

Figure S1. Experimental SPR sensorgrams with corresponding Langmuir 1:1 ligand model simulations (A, C, E, G, I) and residual plots (B, D, F, H, J); (A, B) GPRPAAC, (C, D) GPRFPAC, (E, F) GPRPPERC, (G, H) GPRVVERC, (I, J) GPRVVAAC. Solid lines = experimental SPR response curves, dashed lines = fitted model curves.

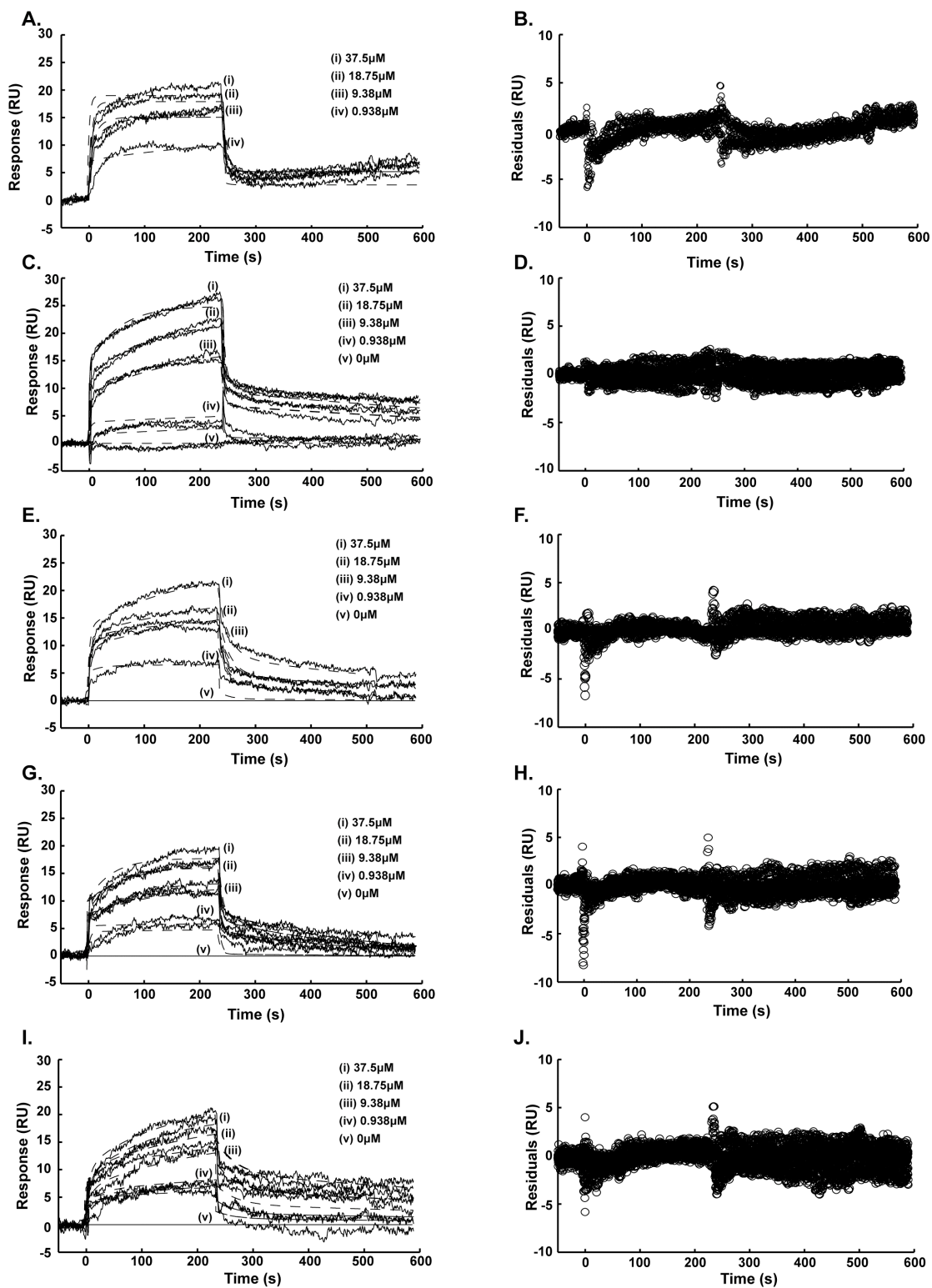
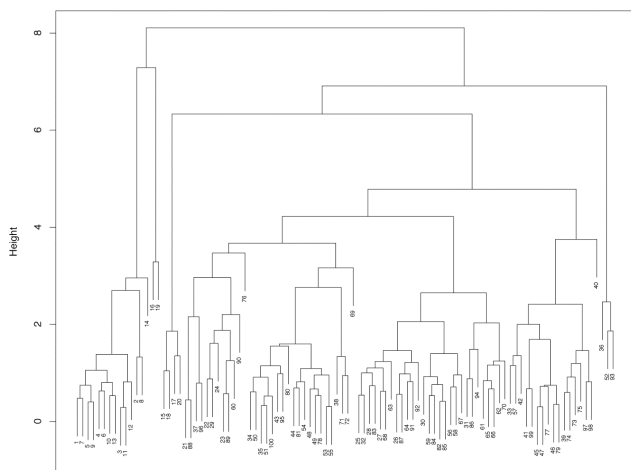
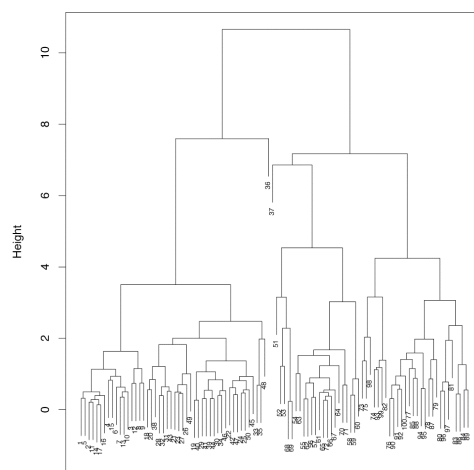


