

Supporting information

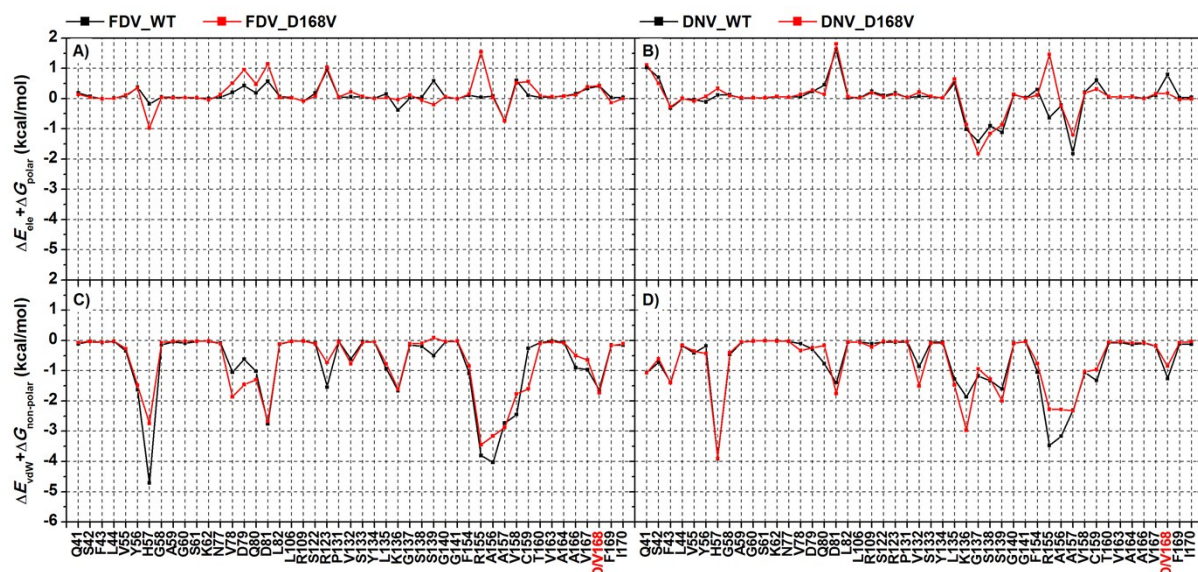


Fig. S1 Energetic components contributed from electrostatic ($\Delta E_{ele} + \Delta G_{polar}$) and van der Waals ($\Delta E_{vdW} + \Delta G_{non-polar}$) terms of NS3 protease domain for wild-type and D168V complexes as shown in black and red lines,