Characterizing the Structure-Activity Relationships of Natural Products, Tanshinones, Reveals their Mode of Action in Inhibiting Spleen Tyrosine Kinase

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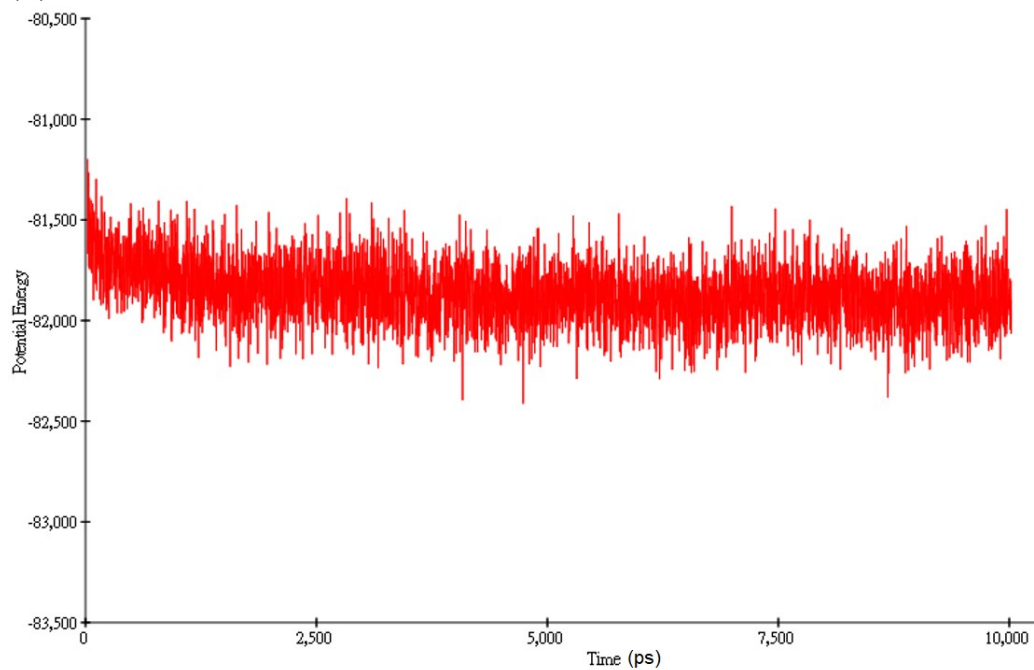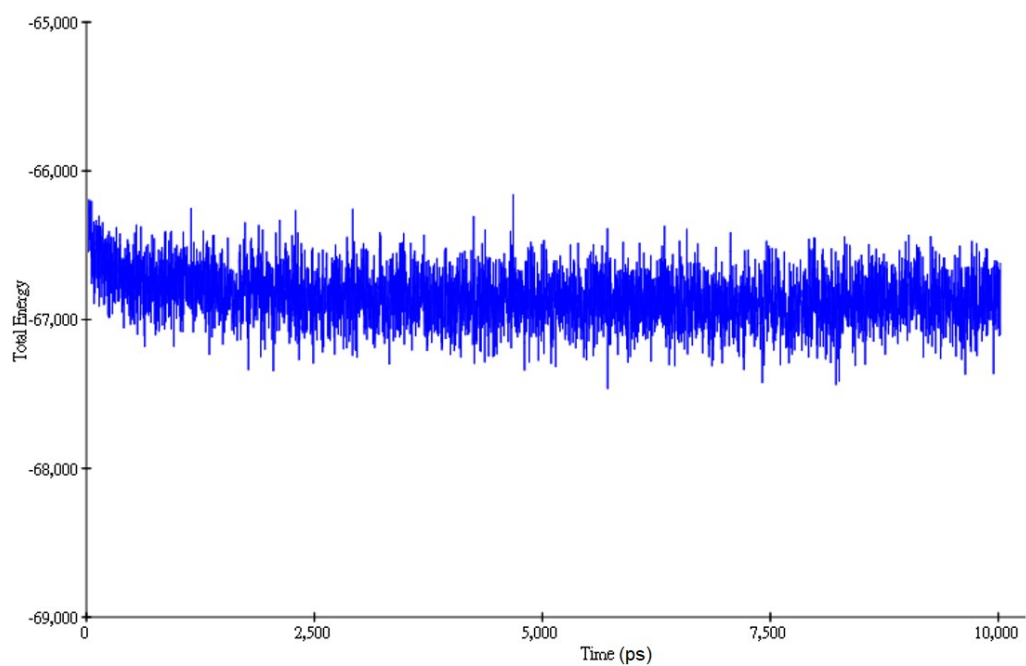
Supporting information

