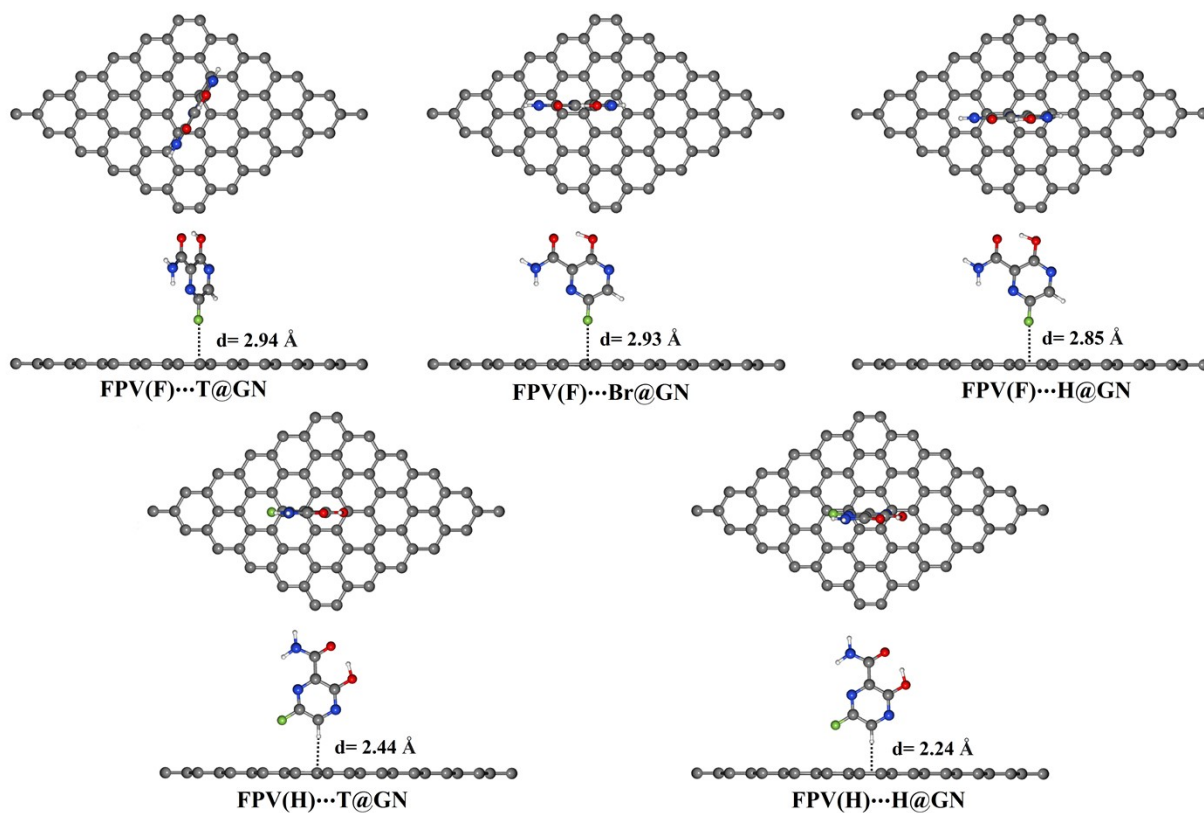


**Figure S1.** Convergence tests plots of the total energy with the (a) cutoff energy, (b) lattice parameter, and (c)  $k$ -point of the unit cell of GN with two C-atoms.



**Figure S2.** Relaxed structures of all FPV...GN complexes in perpendicular and parallel configurations with top and side views. The distance (d) between FPV drug and GN sheet are provided in Å.

