Supporting Information

Dynamics and Fluidity of Amyloid Fibrils: A Model of Fibrous Protein Aggregates

Ami S. Lakdawala, David M. Morgan, Dennis C. Liotta, David G. Lynn, James P. Snyder

Relationship of Peptide Length to Ideal β-sheet Geometry

Residues	AMBER* ΔE^a (kcal/mol)	B3LYP/6-31G** ΔE^a (kcal/mol)
^{16}KL	3.95	3.75
^{16}KLV	4.43	4.09
^{16}KLVF	6.96	7.41
^{16}KLVFF	9.48	8.94
^{16}KLVFFA	11.29	-

[a] ΔE = (constrained geometry) – (unconstrained geometry)

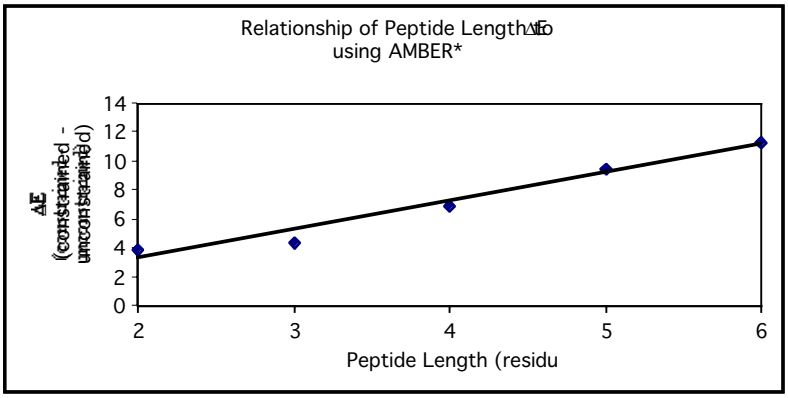

Figure S1. Plot of the energy differences between fully optimized peptides and their idealized β-strand geometries (ΔE(constrained-unconstrained)) for the di-, tri-, tetra-, penta- and hexapeptides from KLVFFA; AMBER*/GBSA/H_2O force field; Slope = 2.0 kcal/mol.

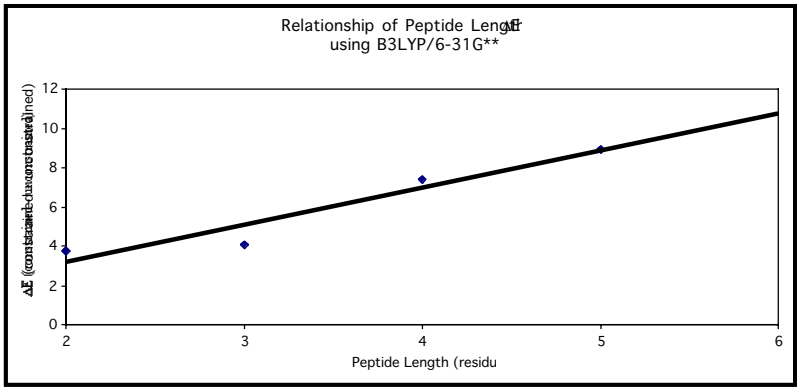

Figure S2. Plot of the energy differences between fully optimized peptides and their idealized β-strand geometries (ΔE(constrained-unconstrained)) for the di-, tri-, tetra-, pentapeptides from KLVFFA; B3LYP/6-31G** single point; Slope = 1.9 kcal/mol.