Electronic Supplementary Material (ESI) for Molecular BioSystems. This journal is © The Royal Society of Chemistry 2016

Supporting information

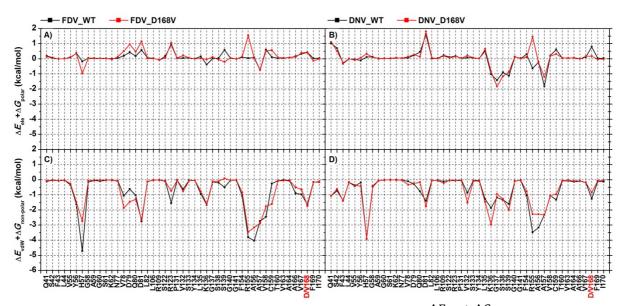


Fig. S1 Energetic components contributed from electrostatic ($^{\Delta E_{ele} + \Delta G_{polar}}$) and van der Waals ($^{\Delta E_{vdW} + \Delta G_{non-polar}}$) terms of NS3 protease domain for wild-type and D168V complexes as shown in black and red lines,