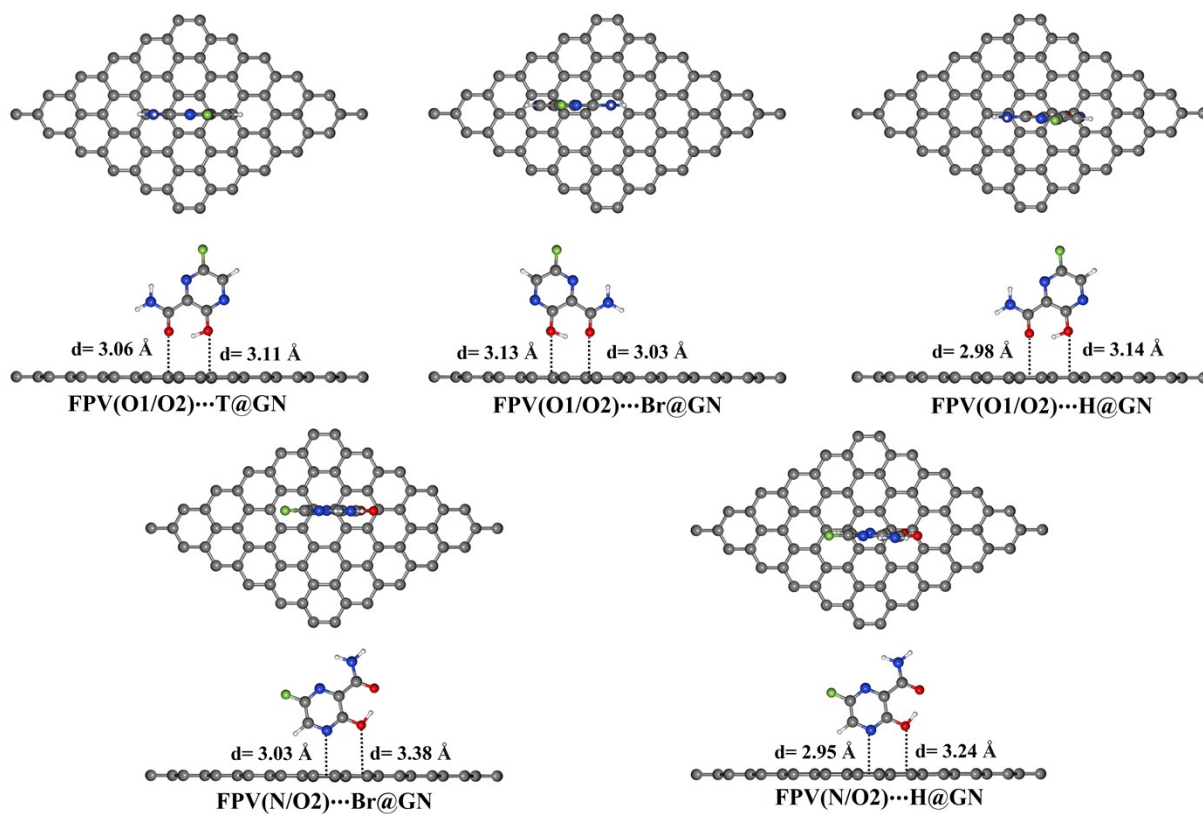


Figure S2. Continue.

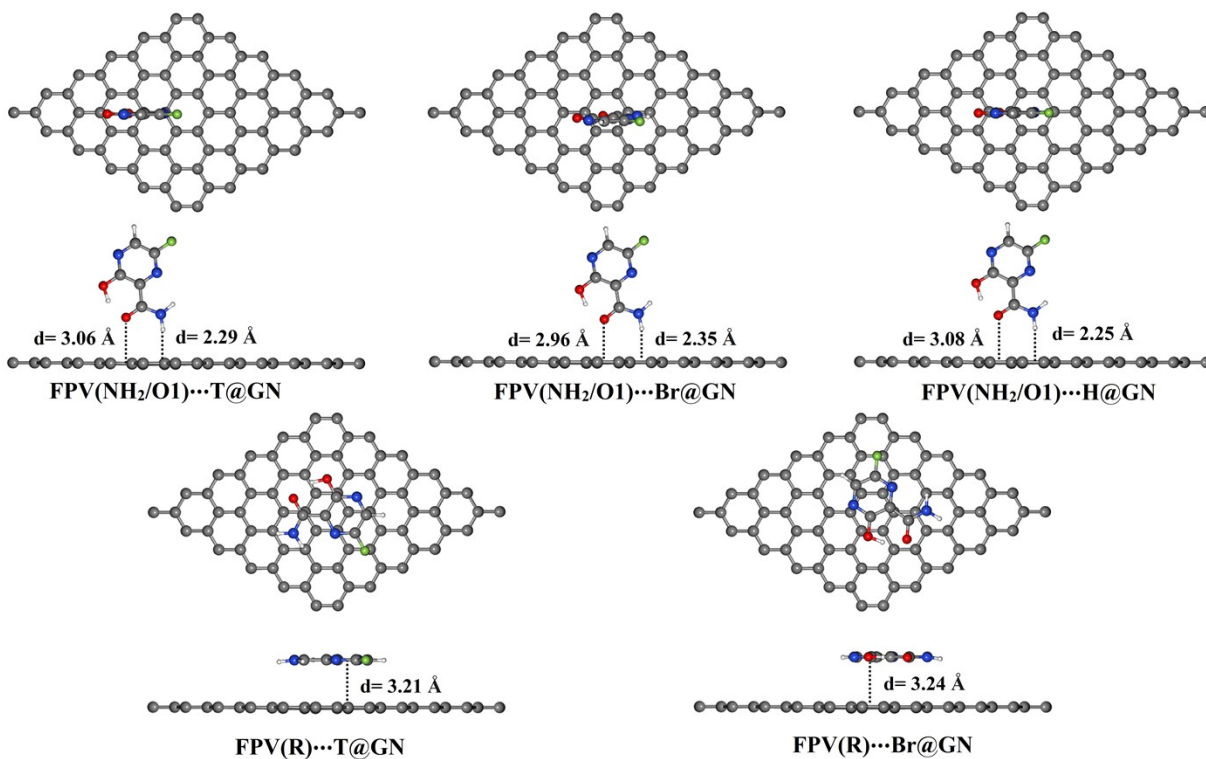


Figure S2. Continue.