(A)
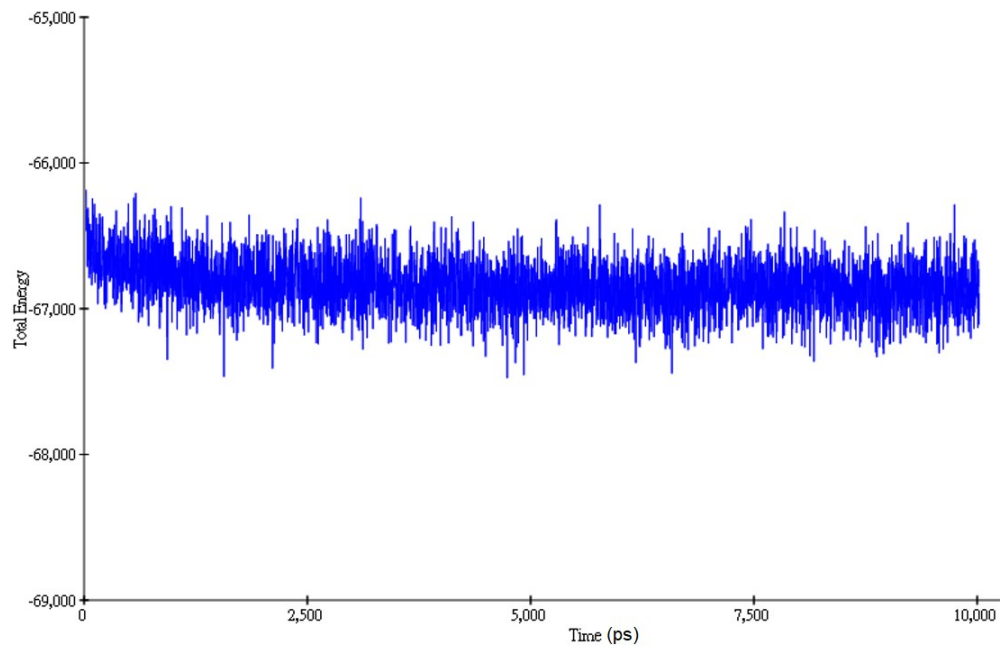
(B)

