Supplementary Material

Reversible α-helix formation controlled by a hydrogen bond surrogate

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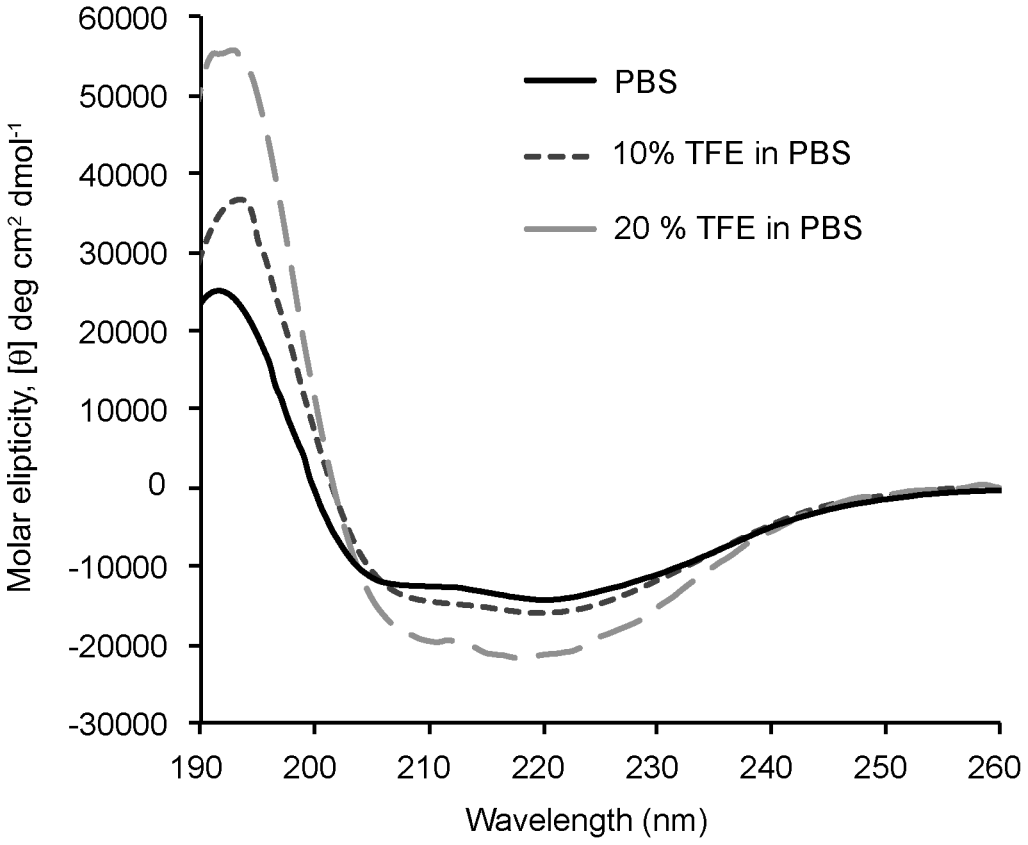

Figure S1. CD spectra of dsHBS **2** in mixtures of PBS and TFE.

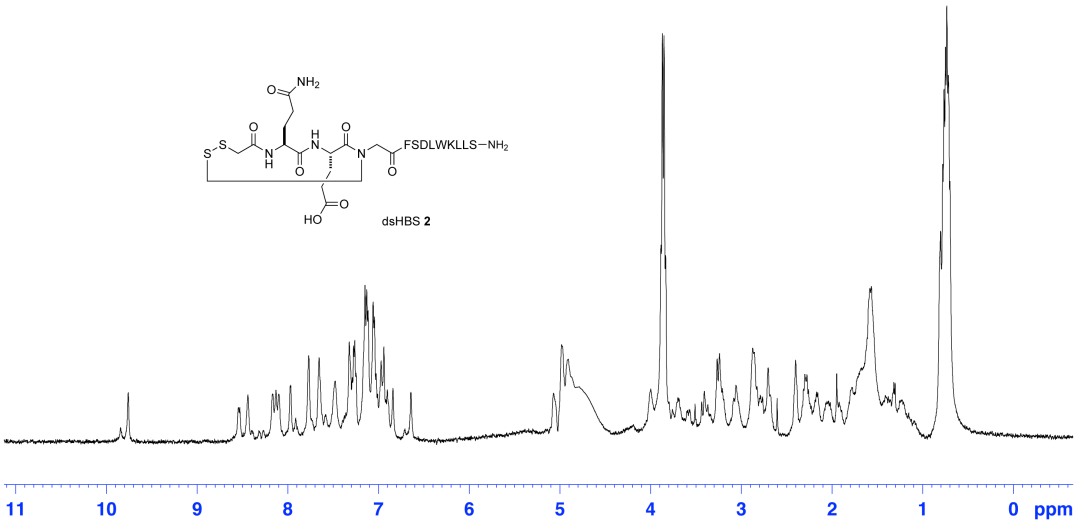

Figure S2. ^{1}H NMR of dsHBS **2** in 20% trifluoroethanol-d3/PBS.

