Supplementary Material
HPLC, Mass spectra and two-dimensional NMR spectra for peptidomimetics.

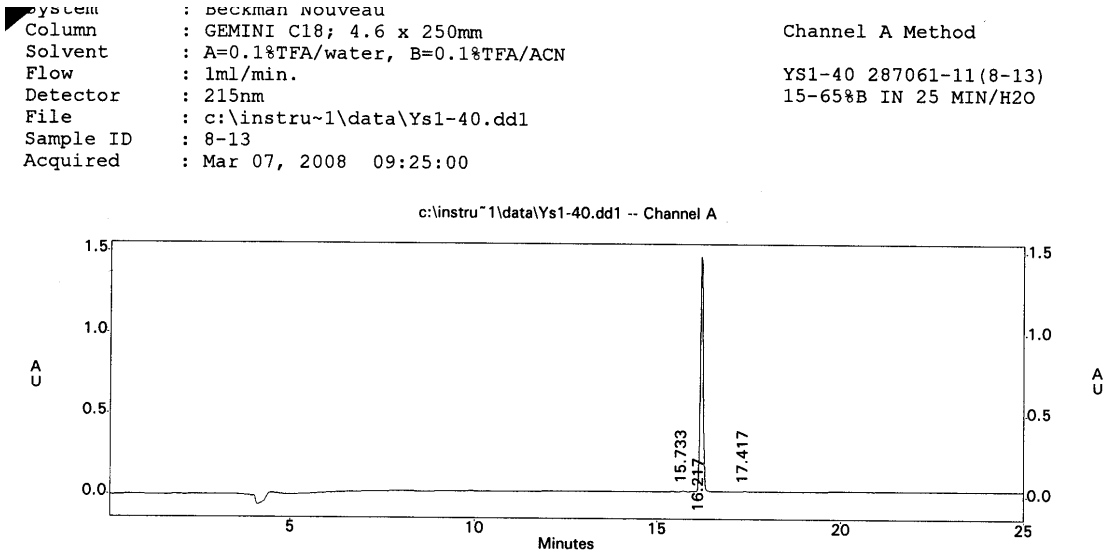

Figure 1. HPLC chromatogram for compound HERP5.