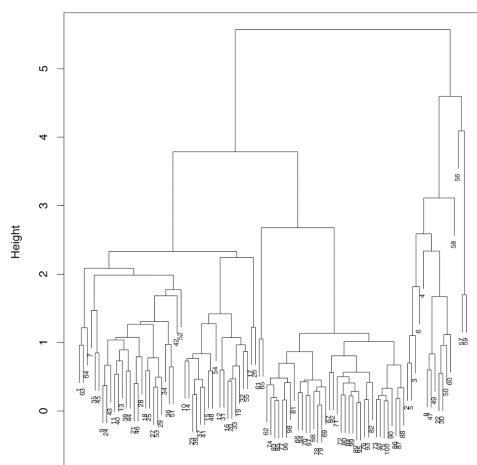
Figure S2. Experimental SPR sensorgrams with corresponding heterogeneous ligand model simulations (A, C, E, G, I) and residual plots (B, D, F, H, J); (A, B) GPRPAAC, (C, D) GPRPFAC, (E, F) GPRPPERC, (G, H) GPRVVERC, (I, J) GPRVVAAC. Solid lines = experimental SPR response curves, dashed lines = fitted model curves.



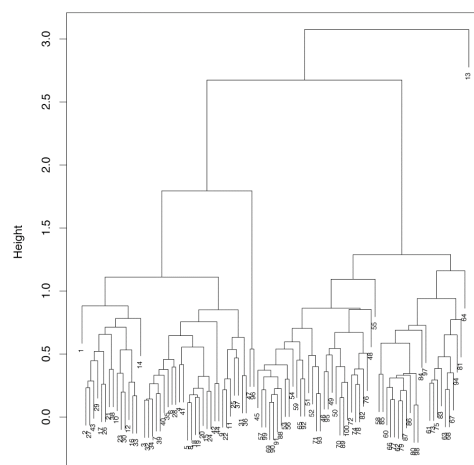
A. GPRFPAC



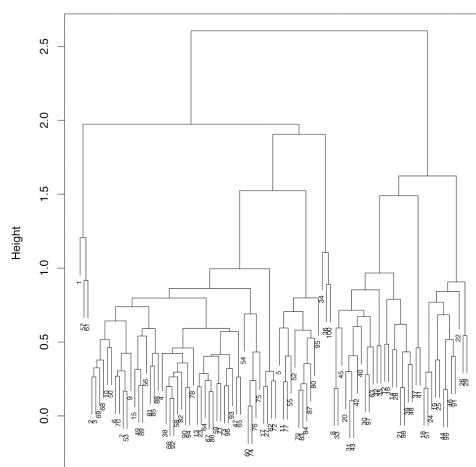
B. GPRVAAC



C. GPRPAAC



D. GPRPPERC



E. GPRVVERC

Figure S3. Dendrograms from hierarchical cluster analysis from a dissimilarity matrix generated from the RMSD between every frame in the trajectory, (A) GPRFPAC, (B) GPRVAAC, (C) GPRPAAC, (D) GPRPPERC, (E) GPRVVERC.

