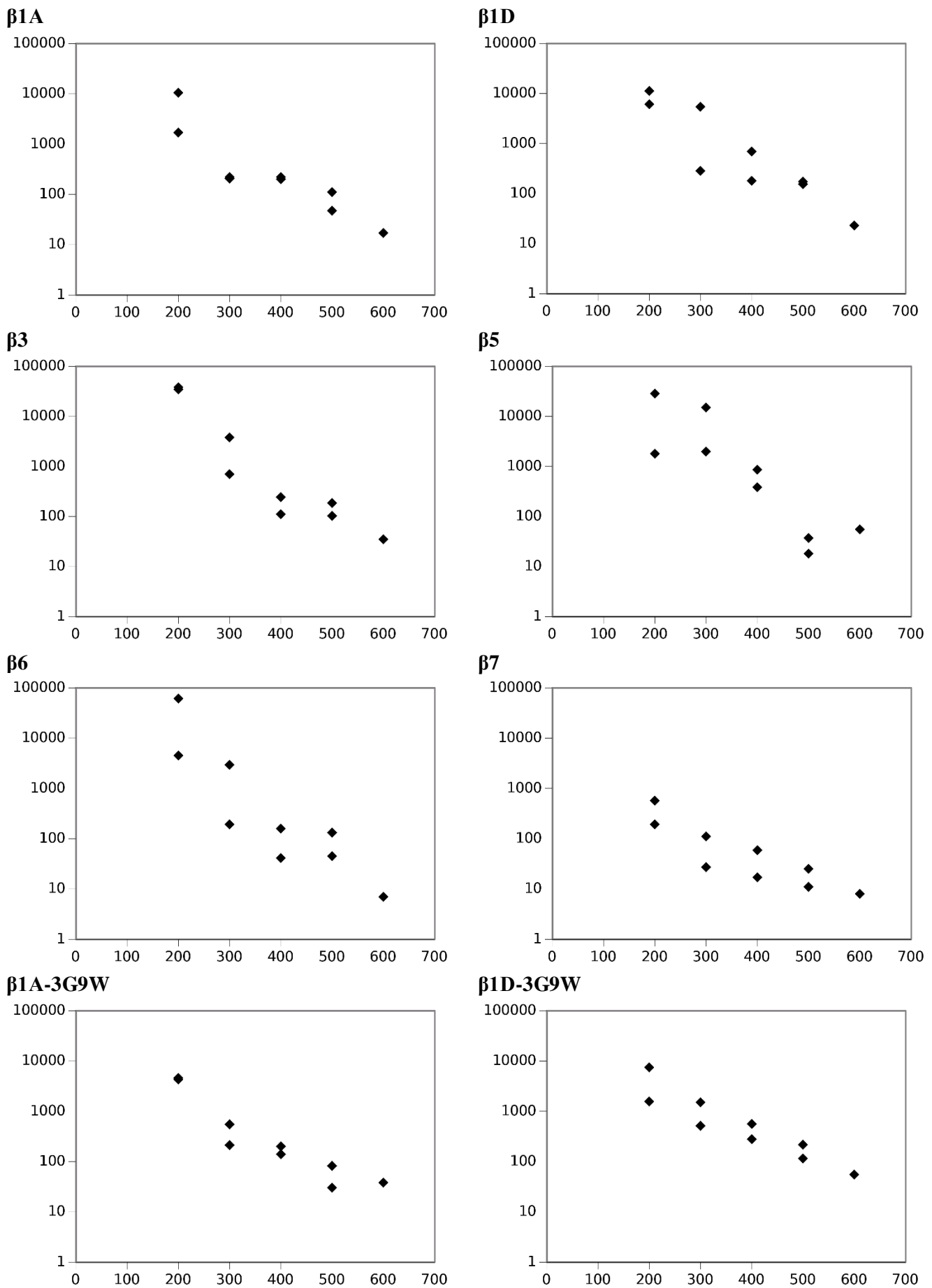Supplementary Material

The talin-integrin interface under mechanical stress

Sampo Kukkurainen, Juha A. Määttä, John Saeger, Jarkko Valjakka, Viola Vogel, Vesa P. Hytönen