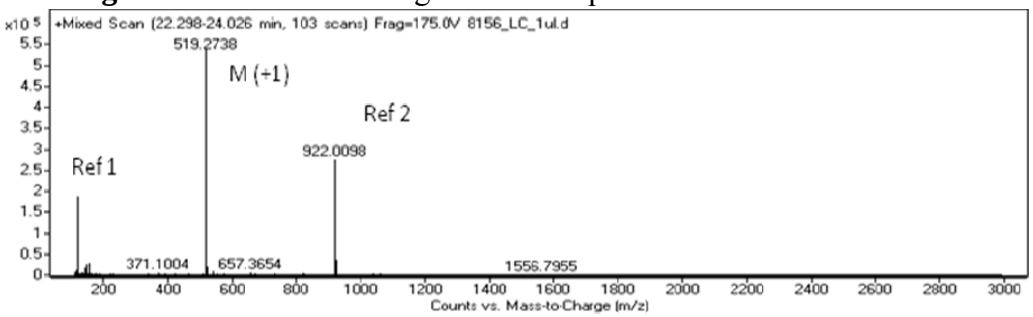

Figure 2. High resolution mass spectrum for compound HERP5

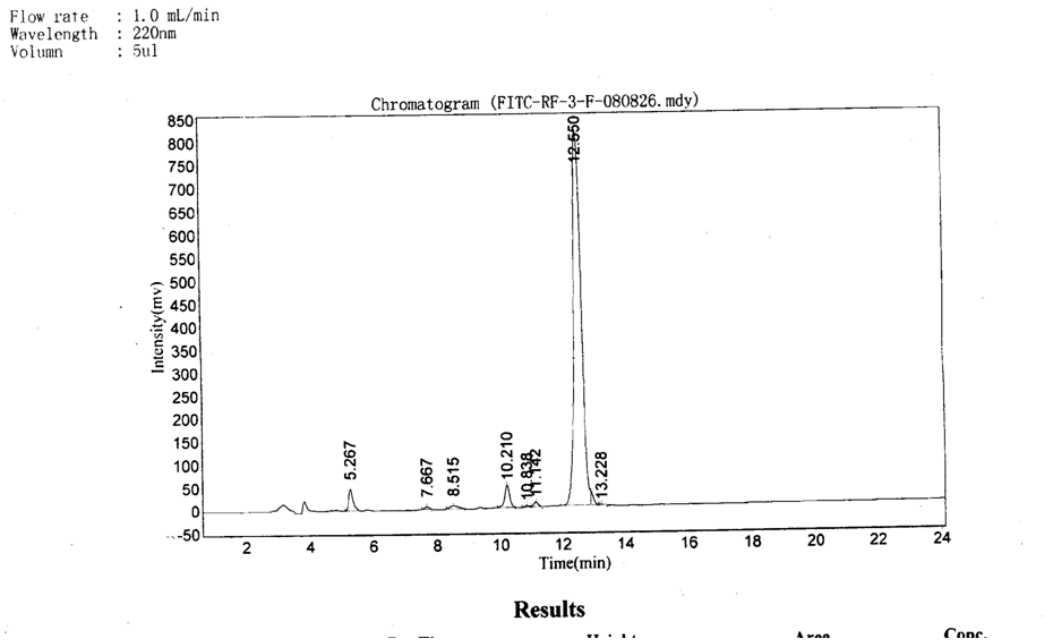

Figure 3. HPLC chromatogram fluorescently labeled compound FITC-HERP5

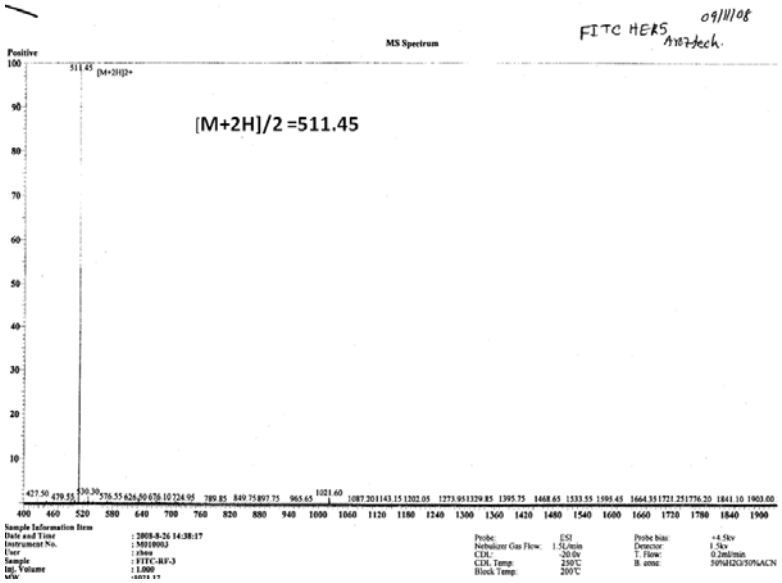

Figure 4. Mass spectrum for fluorescently labeled compound FITC-HERP5.