Figure S1. The molecular dynamics simulations of SYK-TanI complex for 10 ns.
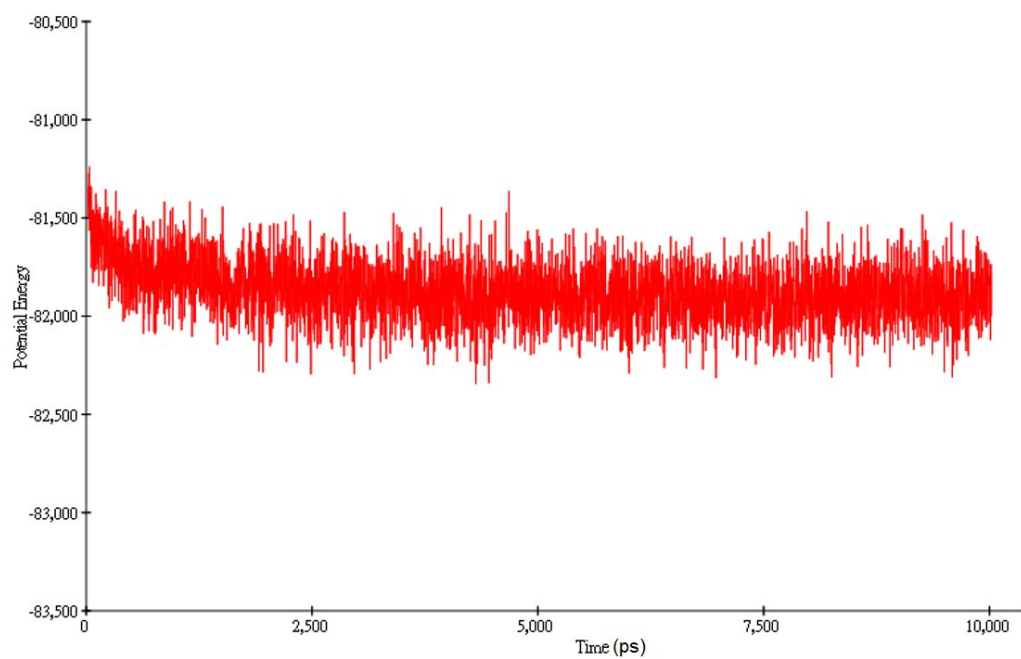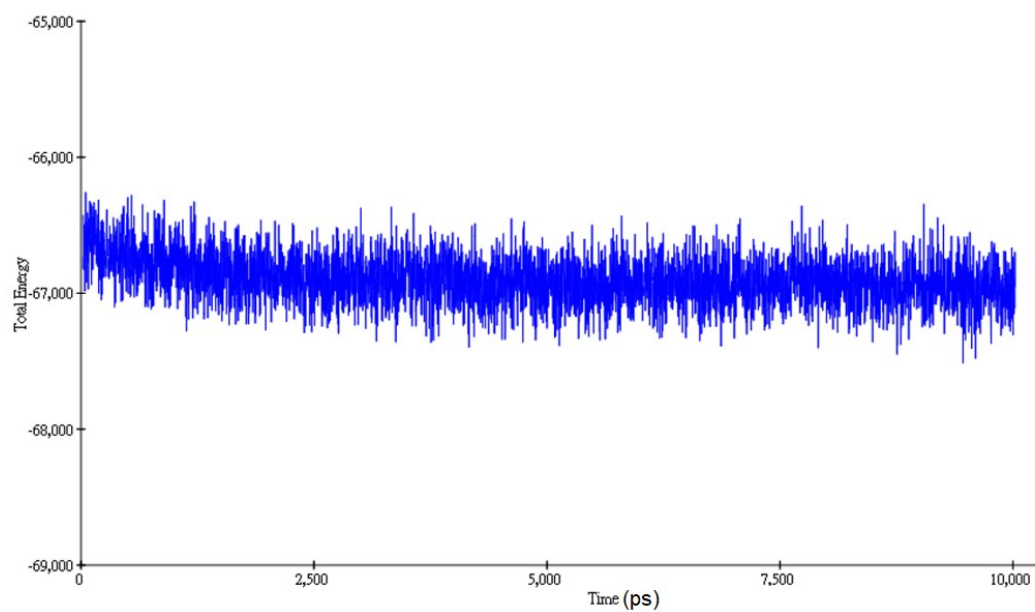(**A**) The total energy as a function of time (**B**) The potential energy as a function of
time.

(A)

(B)

