Supplementary Materials

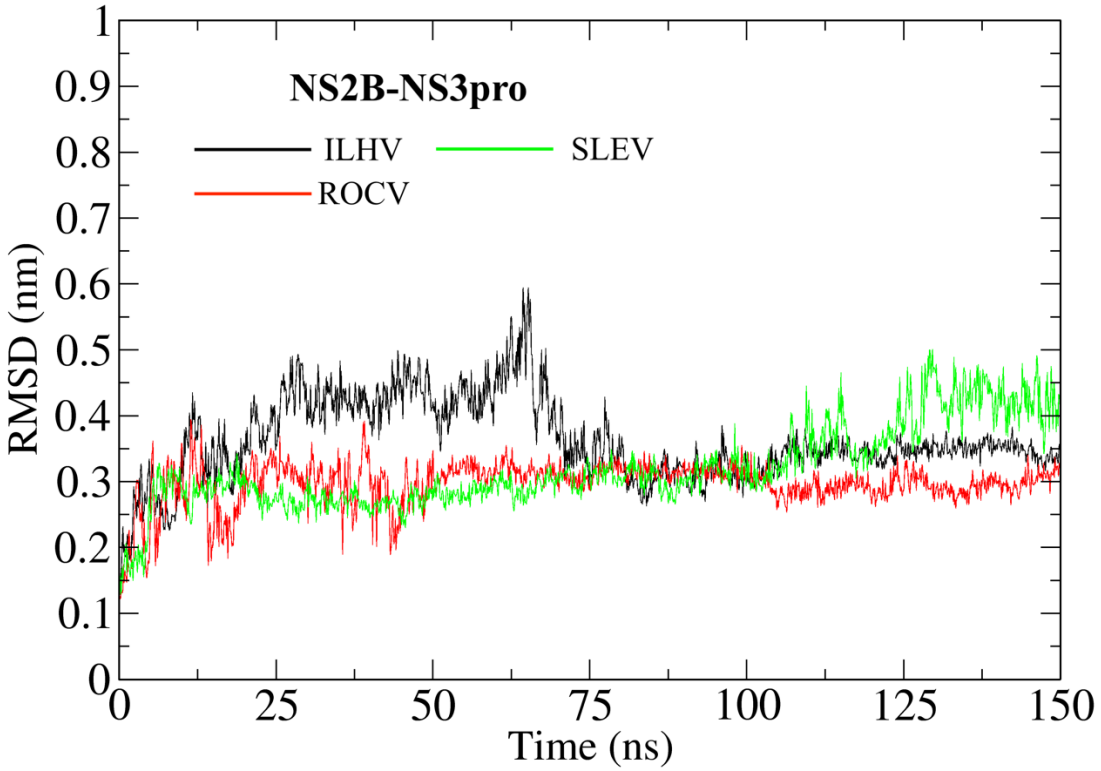


Figure S1—Root mean square deviation (RMSD) analysis from molecular dynamics (MD) simulations. The RMSD evolution was different for each species. The ILHV NS2B–NS3pro protein (black line) is highly unstable until ~80 ns, when the protein becomes stable with an RMSD value of 0.3 to 0.4 nm. The Rocio virus (ROCV) NS2B–NS3Bpro protein becomes stable earlier than the Ilhéus virus (ILHV) protein. At approximately ~60 ns, it is possible to see the protein stability in the RMSD of 0.3 nm. On the other hand, the opposite occurs for the Saint Louis encephalitis virus (SLEV) NS2B–NS3pro protein, where the protein is highly stable at the beginning of the simulation (~0.3 nm) but increases its RMSD value at approximately 100 ns in its trajectory.

