

## **Supporting Information**

### **Tautomeric and Base Pairing Effects of Some of the Vital Antiviral Drugs used Against COVID-19**

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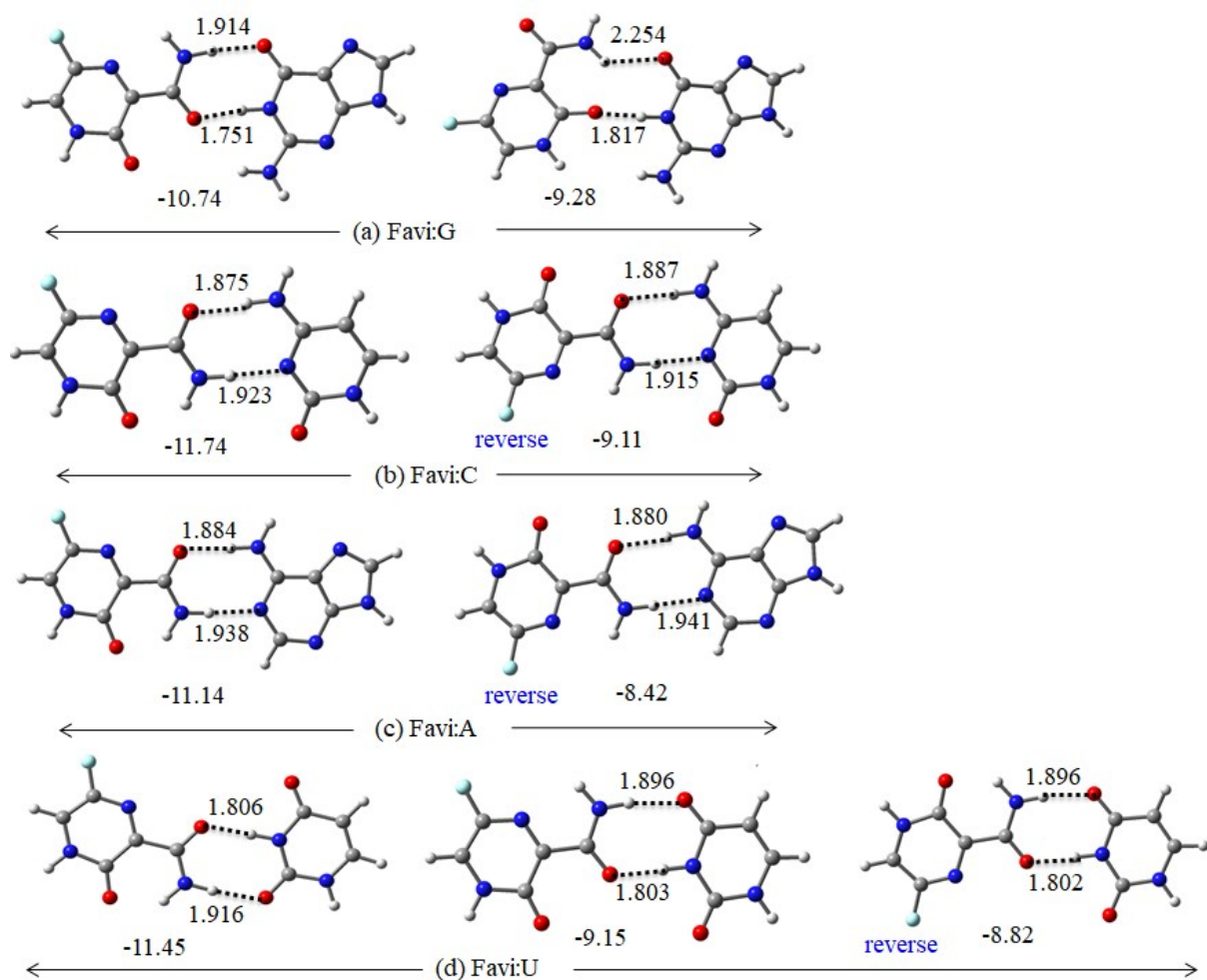


Fig. S1: Structures of different base pairs involving the keto tautomer of Favipiravir (k-Favi) obtained in the aqueous medium. The binding energies (kcal/mol) and hydrogen bond distances obtained at the B3LYP-D3/6-311++G\*\* level of theory in the aqueous medium are also shown.

