Electronic Supplementary Material (ESI) for RSC Advances.

Exploring the mode of action of inhibitors targeting PhoP response regulator of Salmonella enterica through comprehensive pharmacophore approaches

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Supporting information

Molecular dynamics simulations

The MD simulations were conducted through the "**Standard Dynamics Cascade**" module implemented in Discovery Studio 3.5 (Accelrys Software, Inc., San Diego, CA, USA). All the docked inhibitors were subjected to a set of minimization and equilibration steps followed by molecular dynamics using CHARMm forcefield. The parameter settings of the standard dynamics cascade were described as follows. For the first **Minimization**, the "**Steepest Decent**" was chose as the algorithm. The "**Max Steps**" and the "**RMS Gradients**" were set to 1,000 and 1.0, respectively. For the second **Minimization**, "**Adopted Basis NR**" was employed as the algorithm. The "**Max Steps**" and the "**RMS Gradients**" were set to 2,000 and 0.1, individually. About the **Heating**, the **Simulation time (ps), Time Step (fs), Initial temperature, Target Temperature, Adjust Velocity Frequency,** and the **Save Results Interval (ps)** were set to 4, 2, 50, 300, 50, and 2, respectively. After that, the **Equilibration** was done with the **Simulation Time, Time Step (fs), Target Temperature, Adjust Velocity Frequency,** and the **Save Results Interval (ps)** set to 10, 2, 300, 50, and 2, individually.

For the "**Production"**, all the parameters were set as defaults. The "**Nonbond List Radius**" was set to 14, and "**Electrostatic**" was set to "**Automatic**".

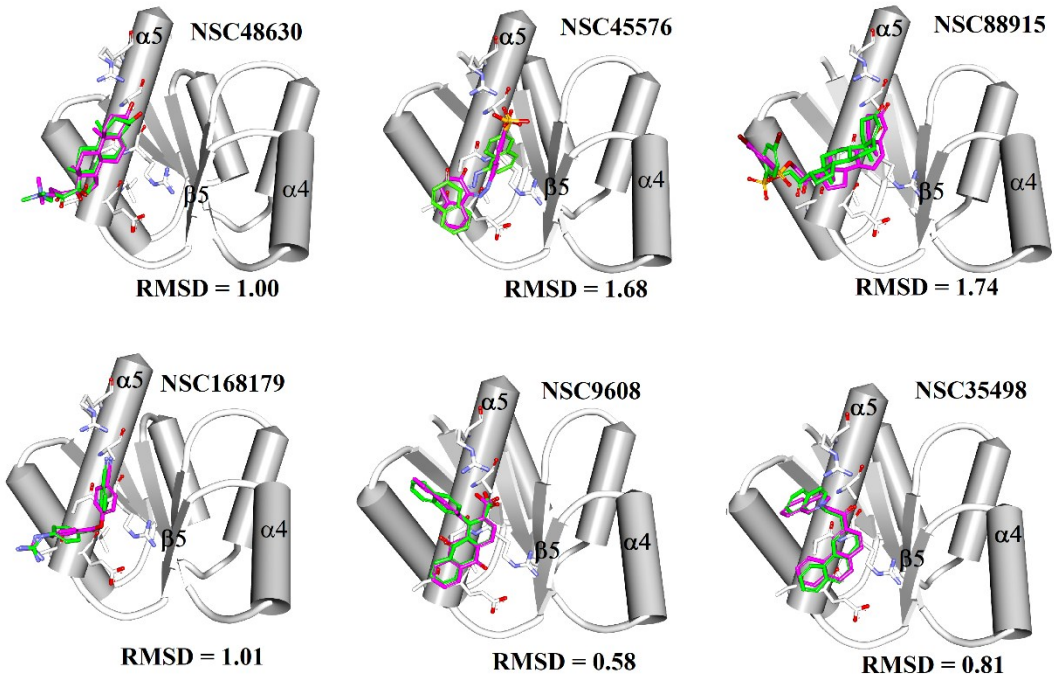

Fig. S1. The diagrammatic representations of the superimpositions of the docked PhoP inhibitors before and after molecular dynamic simulations. The docked PhoP inhibitors from ligand-pharmacophore mapping were subjected to molecular dynamic simulations. The inhibitors shown in magenta and green are the poses before and after molecular dynamic simulations, respectively.