Figure S2. The molecular dynamics simulations of SYK-TanIIA complex for 10 ns. (**A**) The total energy as a function of time (**B**) The potential energy as a function of time.
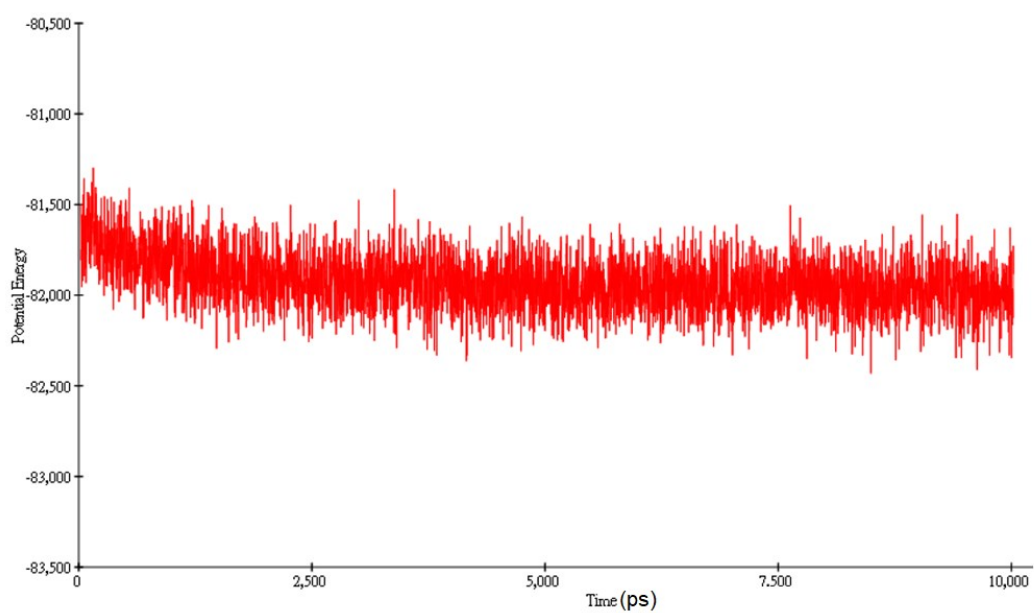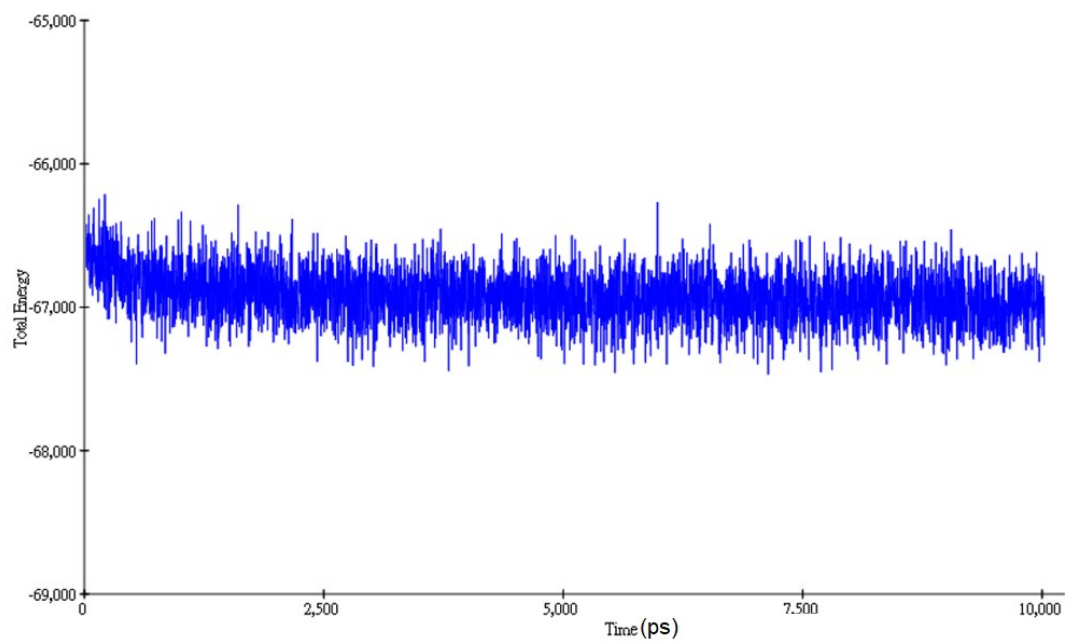
(A)

(B)