Table S1. ^{1}H NMR assignments and chemical shifts (δ, ppm) for dsHBS **2** in 20% trifluoroethanol-d3/PBS.

Residue	NH	Hα	Hβ	Hγ	Hδ	Hε
Q^{1}	8.54	4.47	1.93	2.27	-	-
E^{2}	8.40	4.24	2.1	2.38	-	-
G^{3}	-	*	-	-	-	-
F^{4}	7.13	4.27	3.06, 2.85	-	-	-
S^{5}	7.98	4.18	3.89	-	-	-
D^{6}	8.17	4.44	2.75	-	-	-
L^{7}	8.14	3.99	1.59	1.33	0.72	-
W^{8}	8.10	4.20	3.20	-	-	-
K^{9}	7.66	4.01	1.75	1.57	1.37	3.25
L^{10}	7.77	3.98	1.49	1.74	0.77	-
L^{11}	8.12	3.99	1.59	1.33	0.72	-
S^{12}	7.65	4.00	3.67	-	-	-

*αCH for glycine could not be unambiguously assigned.

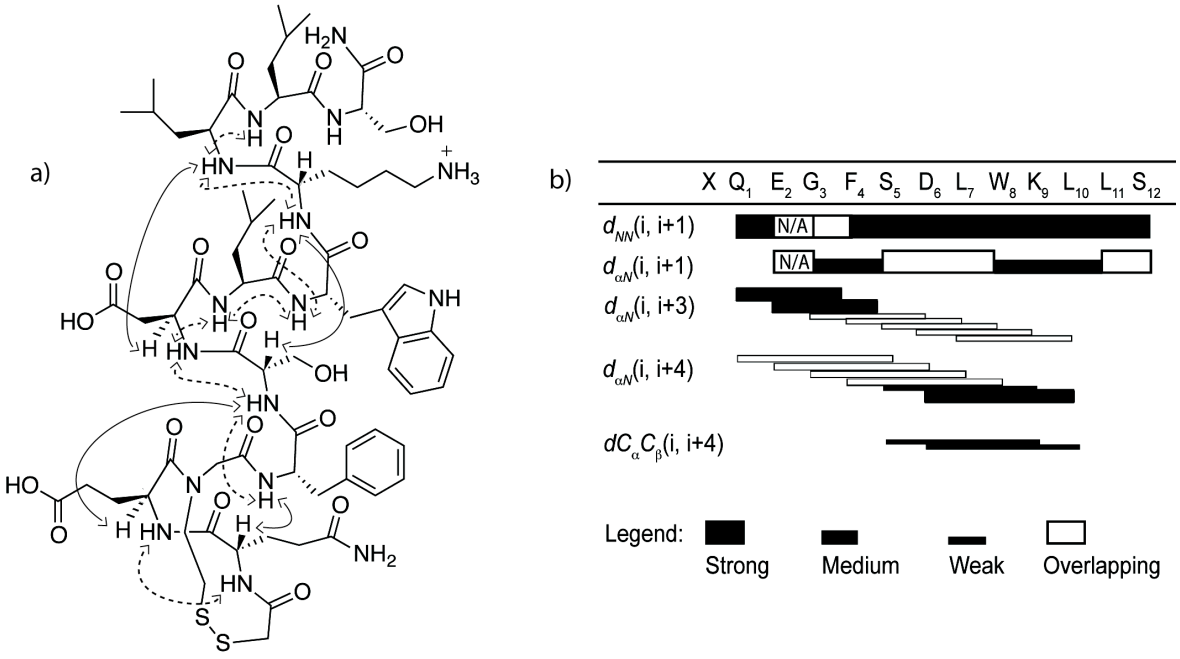

Figure S3. Observed NOE's for dsHBS **2**. a) arrows depicting short (dashed) and medium (solid) range NOE's. b) complete NOESY correlation chart. Note: the glycine-3 residue is N-alkylated. Filled rectangles indicate relative intensities of NOE cross-peaks. Empty rectangles indicate NOEs that could not be unambiguously assigned because of overlapping signals.