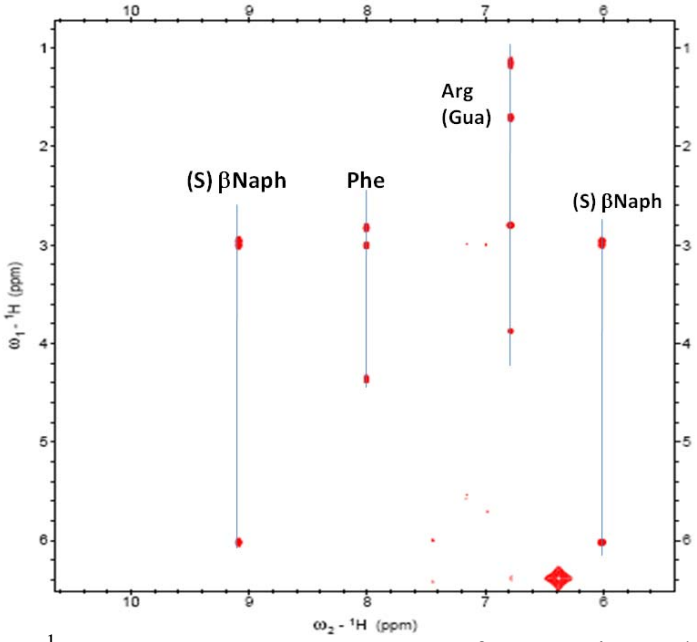

Figure 5. ^{1}H 2D-TOCSY NMR spectrum of HERP5 in H_20/D_2O at 298 K showing fingerprint region.

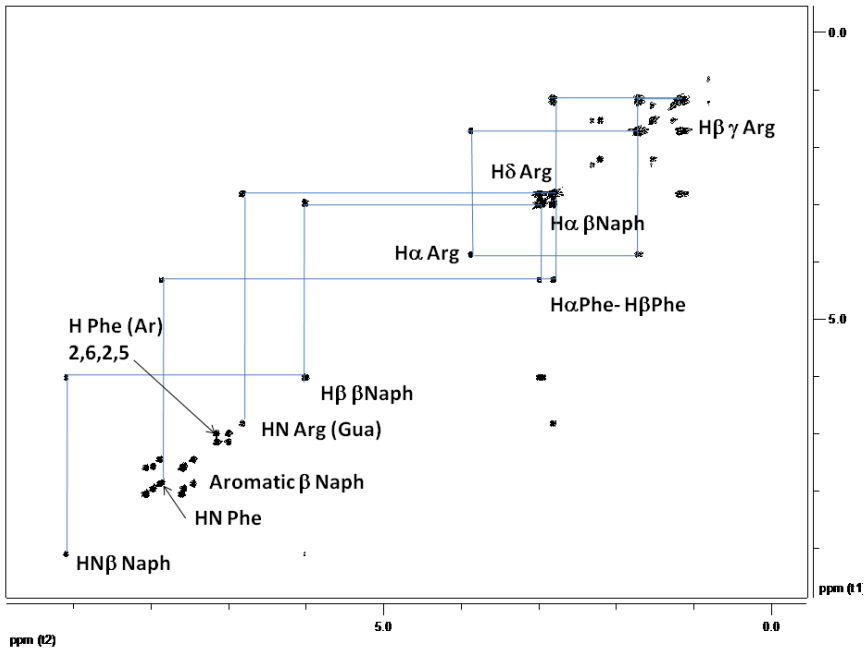

Figure 6. ^{1}H 2D-DQF-COSY NMR spectrum of HERP5 in H_20/D_2O at 298 K showing assignments. Ar –aromatic resonances, Gua-guanidine group.