Figure S3. The molecular dynamics simulations of SYK-ST32da complex for 10 ns. (**A**) The total energy as a function of time (**B**) The potential energy as a function of time.
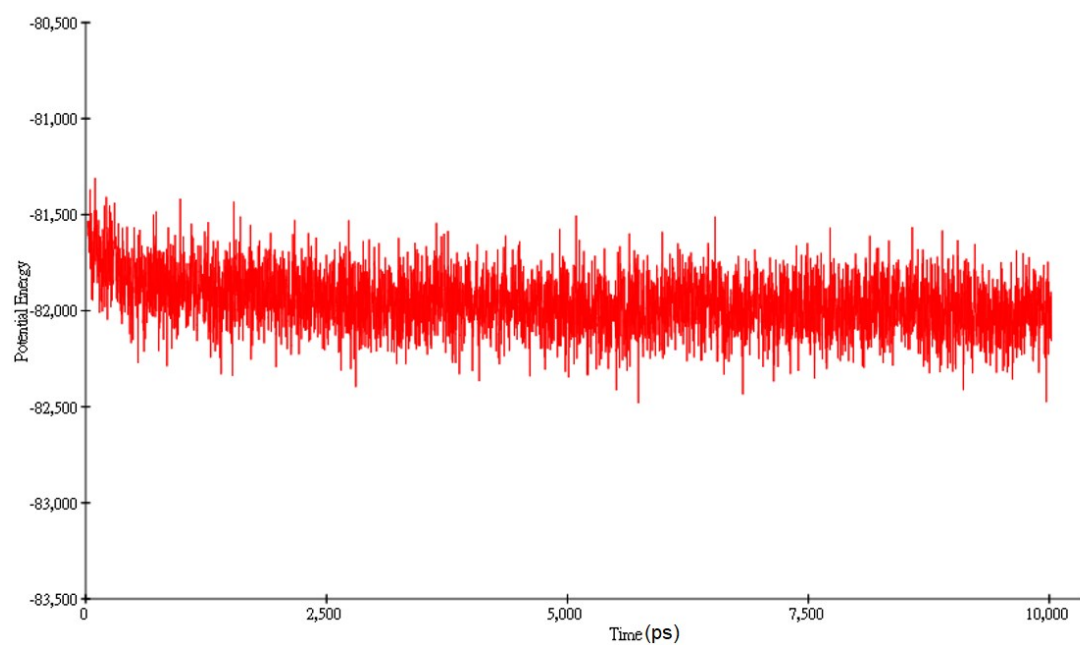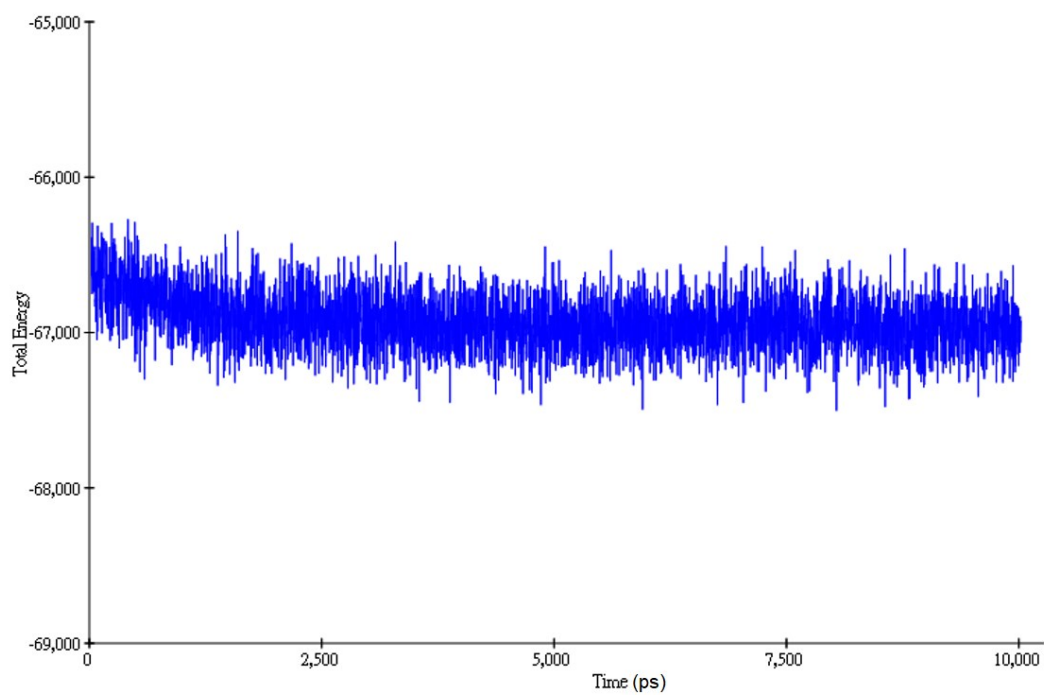
(A)

