

Myricetin allosterically inhibits Dengue NS2B-NS3 protease by disrupting the active and locking the inactive conformations

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Short title: Mechanism for myricetin to allosterically inhibit Dengue protease

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Supplementary Figures

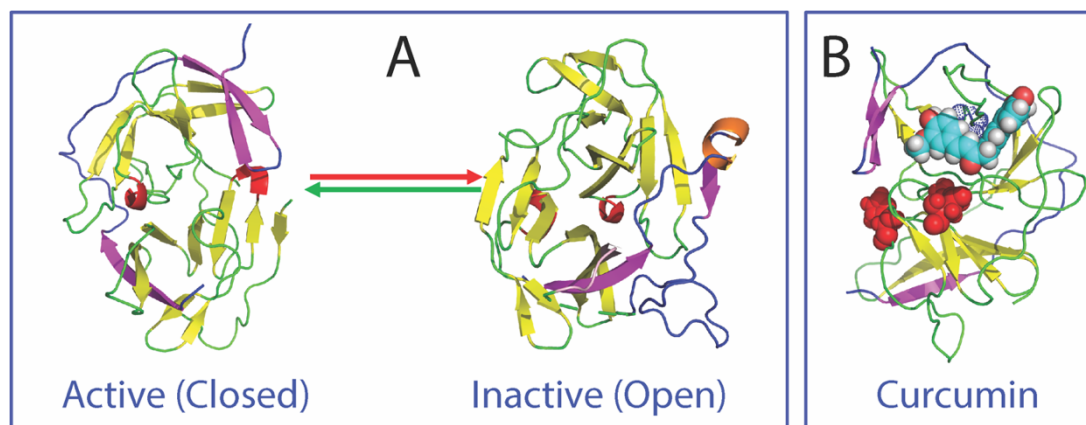


Figure S1. Conformational equilibrium and allosteric inhibition by Curcumin.

(A) Conformational equilibrium of the active (closed) and inactive (open) forms of Dengue NS2B-NS3 protease. (B) The active form of Dengue protease in complex with Curcumin (in spheres) at AS1. Red spheres are used to indicate the catalytic triad composed of His51, Asp75 and Ser135.

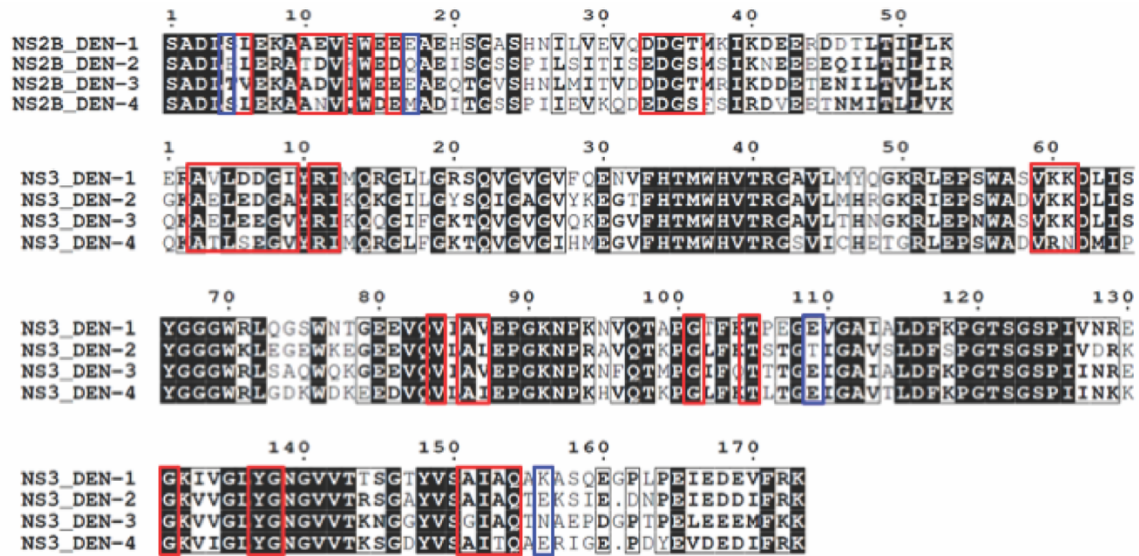


Figure S2. Alignment of NS2B and NS3 sequences of four serotypes of DENV.
 The significantly perturbed residues were boxed with different colors: red for the identical or consensus residues and blue for the different residues.