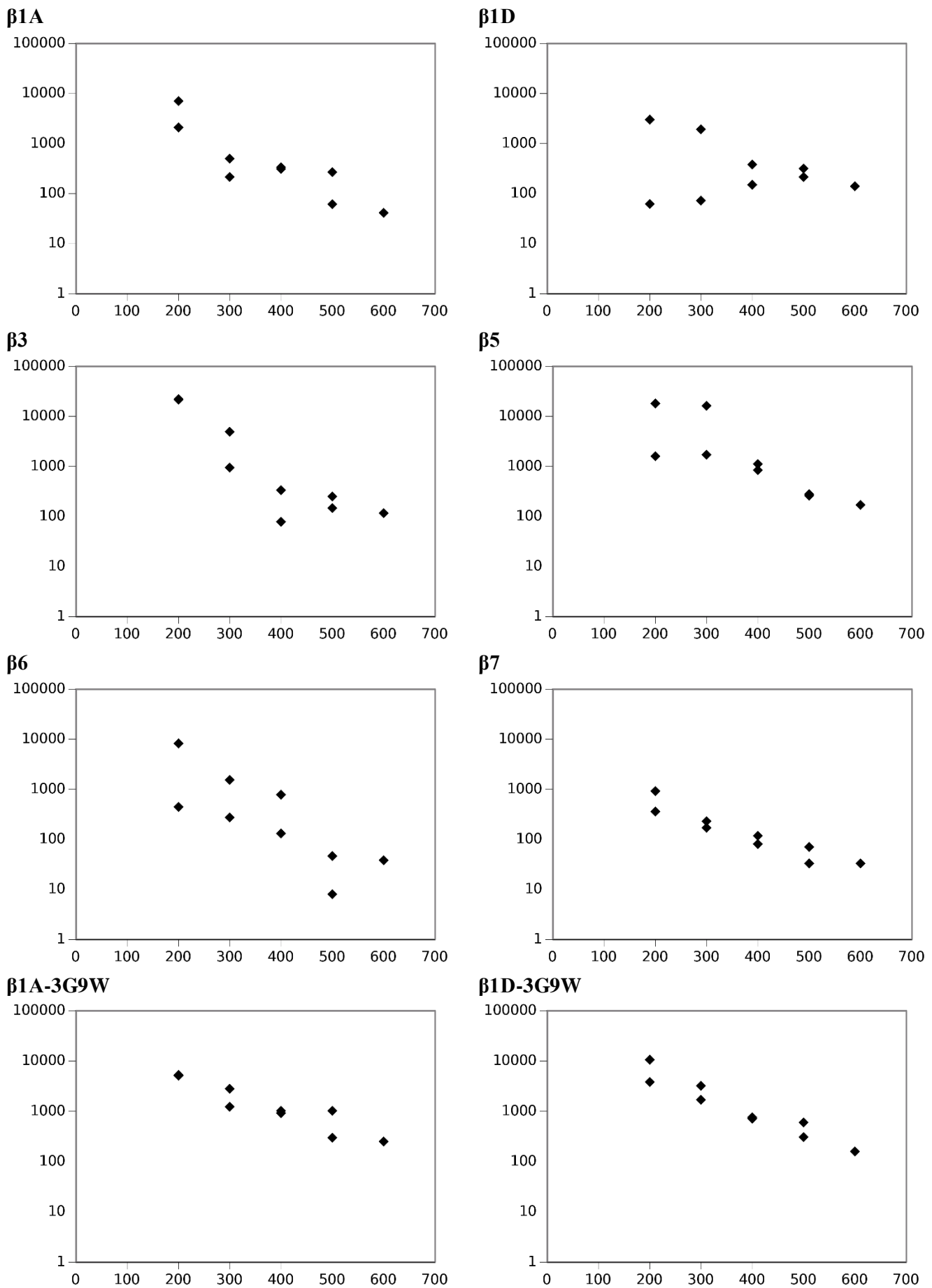**β1A**

β1D

β3

β5

β6

β7

β1A-3G9W

β1D-3G9W

Figure S1 W739(β3)-R358(tal) side chain center of mass distance. Bound state lifetime in picoseconds in the different simulations. Distance cutoff for the bound state: 5 