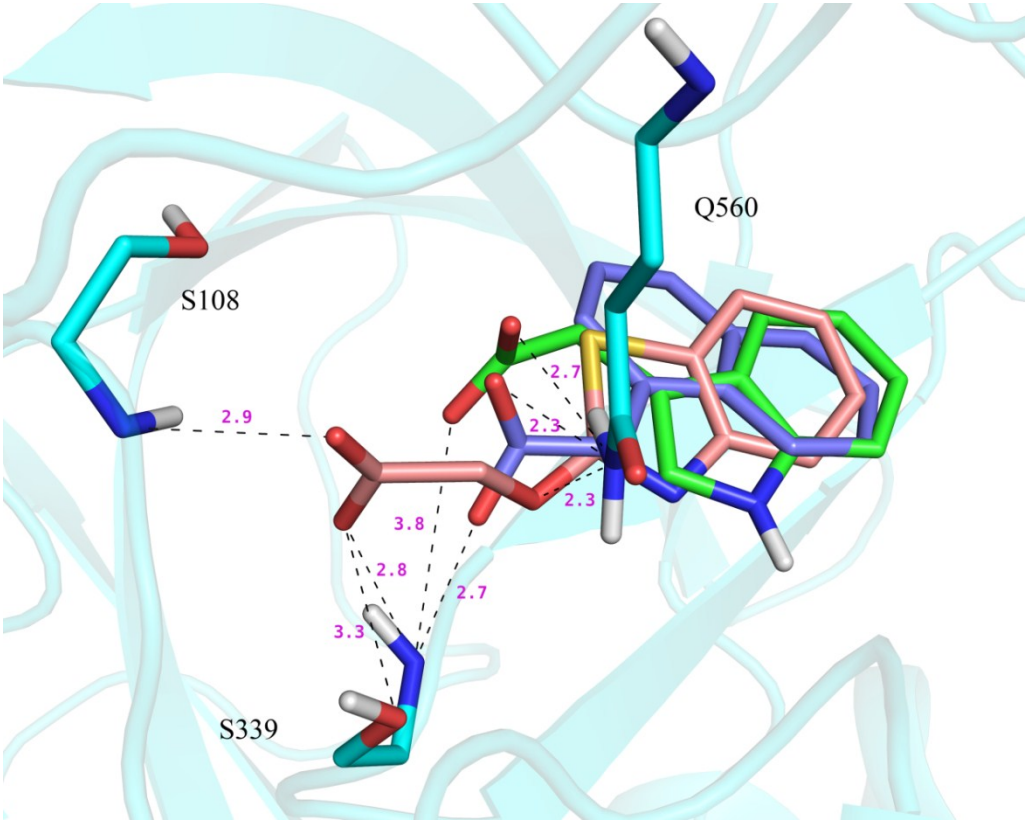

Fig.S1. Binding modes of the three substrates to the open form of VvGH3.1 predicted by molecular docking. The carbon atoms of substrates are colored in green (IAA), slate (NAA), salmon (BTOA).

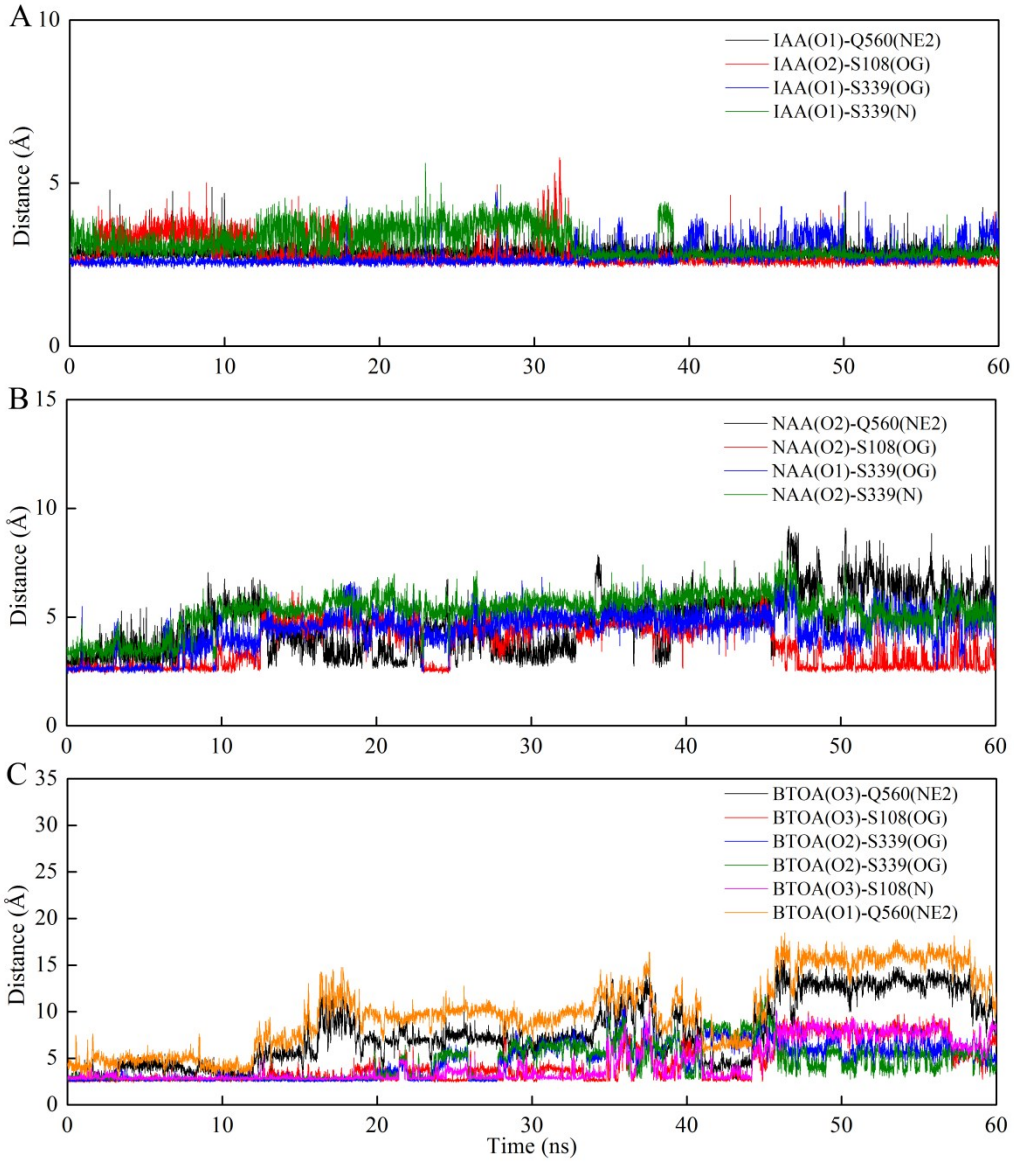

Fig. S2. Monitoring for the intermolecular hydrogen bonds between GH3.1 and substrates during the MD simulation, (A) GH3.1-ATP-IAA system; (B) GH3.1-ATP-NAA system; (C) GH3.1-ATP-BTOA system.