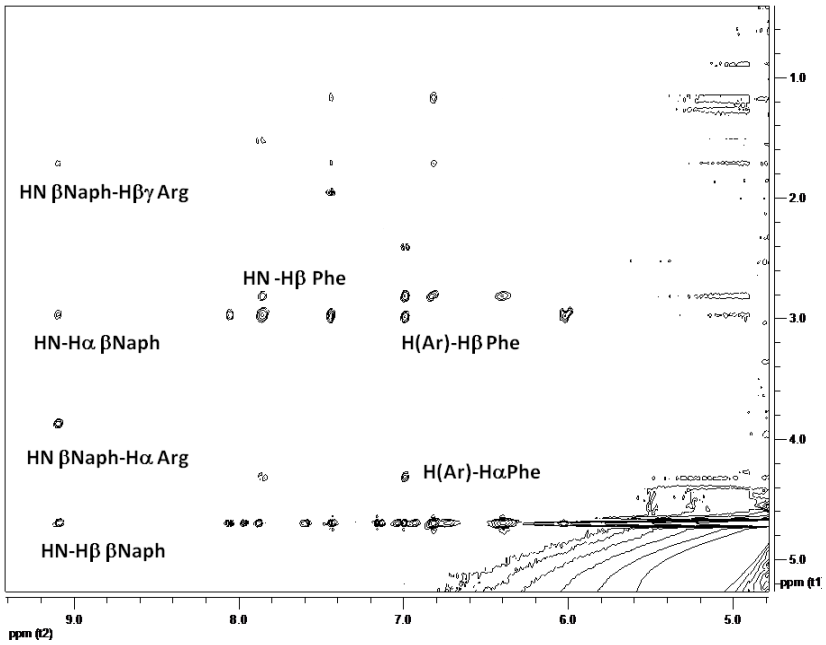

Figure 7. ^{1}H 2D-ROESY NMR spectrum of HERP5 in H_20/D_2O at 298 K showing amide to aliphatic connectivities with assignments.

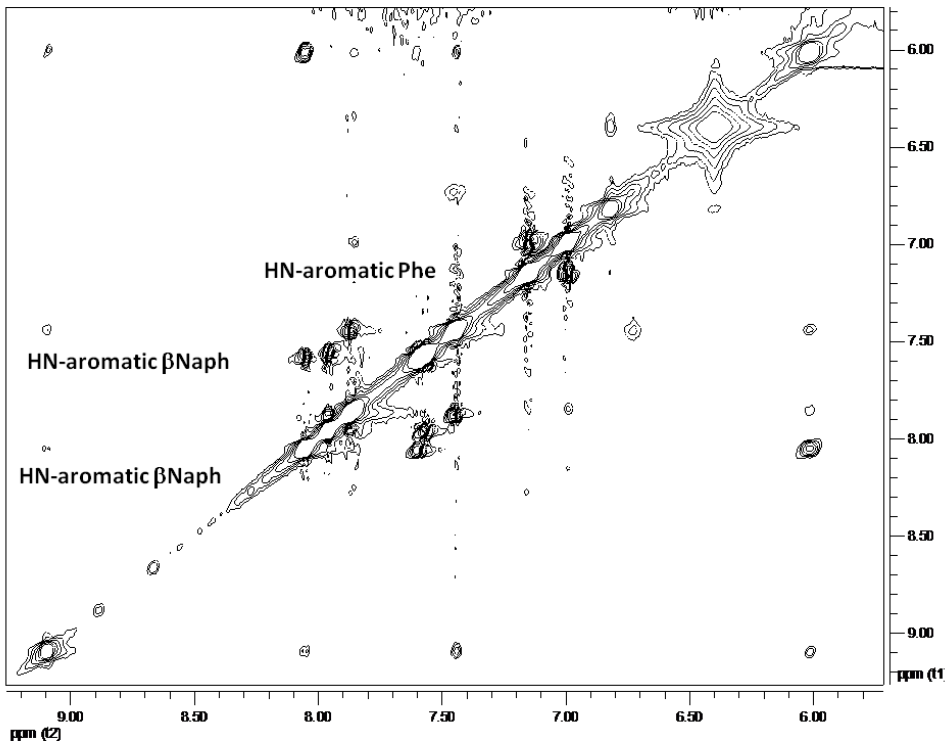

Figure 8. ^{1}H 2D-ROESY NMR spectrum of HERP5 in H_20/D_2O at 298 K showing amide and aromatic region.

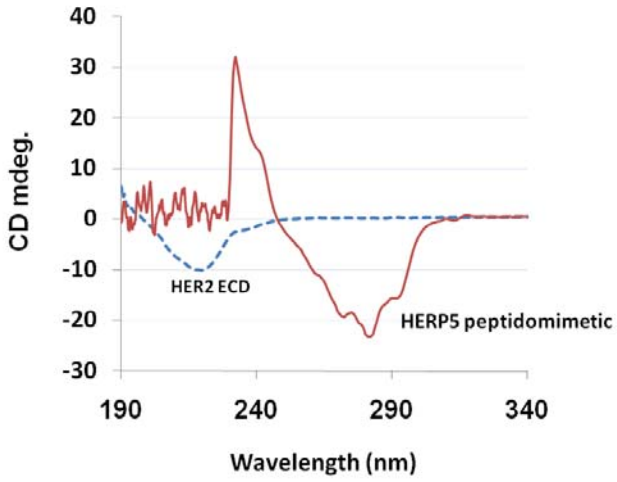

Figure 9. CD spectra of HER2 protein extracellular domain at 6.5 μM and HERP5 peptidomimetic at 1.3 mM in water. Notice that the CD spectra of HER2 protein and HERP5 peptidomimetic do not have overlapping CD bands.