Å. X-axis: force (pN). Y-axis: time (ps).
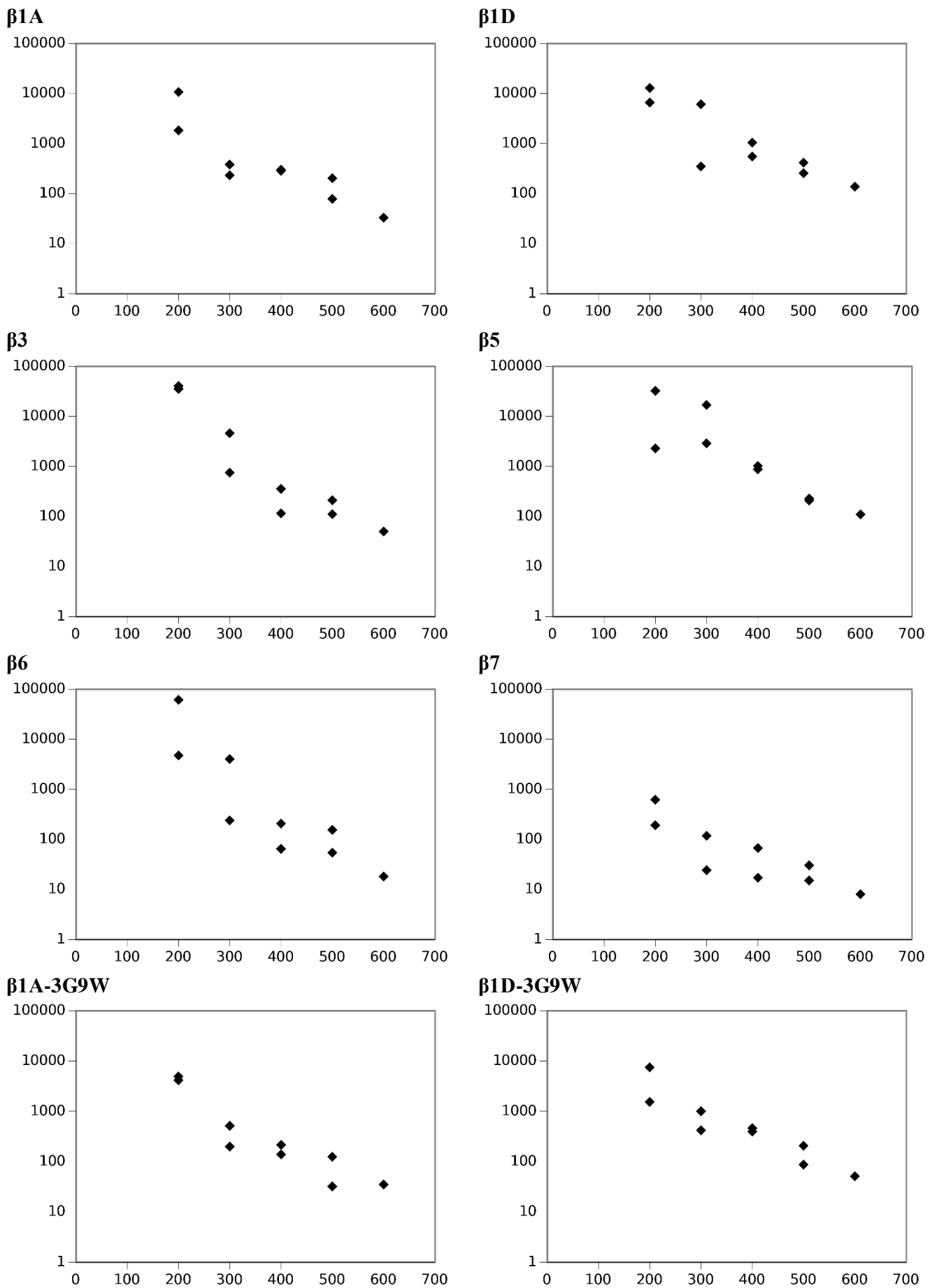
Figure S2 D740(β3)-W359(tal) Cα-Cα distance. Bound state lifetime in picoseconds in the different simulations. Distance cutoff for the bound state: 7 Å. X-axis: force (pN). Y-axis: time (ps).