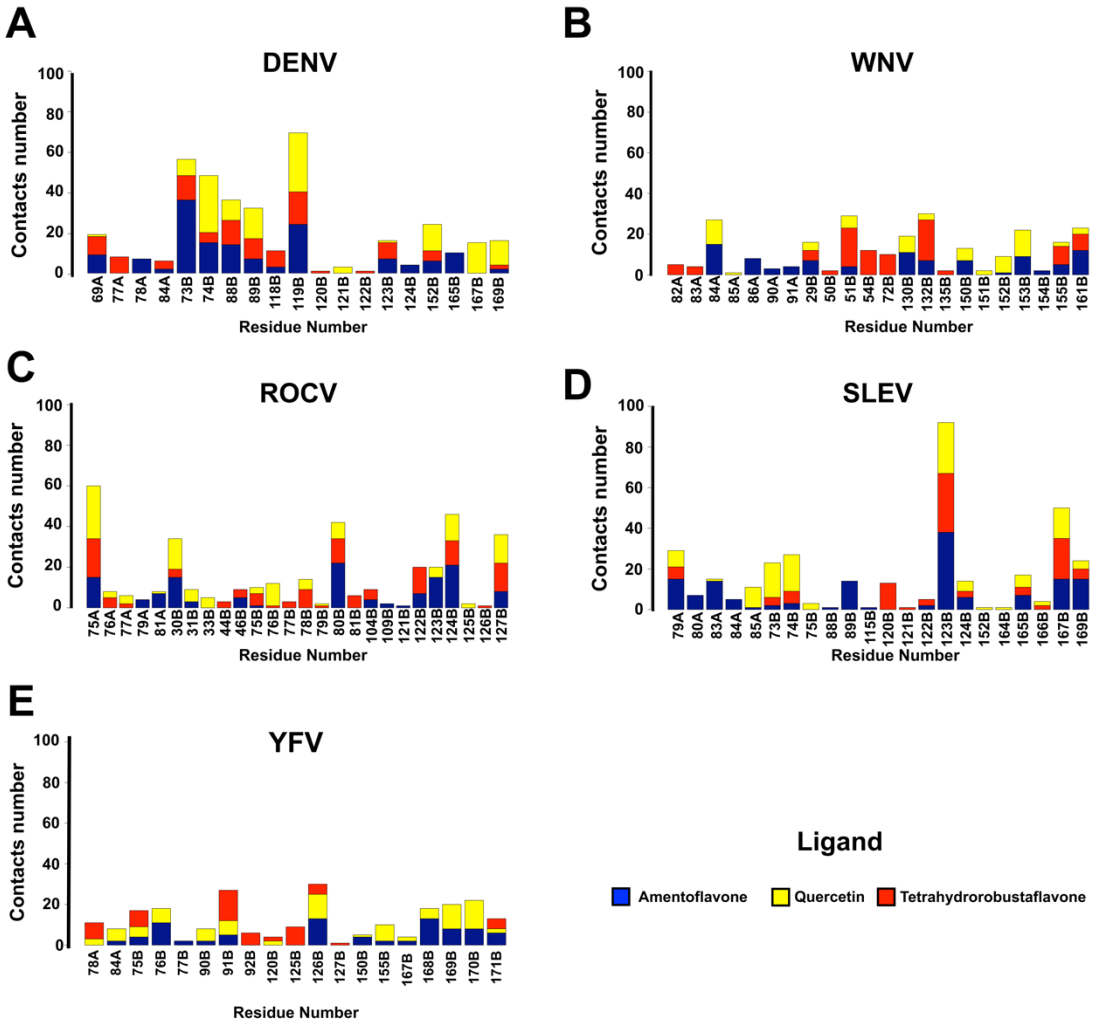


Figure S2—Stacked bar plot version of Figure 7, showing the number of contacts per residue of the NS2B–NS3pro protein complex of the dengue virus (DENV), West Nile virus (WNV), Rocio virus (ROCV), Saint Louis encephalitis virus (SLEV) and yellow fever virus (YFV). In this case, it is easier to see the most contacted residues for all molecules.