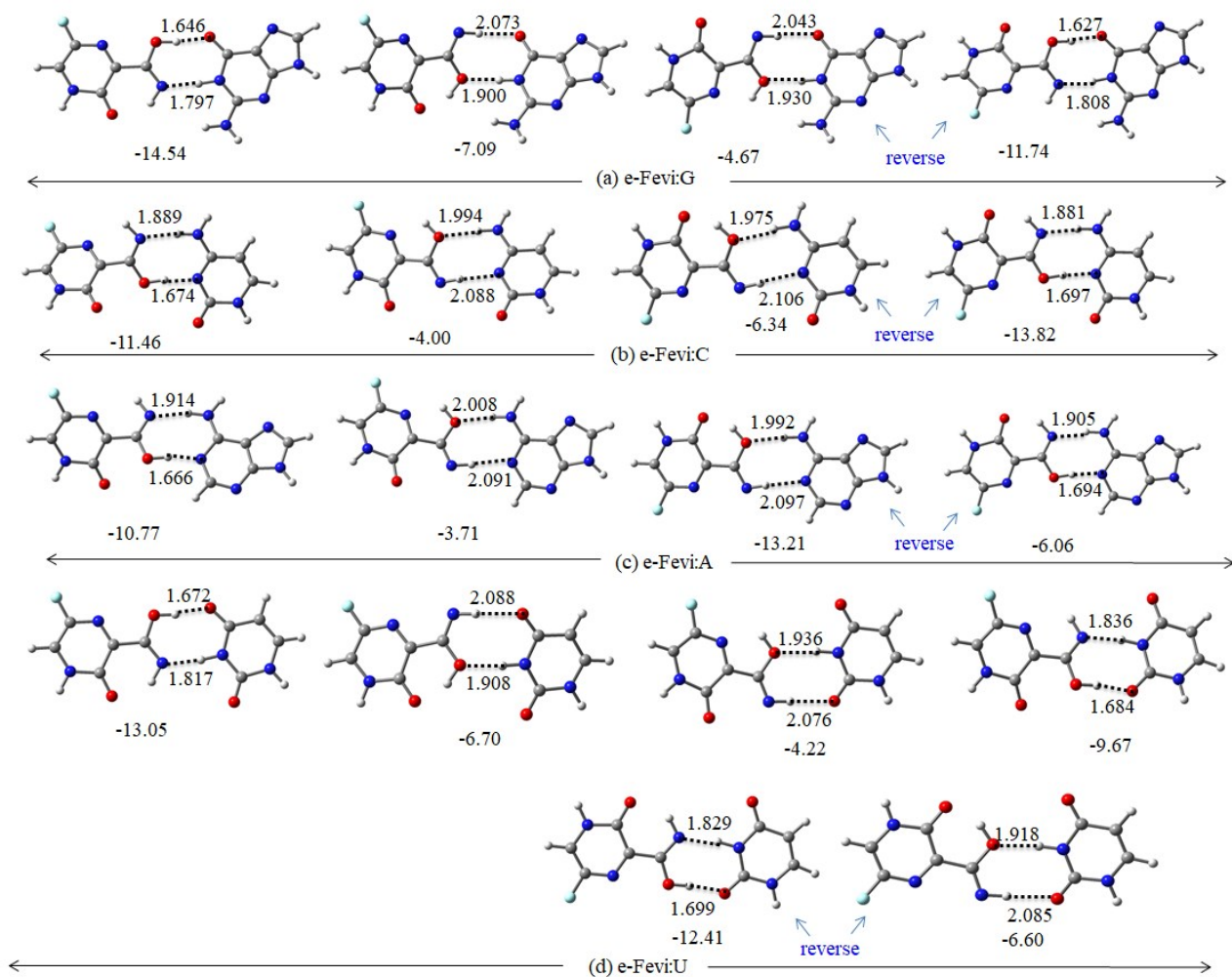


Fig. S2: Structures of different base pairs involving the enol tautomer of Favipiravir (e-Favi). The binding energies (kcal/mol) obtained at the B3LYP-D3/6-311++G\*\* level of theory in aqueous medium and hydrogen bond distances are also shown.