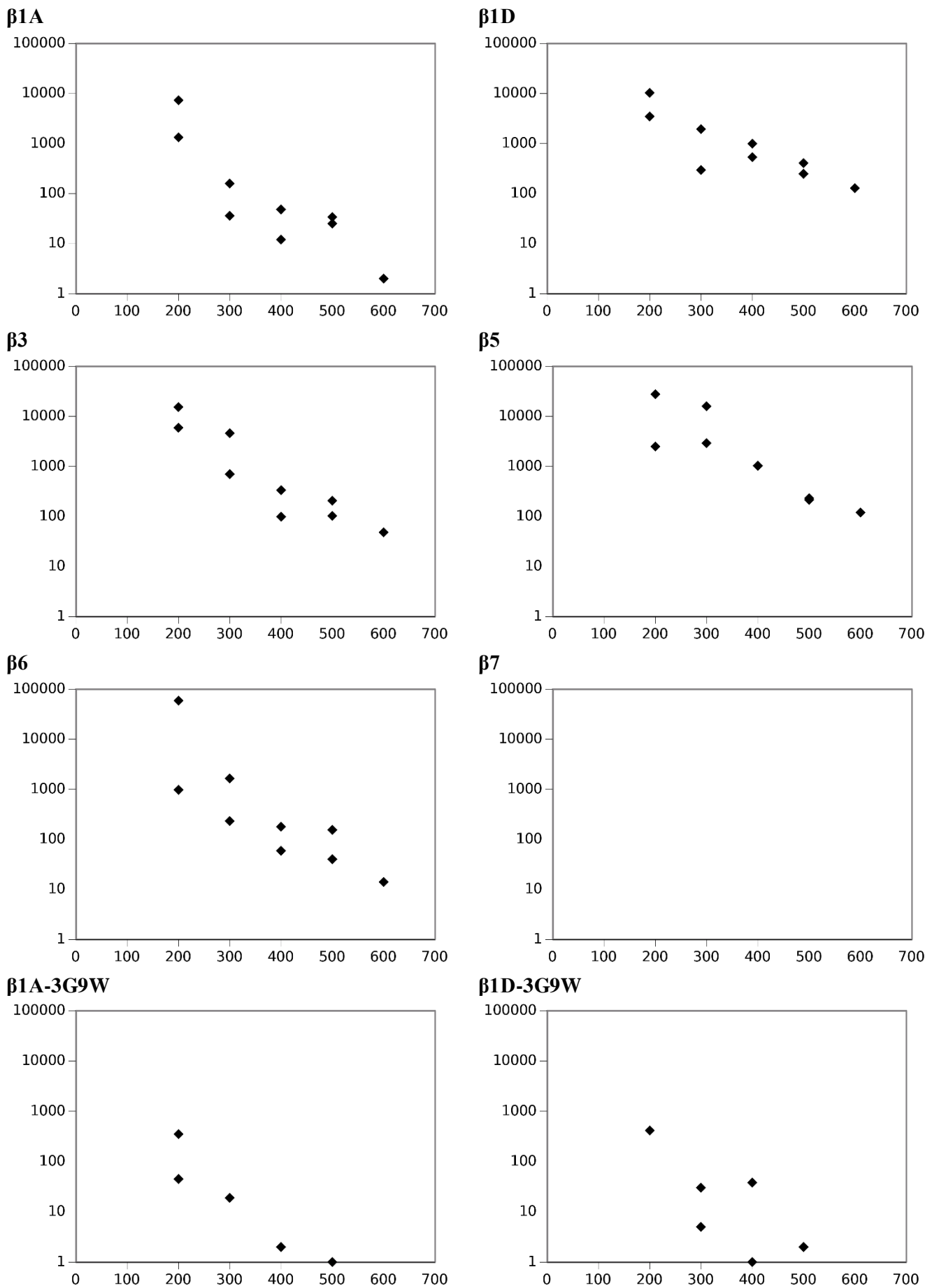
Figure S3 A742(β3)-K357(tal) Cα-Cα distance. Bound state lifetime in picoseconds in the different simulations. Distance cutoff for the bound state: 7 Å. X-axis: force (pN). Y-axis: time (ps).