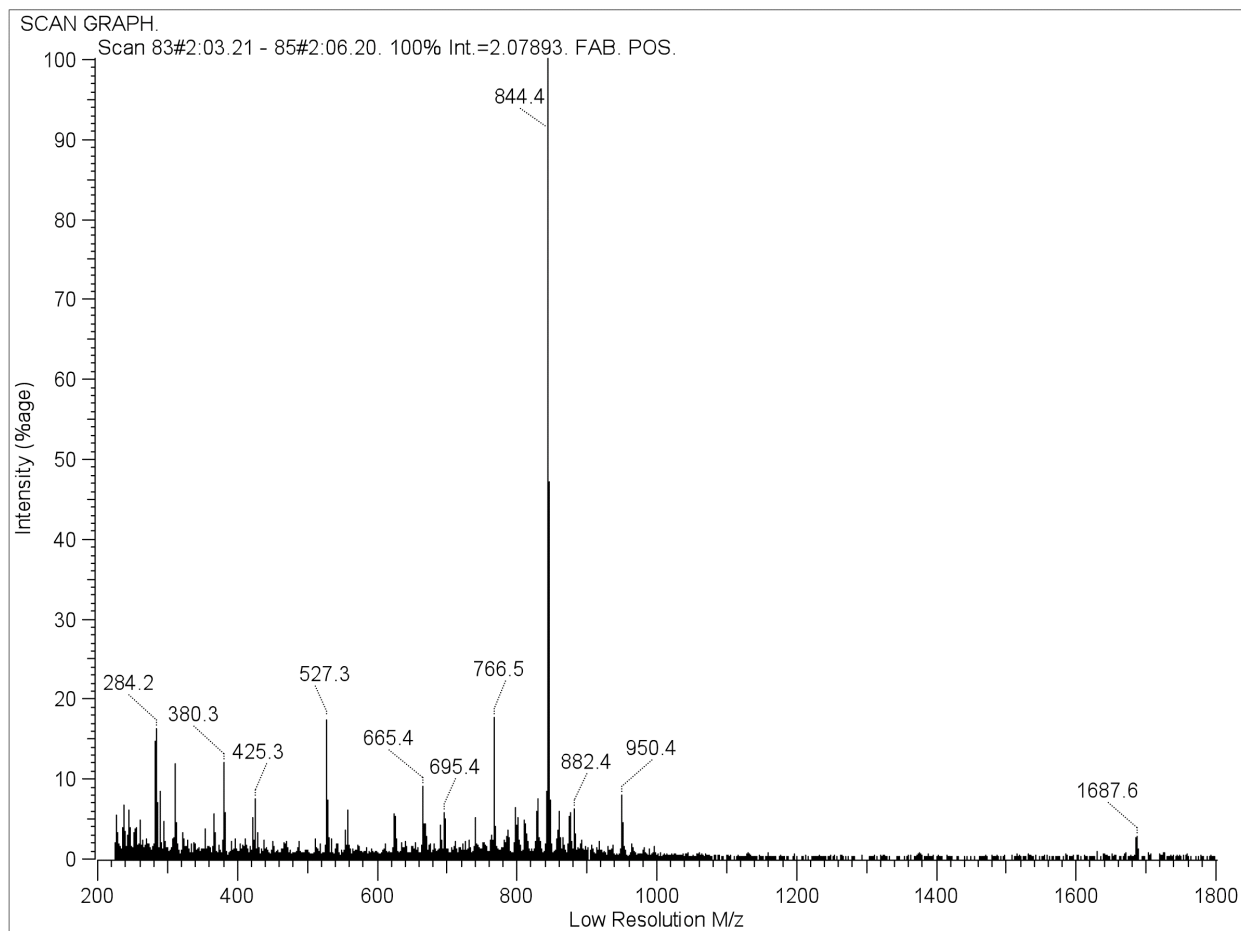


Figure S4. Representative fast atom bombardment (FAB) mass spectrometry analysis on GPRPFAC peptide solution remaining after a SPR experiment. The analysis revealed an intense ion peak at 844.4 presumably the $[M+H]^+$ (nominal molecular weight = 843.4Da), indicative of a monomer peptide solution. Additionally, a minor intensity ion peak was at 1687.6, indicating minimal dimerization in the solution.