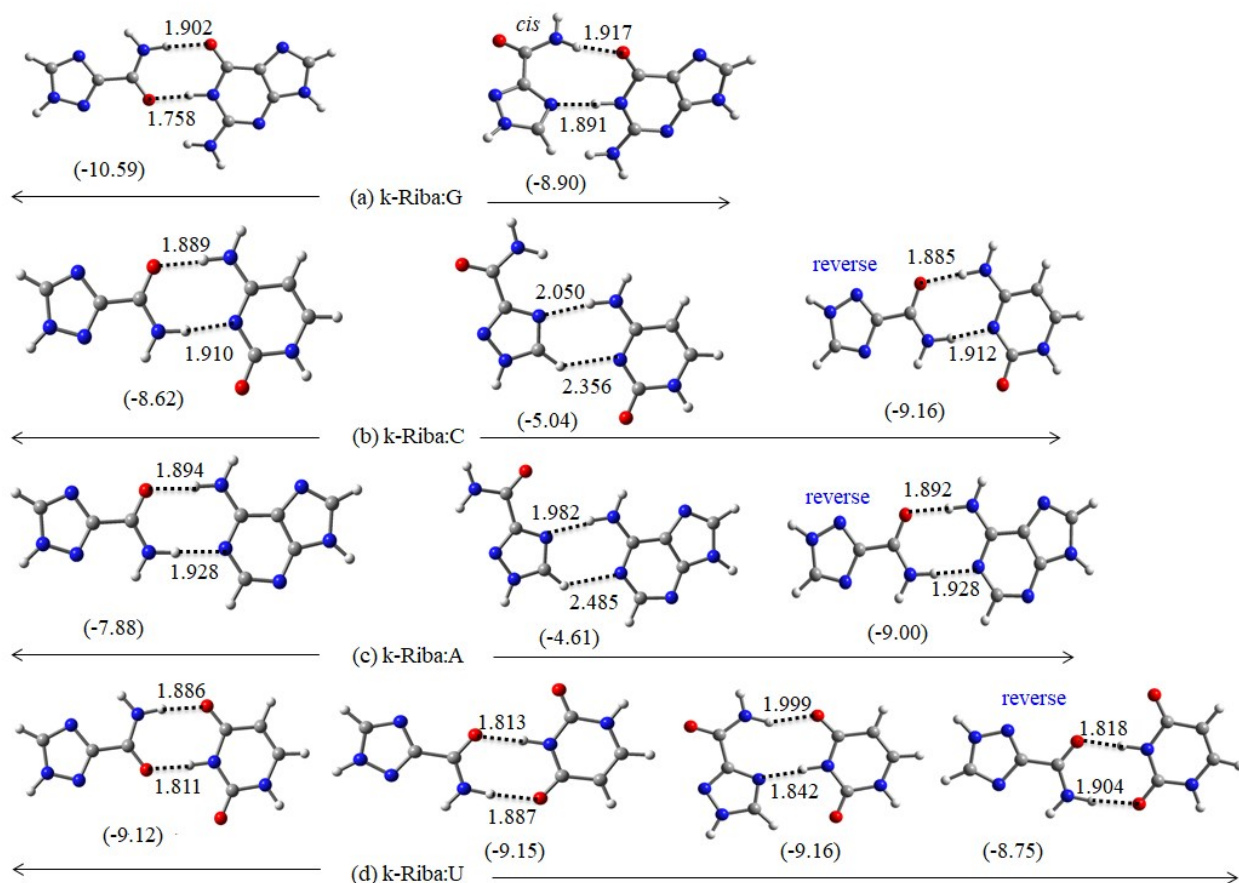


Fig. S3: Structures of different base pairs involving the keto tautomer of Ribavirin (k-Riba). The binding energies (kcal/mol) obtained at the B3LYP-D3/6-311++G\*\* level of theory in aqueous medium and hydrogen bond distances are also shown.