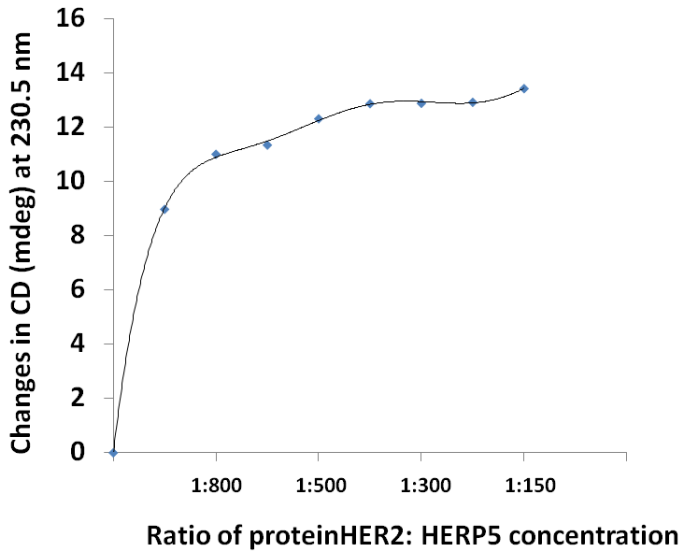

Figure 10. Changes in the CD signal of the peptidomimetic HERP5 at 230.5 nm upon addition of HER2 protein extracellular domain at different proteinHER2: HERP5 ratio. Changes in CD spectra are calculated by subtracting the different spectra from HERP5 spectra without the protein.

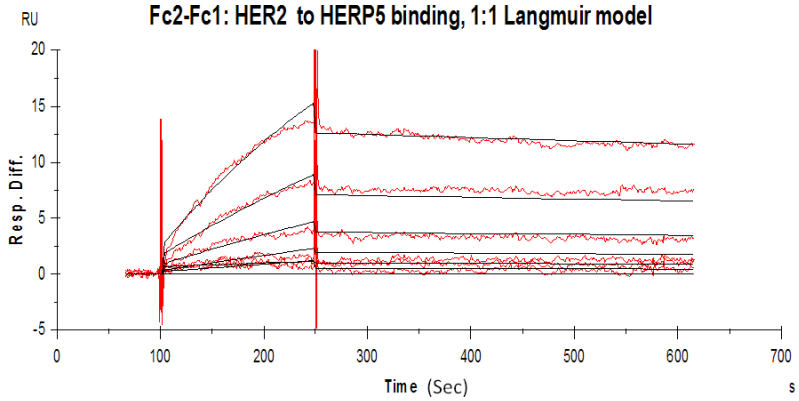

Figure 11. Preliminary results of Surface Plasmon Resonance (SPR) analysis of interaction between the HER2 extracellular domain and the HERP5 peptidomimetic. Difference in dose response compared to the control is shown in the figure. 1:1 Langmuir model was used to fit the data to obtain k_{on} and k_{off} values. K_d value calculated was around 1 µM. Peptidomimetic was immobolized on CM5 chip with 10 µg/mL in 10 mM sodium acetate pH 5.0 at a flow of 10 µL/min for 7 min. An analogue of HERP5 was used as negative control. Different concentration of extracellular domain of the HER2 protein (0, 5, 10, 20, 40, 80, 160 µM) was injected to flow on the chip at a flow rate of 30 µL/min.