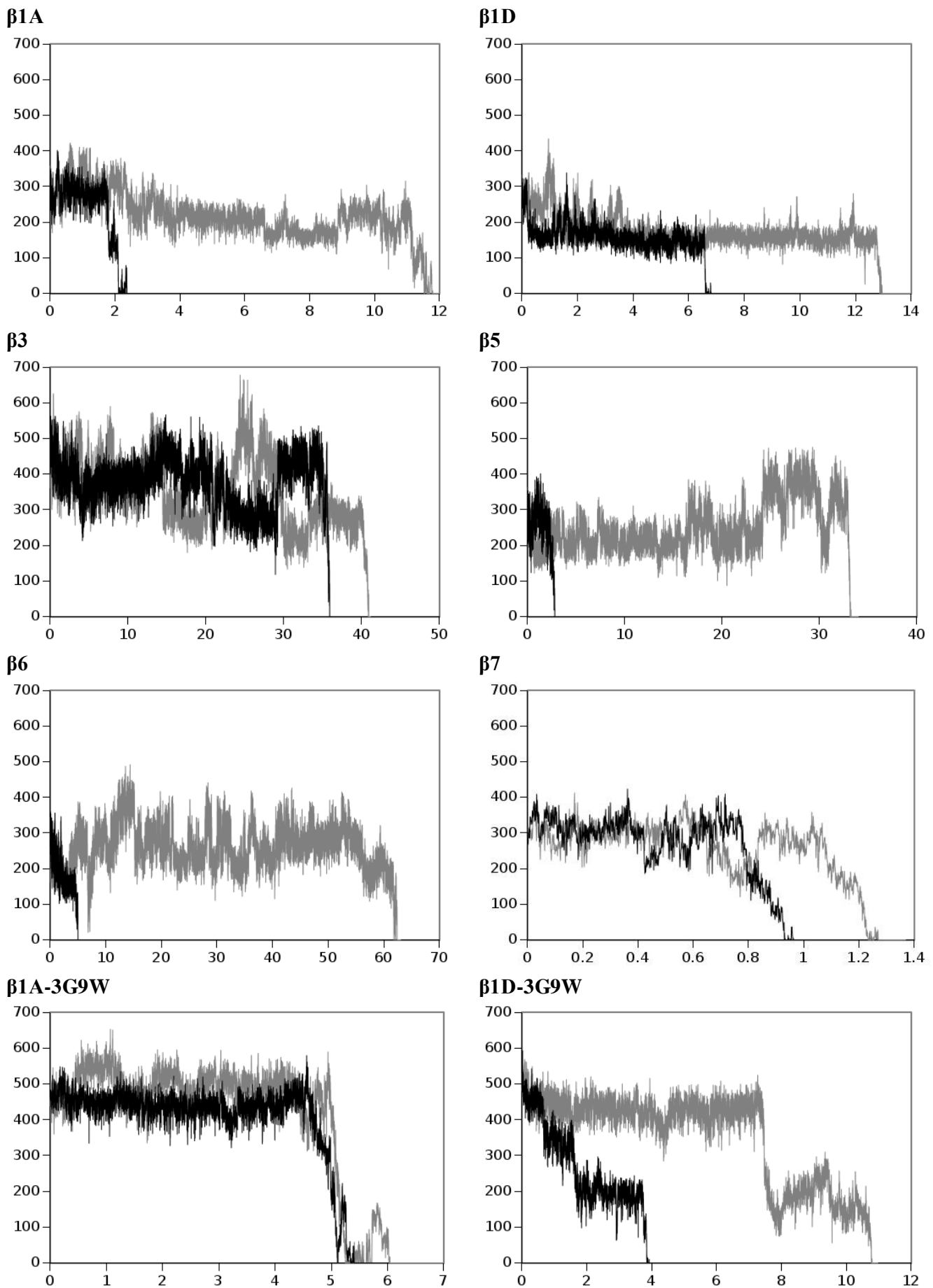
Figure S4 Y747(β3) side chain center of mass distance from N355(tal) backbone O. Bound state lifetime in picoseconds in the different simulations. Distance cutoff for the bound state: 7 Å. X-axis: force (pN). Y-axis: time (ps).

