

## Supplemental Material:

### FIGURES:

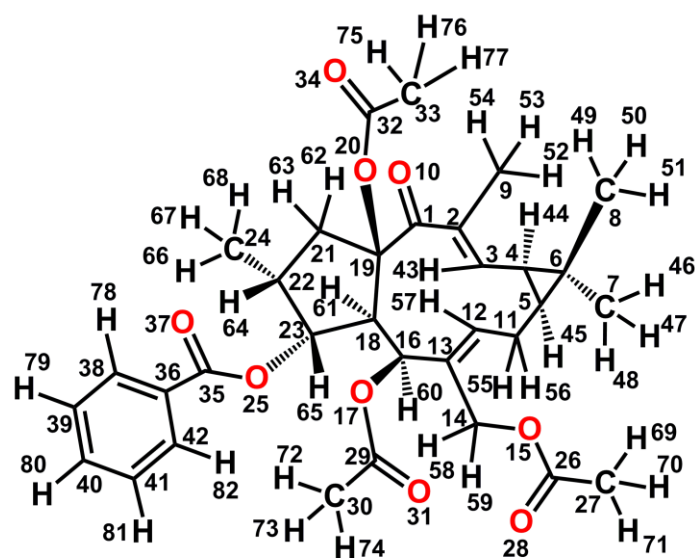


FIGURE S1: The structure of L713283 with atomic number.

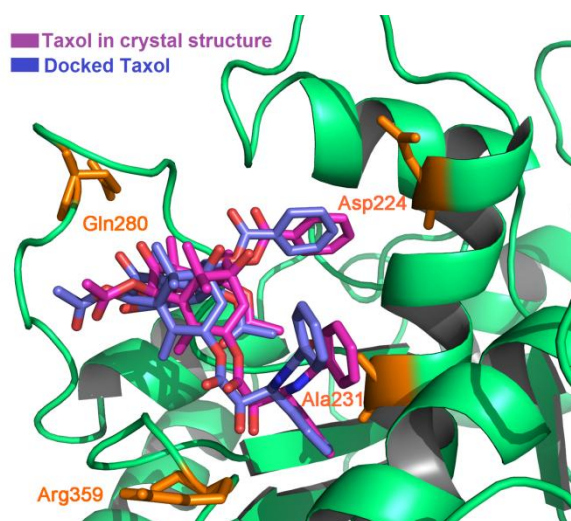


FIGURE S2: Superimposition between 1JFF crystal structure and the re-docked model of Taxol molecule with  $\beta$ -tubulin.

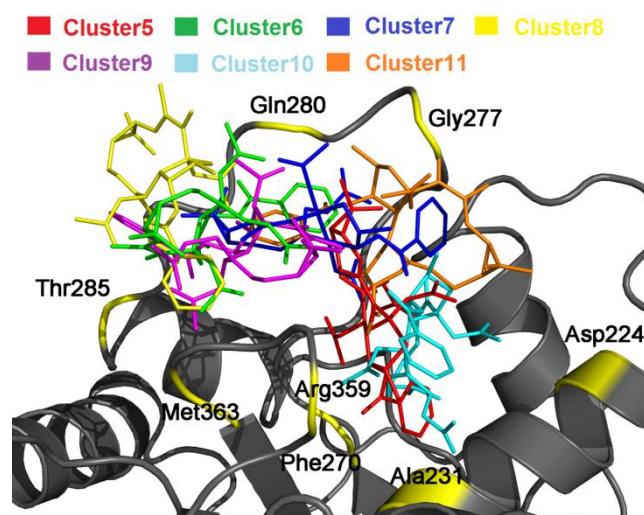


FIGURE S3: The binding modes of  $\beta$ -tubulin with the representative conformation of L713283 in the 5th~11th cluster, which are shown in red, green, blue, yellow, violet, cyan, orange, respectively.

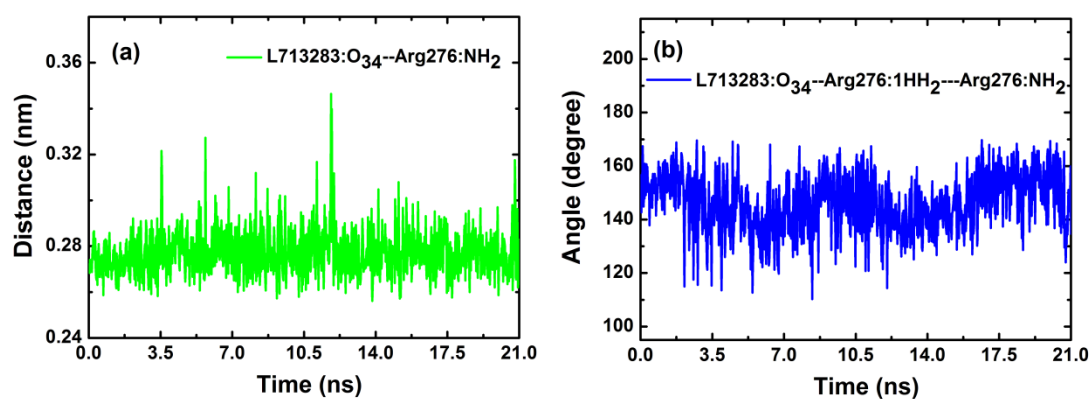


FIGURE S4: The geometry parameter for the hydrogen bond between L713283 and  $\beta$ -tubulin. (A) Distance of donor atom with acceptor atom. (B) Angle of donor atom, hydrogen atom and acceptor atom.