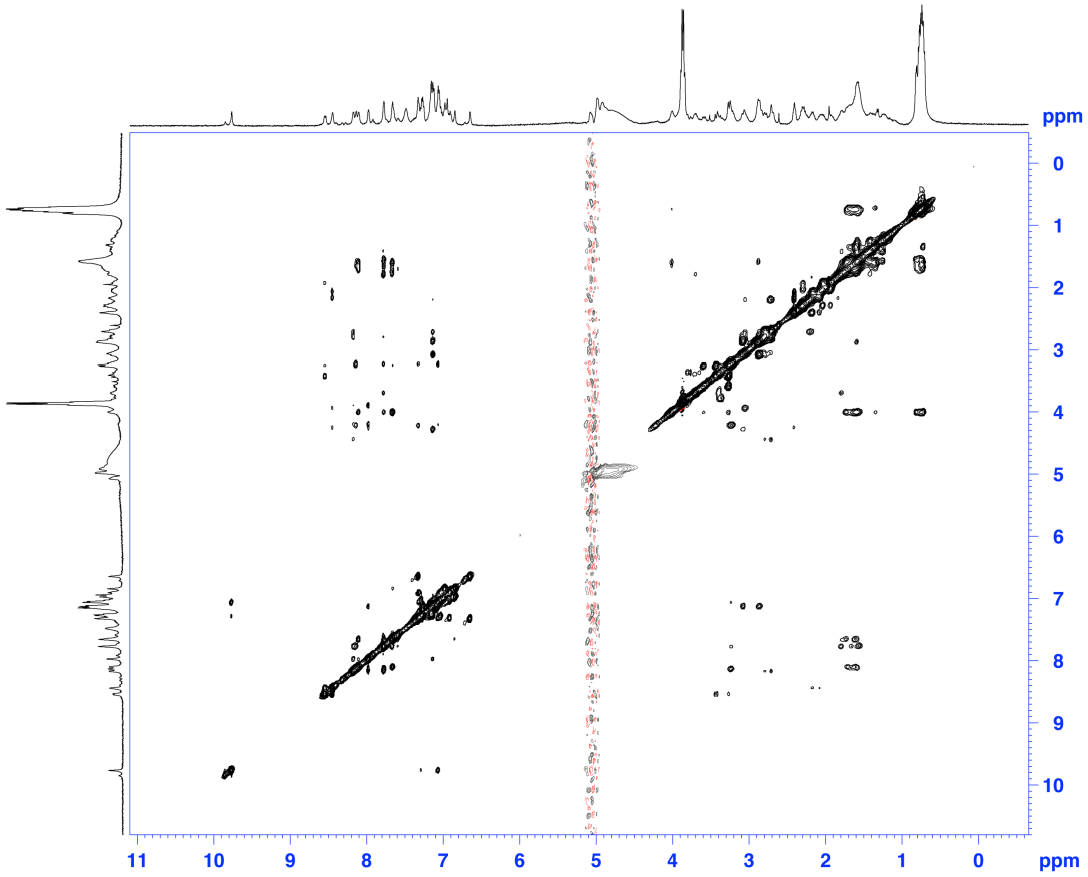

Figure S4. NOESY spectrum for dsHBS **2** in 20% TFE/PBS

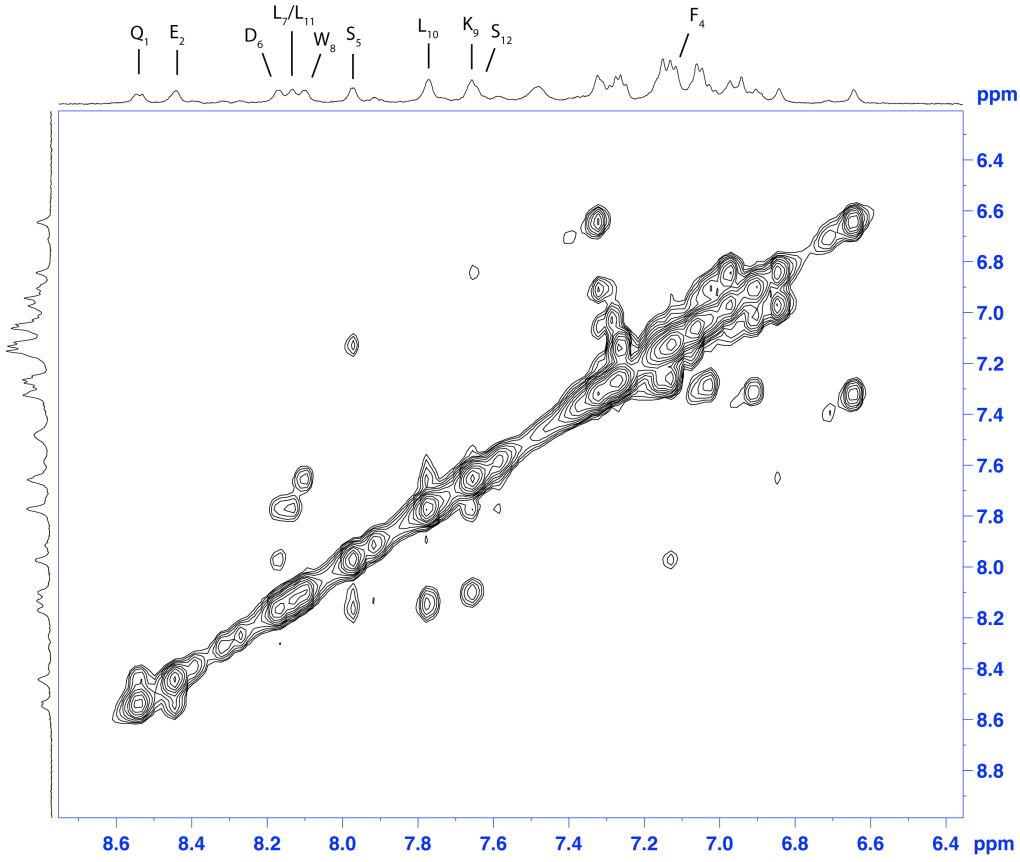

