



S2 Fig. Illustration of the binding patterns between the MHC molecule and acyclovir predicted by molecular docking studies.

Hydrogen bond interactions between the Ile 124 (MHC molecule) main chains and acyclovir is represented by green dashed arrow. Hydrogen bond interactions between side-chains of Ser 116, Asp 114 (MHC molecule) and acyclovir is represented by blue dashed arrow. Pi interactions between the Trp147, Tyr74 of the MHC molecule and acyclovir is shown in orange line. Figure prepared by using Discovery Studio software (version 3.1; Accelrys Inc., USA).

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