(B)

Figure S4. The molecular dynamics simulations of SYK-ST32db complex for 10 ns. (A) The total energy as a function of time (**B**) The potential energy as a function of time.
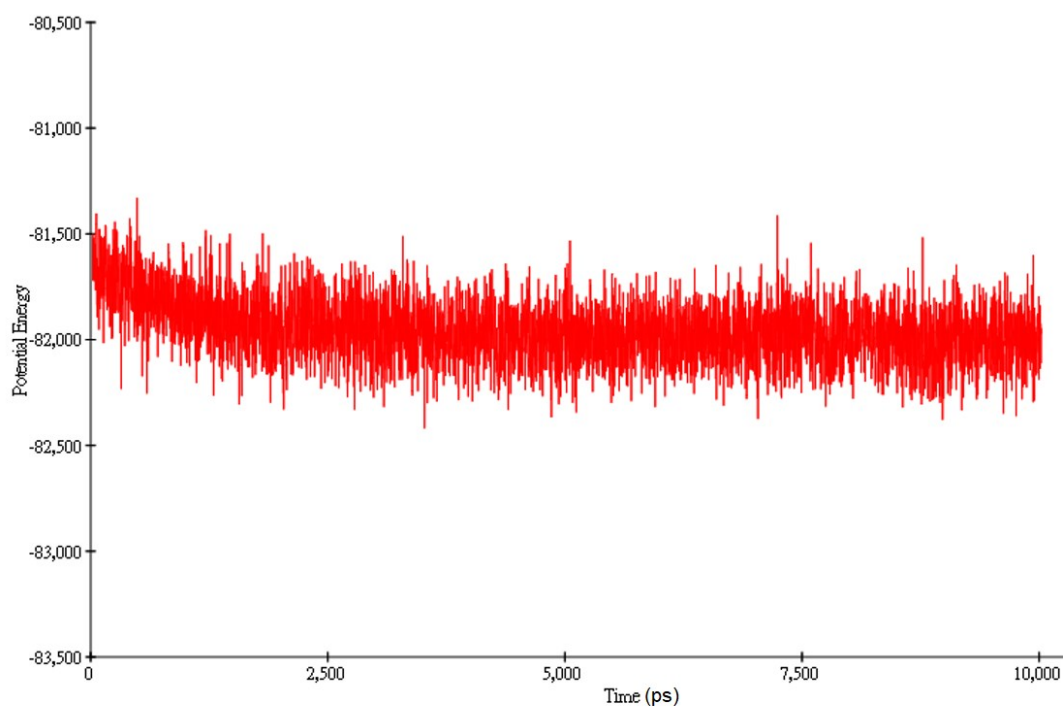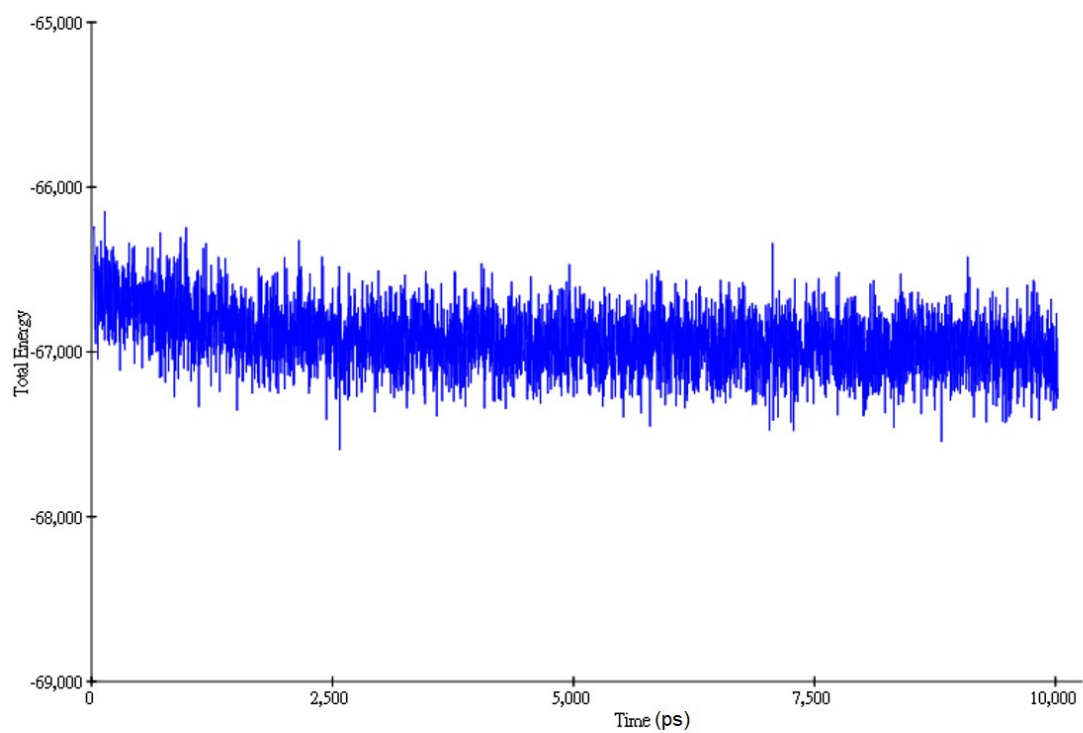
(A)