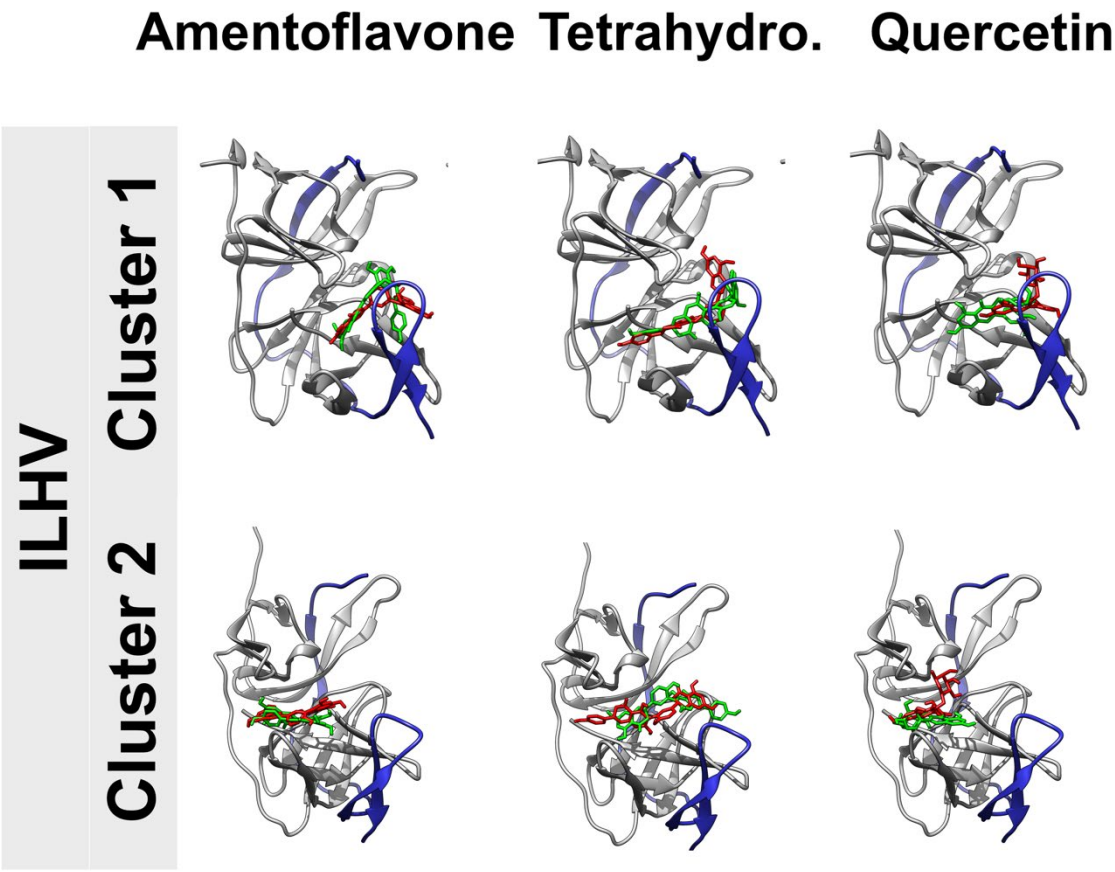


Figure S3—Representation of the binding modes of the molecules in the NS2B–NS3pro proteins from Ilhéus (ILHV). On the right of NS2B (blue ribbon) is the allosteric site and on the left is the active site.

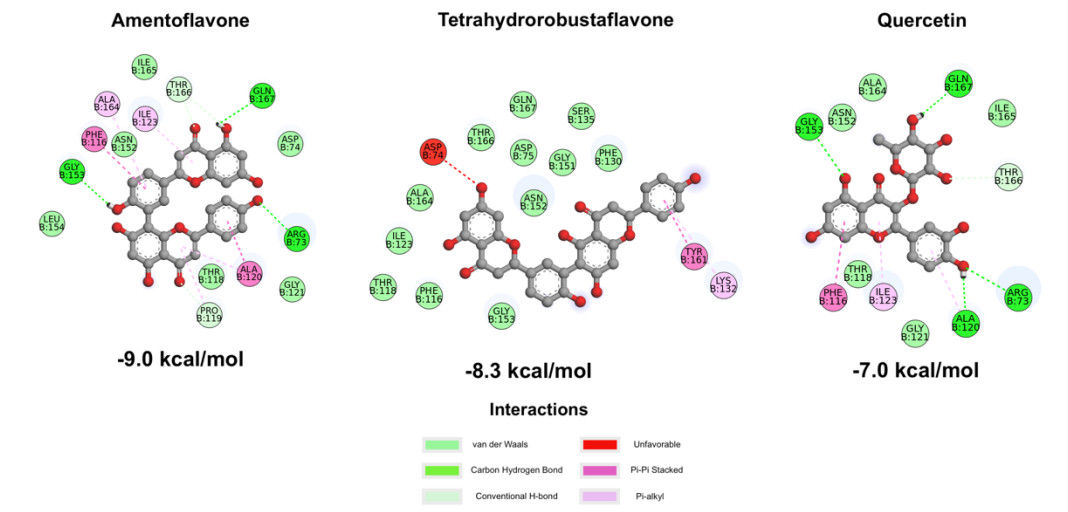


Figure S4—Interaction analysis of flavonoids and NS2B–NS3pro proteins from Ilhéus (ILHV), Cluster 2.