**Figure S1.** A) $^1$H-$^1$N HMQC spectra of apo-hPD-L1 (18-134) (blue) and hPD-L1 (18-134) with AUNP-12 (red) in the molar ratio 1/5. B) $^1$H NMR spectra of apo-hPD-L1 (18-134) (blue), hPD-L1 (18-134) with AUNP-12 (red) in the molar ratio 1/5, apo-hPD-L1 (18-239) (purple), and hPD-L1 (18-239) with AUNP-12 (green) in the molar ratio 1/5.
Figure S2. A) $^1$H-$^1$N HMQC spectra of apo-hPD-1 (blue) and hPD-1 with AUNP-12 (red) in the molar ration 1/5. B) $^1$H NMR spectra of apo- hPD-1 (blue), hPD-1 with AUNP-12 (red) in the molar ration 1/5.

Figure S3. $^1$H NMR spectra of apo-hPD-L1 (18-134) (blue) and with BMS-1166 compound (green) and peptide-57 (red) in the molar ration 1/1, respectively.