(B)

Figure S5. The molecular dynamics simulations of SYK-ST64 complex for 10 ns.
(**A**) The total energy as a function of time (**B**) The potential energy as a function of
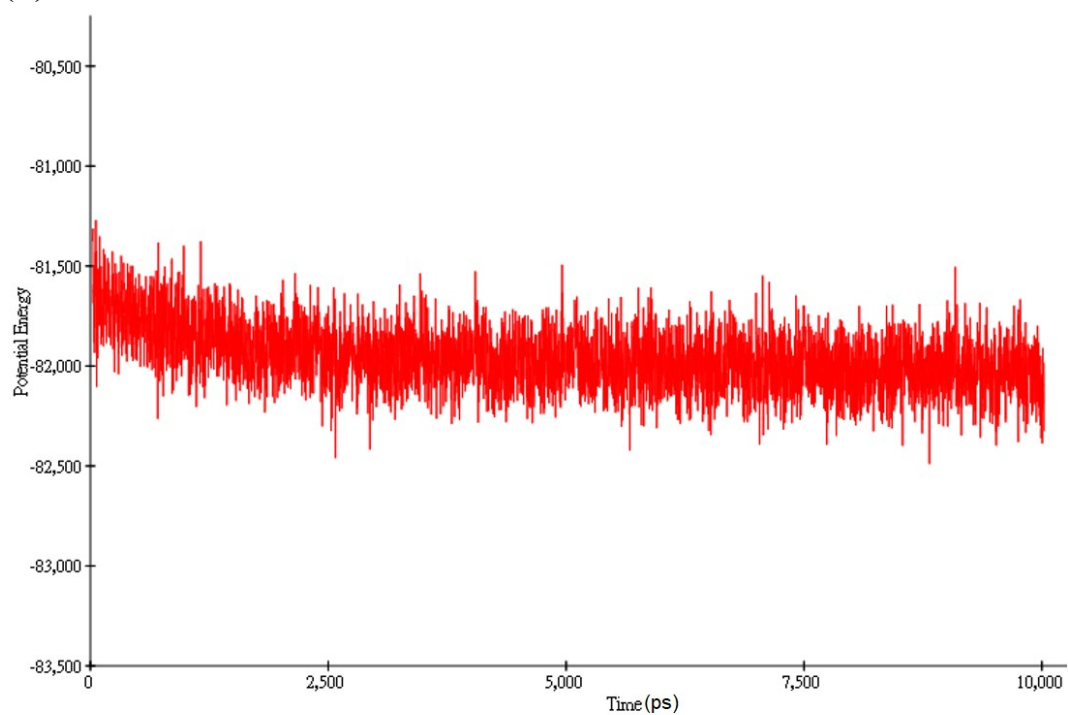time.

(A)

(B)

Figure S6. The molecular dynamics simulations of SYK-WST23 complex for 10 ns. (**A**) The total energy as a function of time (**B**) The potential energy as a function of time.