**Supplementary Information**

**Structural Insights into the Zika Virus NS1 Protein Inhibition Using a Computational Approach.**

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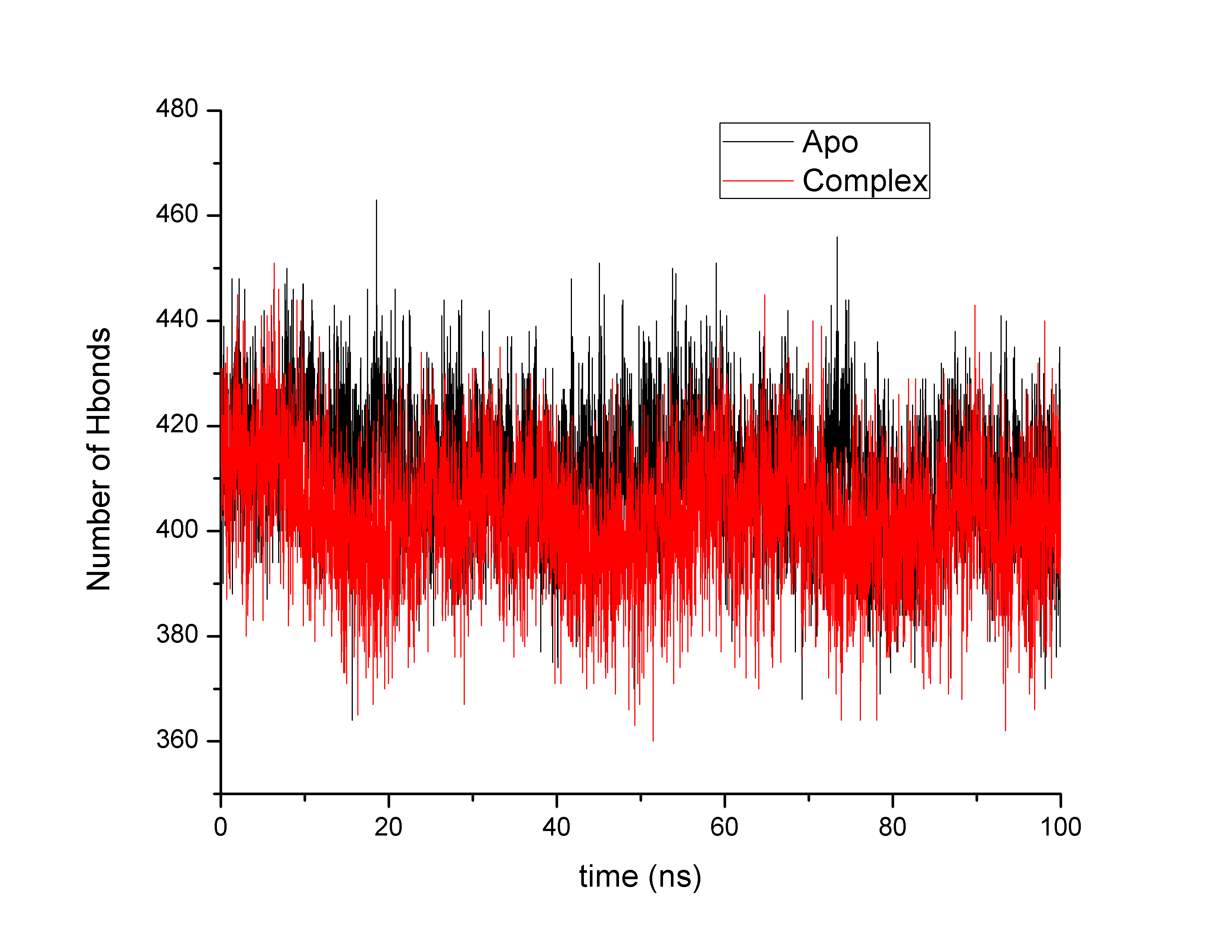
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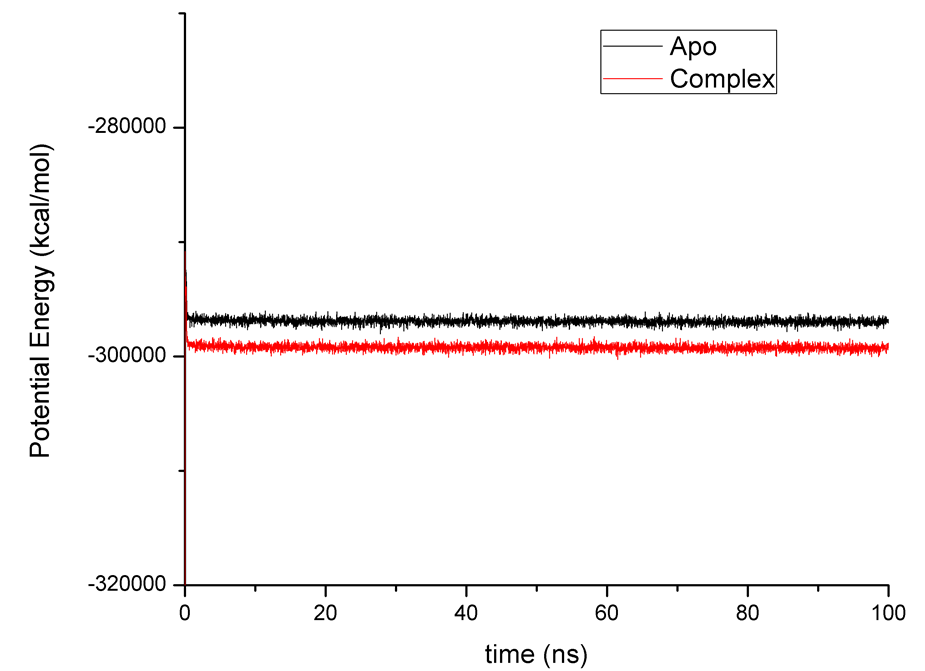
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**Supplementary figure 1.** Structures of flavonoid derivatives from F1 to F10.



**Supplementary figure 2.** The number of hydrogen bonds in Apo (black) and complex (red) during 100 ns simulation.



**Supplementary figure 3.** Potential energy of Apo (back) and complex (red) over a period of 100 ns simulation time.

|  |  |  |
| --- | --- | --- |
| **Apo** | **Apo** | **Apo** |
| **Complex** | **Complex** | **Complex** |

**Supplementary figure 4.** Principal component (PC) analysis of apo-protein of NS1 and NS1-flavonoid complex during100 ns simulation for three components PC1, PC2, PC3.