Figure S5 Buried area of hydrophobic residues in the talin-integrin interface. The buried area was calculated for every picosecond in two 200 pN simulations, using the 'sasa' function in VMD. The hydrophobic residues were defined as Ala, Ile, Leu, Met, Phe, Pro, Trp, and Val. Areas from two simulations are shown in black and gray. X-axis: time (ns). Y-axis: buried area of hydrophobic residues (Å^2).
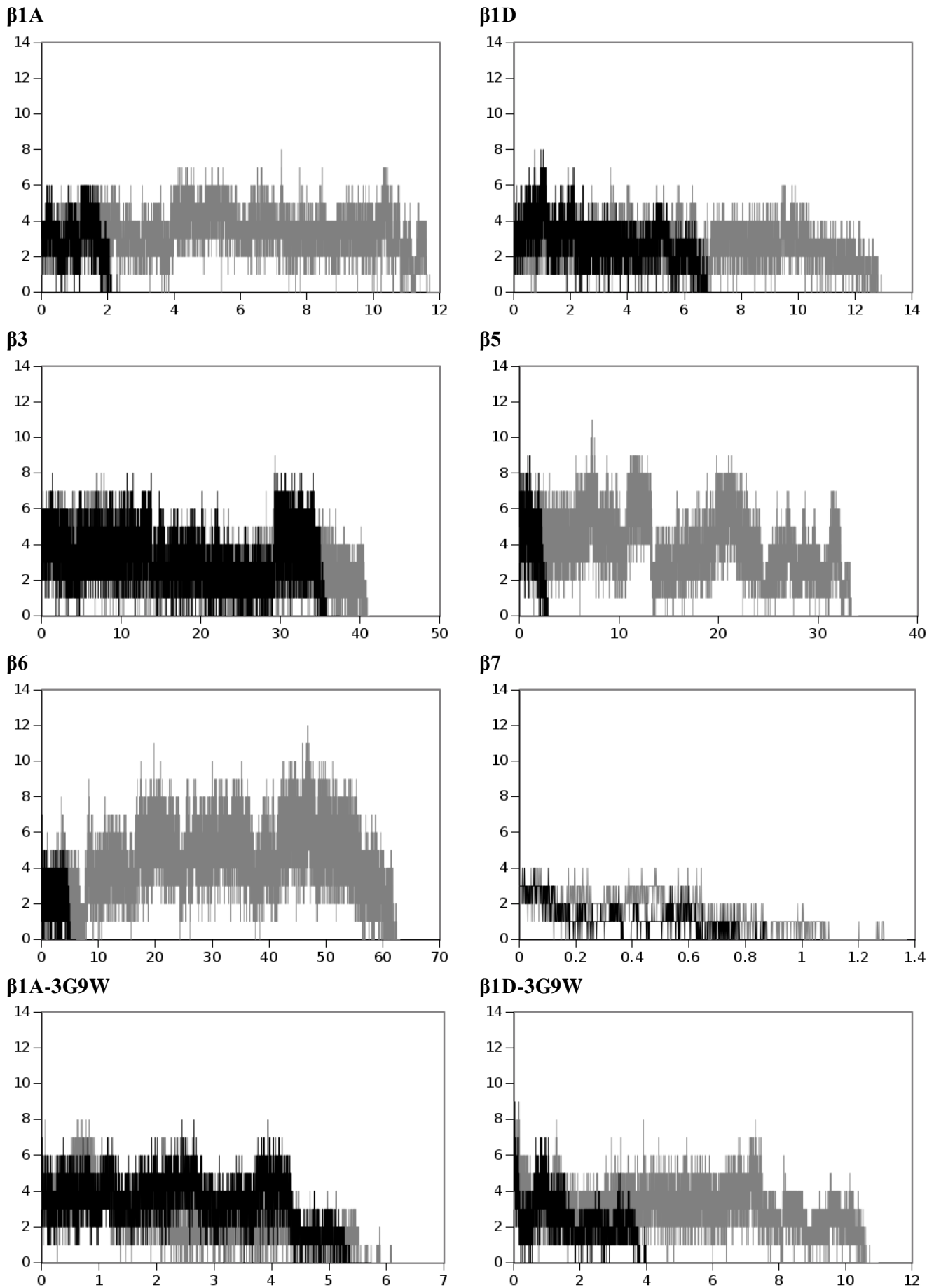
Figure S6 Number of hydrogen bonds in the talin-integrin interface. The hydrogen bonds were calculated for every picosecond in two 200 pN simulations for each complex using the Hydrogen Bonds tool in VMD, with cutoff distance 3.51 Å and cutoff angle 30.1°. The numbers of hydrogen bonds from two simulations are shown in black and gray. X-axis: time (ns). Y-axis: number of hydrogen bonds.