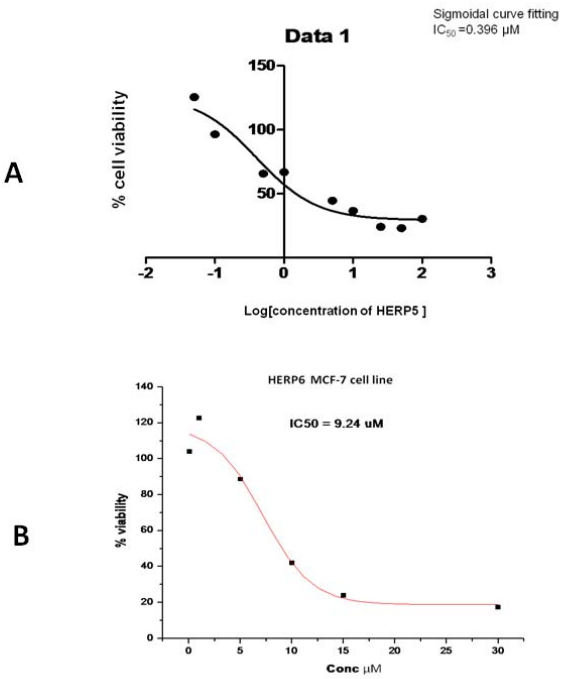

Figure 12. Example of different dose response curves plotted to calculate IC_{50} values for the compounds. A) plot of log of concentration of the compound vs % cell viability. B) concentration of compound vs cell viability

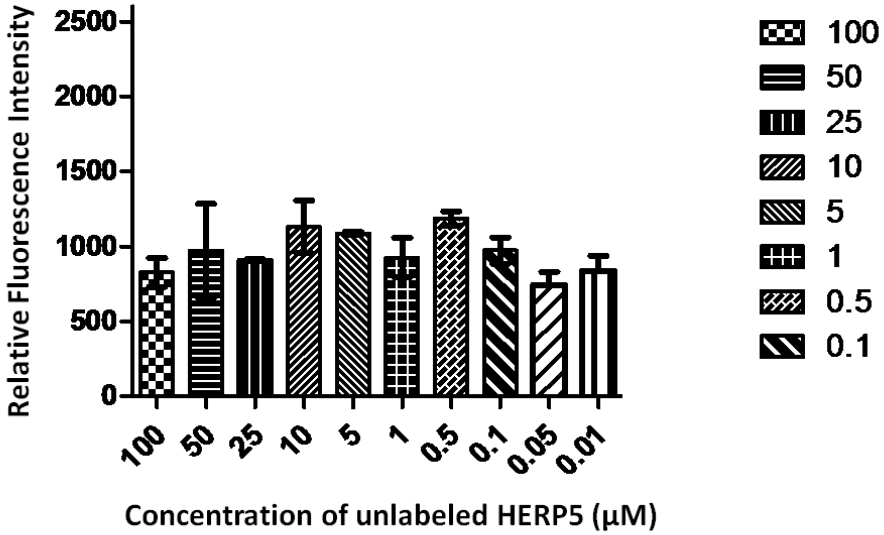

Figure 13. Competitive binding of unlabeled HERP5 to MCF-7 cells. Fluorescence of the FITC-labeled HERP5 is monitored to observe competitive binding. Concentration of unlabeled HERP5 was varied (100 μM to 0.01 μM). Graph indicates that binding of HERP5 to MCF-7 cells is non-specific.

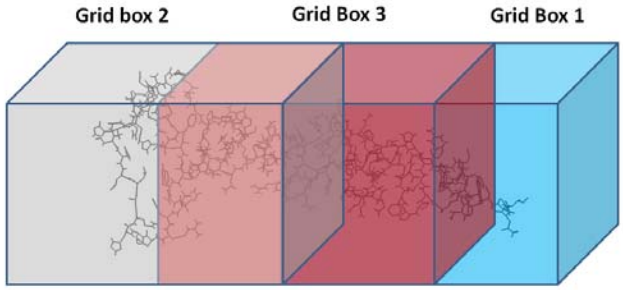

Figure 14. Schematic diagram of three-grid boxes used for docking of HERP5 to the entire domain IV of HER2 protein. Notice the overlapping in grid boxes. Grid box 2 contains interface of domain III and domain IV.