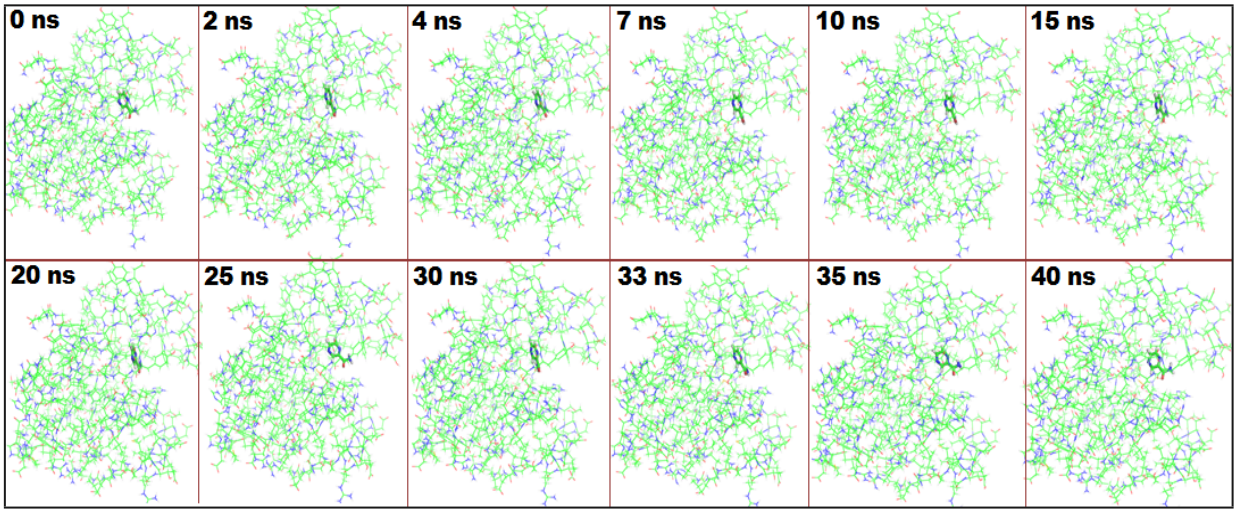

Fig. S5. The snapshots corresponding to simulation of PZA/pncA protein with PZA docked within the binding pocket of pncA for 40 ns time frame.

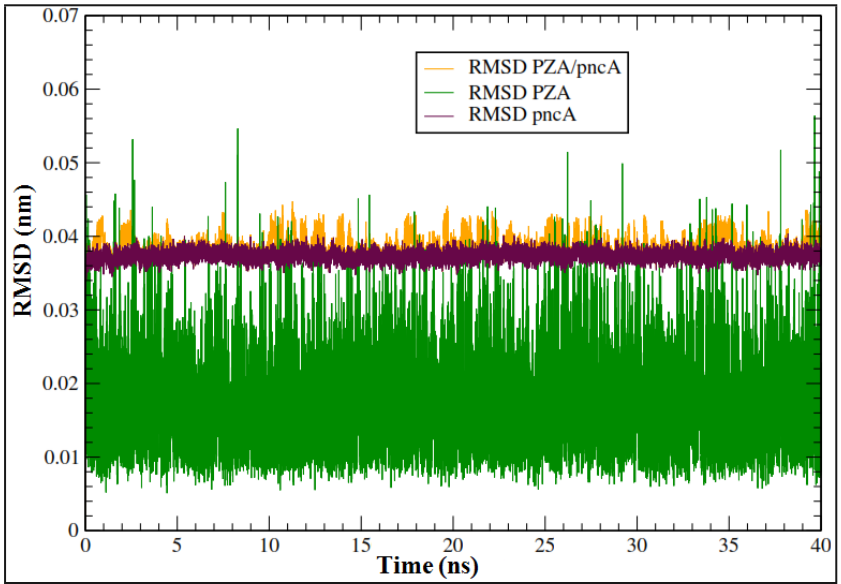

Fig. S6. The RMSD vs. time (ns) plot for PZA, pncA and PZA/pncA combined with PZA docked within the binding pocket of pncA.

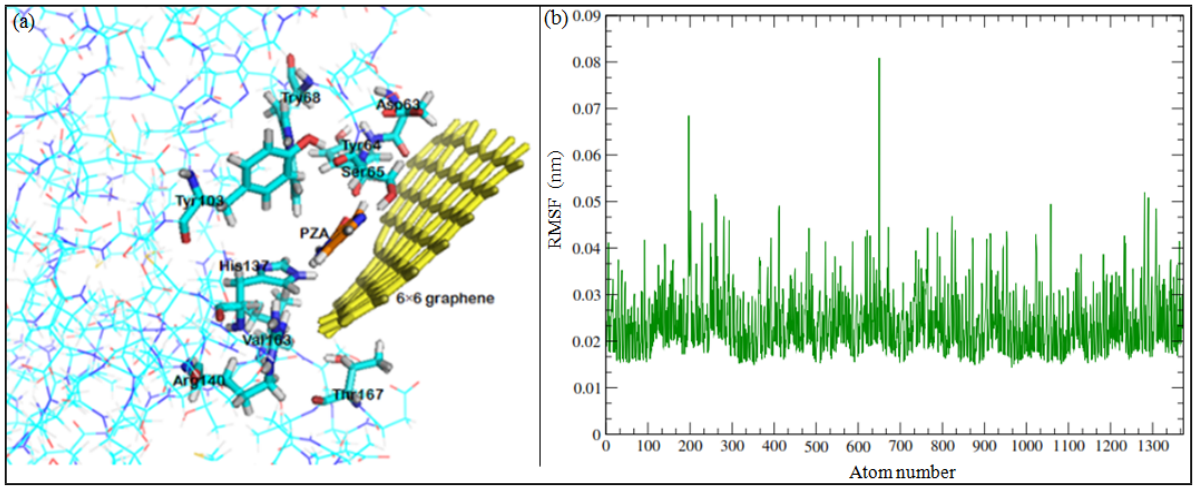

Fig. S7. (a) Interaction of PZA and graphene with some of the ligand binding residues of pncA, (b) RMSF of non H atoms of pncA with respect to the residue number of the protein atoms.