Figure S5. NH region of NOESY spectrum for dsHBS **2**.

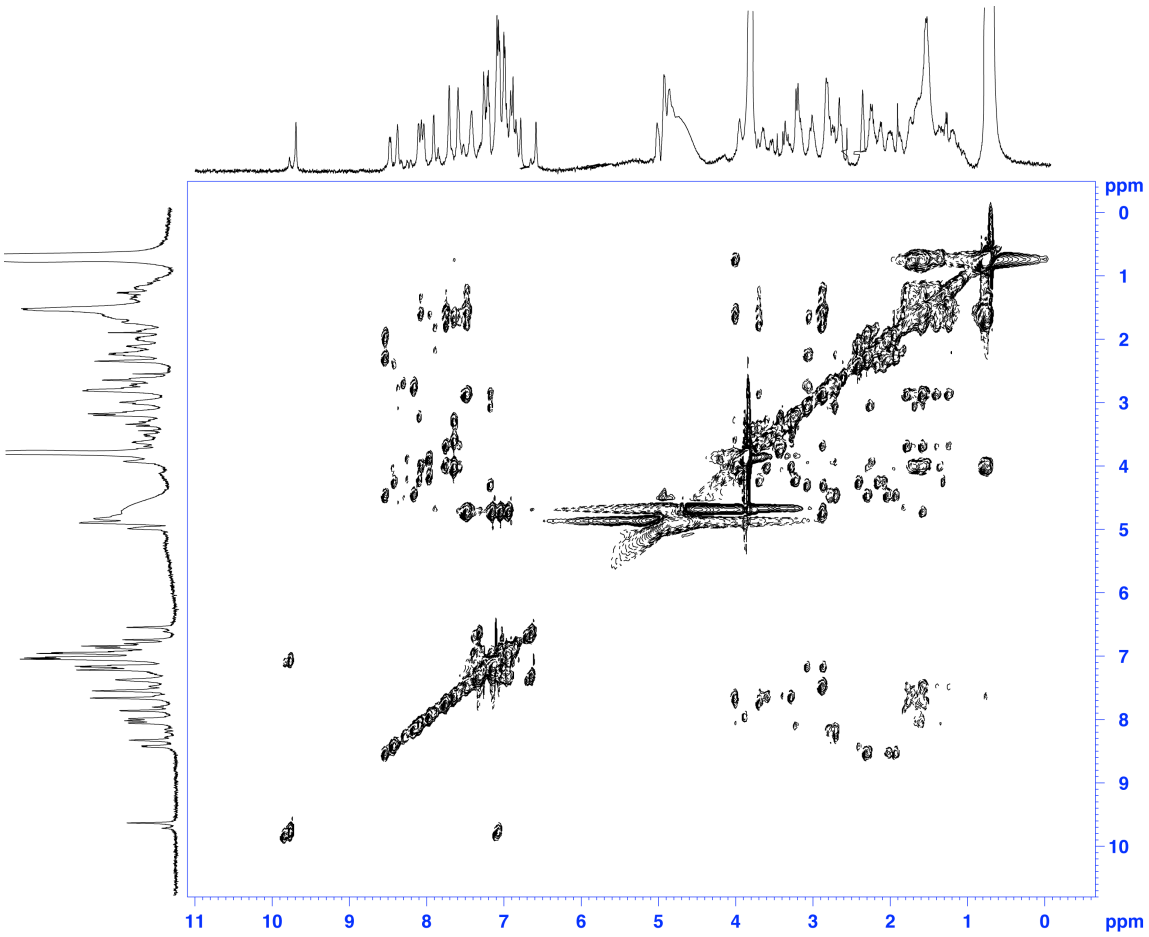

Figure S6. TOCSY spectrum for dsHBS **2** in 20% TFE/PBS.