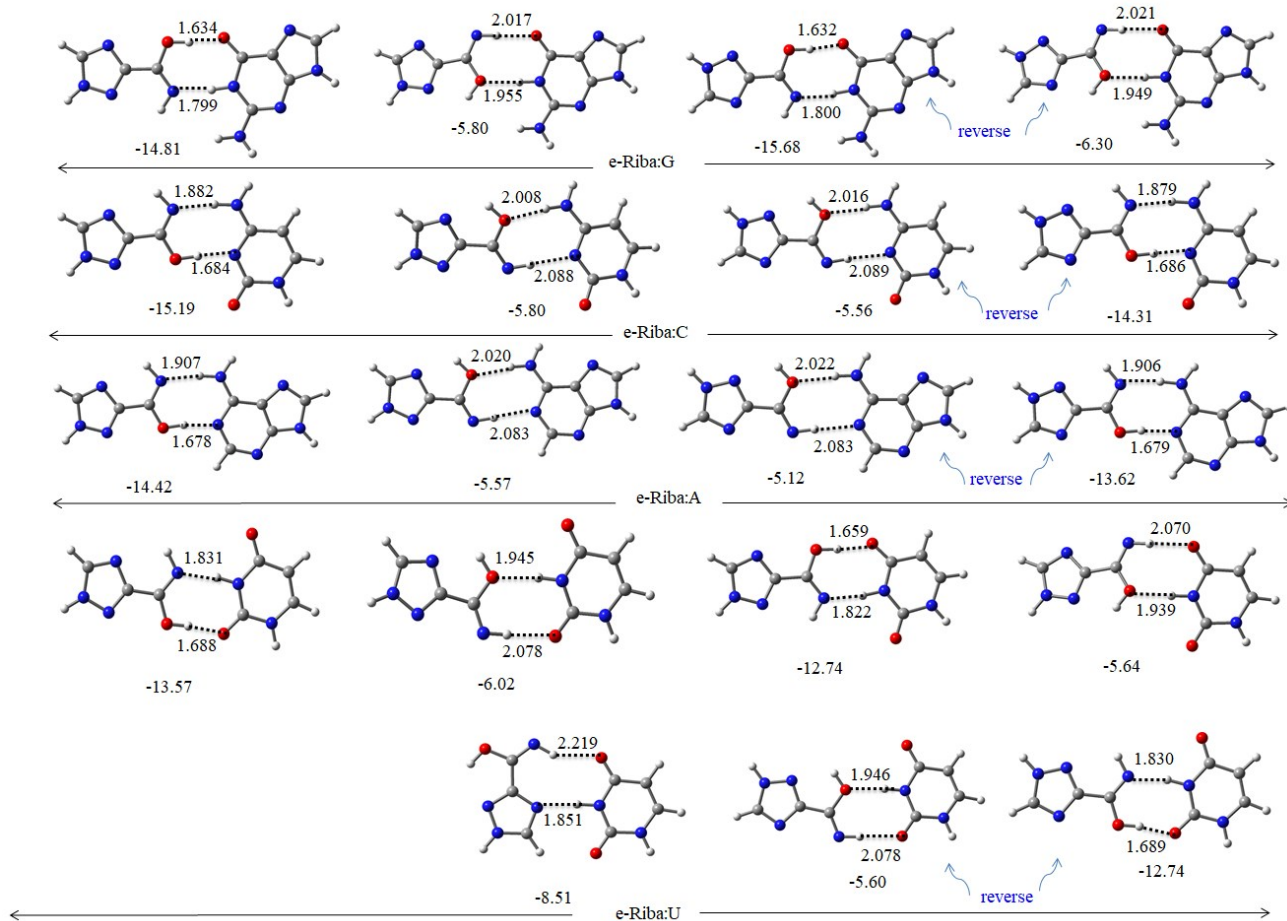


Fig. S4: Structures of base pairs involving the enol tautomer of Ribavirin (e-Riba). The binding energies (kcal/mol) obtained at the B3LYP-D3/6-311++G\*\* level of theory in aqueous medium and hydrogen bond distances are also shown.