De Novo Self-Assembling Collagen Heterotrimers using Explicit Positive and Negative Design

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SUPPLEMENTARY DATA

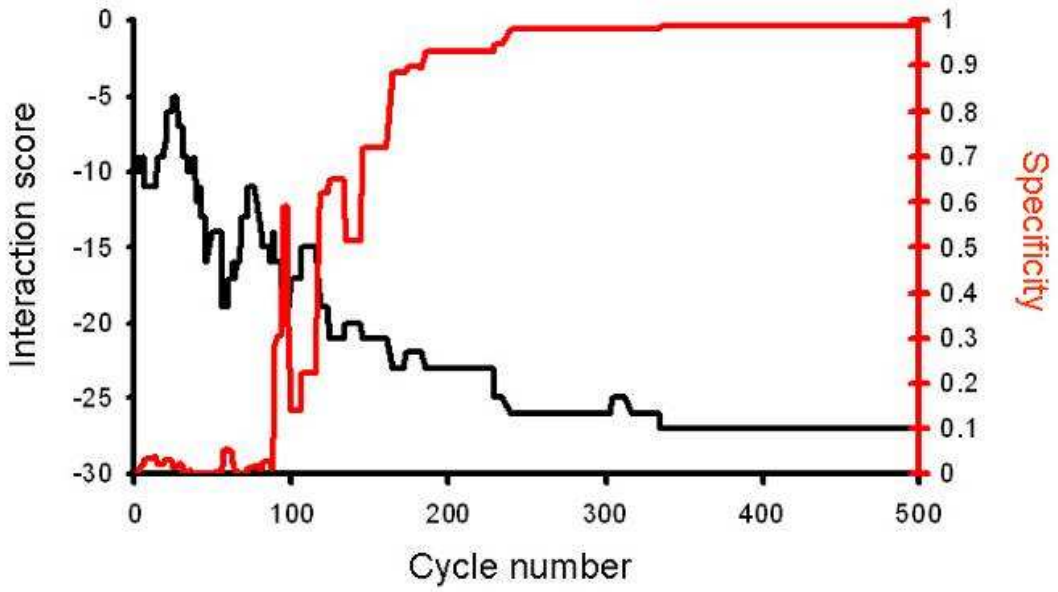

Figure S1: Trajectory of stability, E_{ABC}, and specificity, P_{ABC}, for a single optimization. Energies calculated using the sequence-based scoring function (Eq. 1).

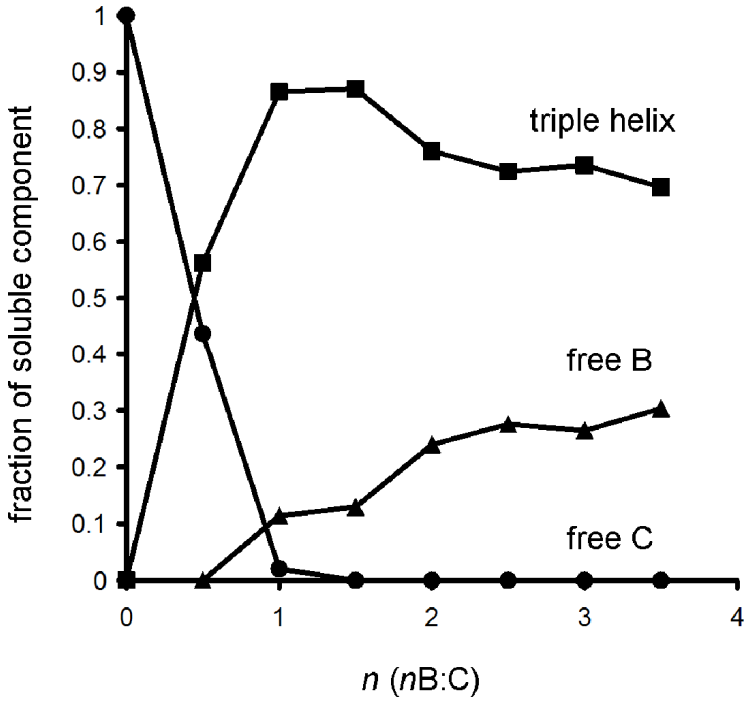

Figure S2: Separation of the *n*B:C Job plot (Figure 7B) into components for the triple-helix, B-type monomer and C-type monomer CD spectra. Using a conjugate gradient optimization, experimental spectra for each ratio *n* of *n*B:C were fit to $\alpha_{helix}S_{helix} + \alpha_{freeB}S_{freeB} + \alpha_{freeC}S_{freeC}$. 0.2 mM CD spectra for free B and C were used for S_{freeB} and S_{freeC}. $(POG)_{10}$ was used for S_{helix}. α's were normalized to total soluble concentration.

Table S1. The top 5 sequences of chains A, B, and C (sorted by E_{GAP}) from the simultaneous optimization of interaction score of species ABC and its specificity.

Sequences	E_{ABC}	E_{GAP}	Number of Glu	Number of Arg
A: EOGROGPEGPEGPEGEOGEOGPEGROGPRG B: PEGEOGROGROGPRGPRGPRGROGROGPRG C: PRGROGROGROGPRGEOGPEGPEGEOGEOG	–29	22	14	16
A: PRGEOGROGROGPEGPEGEOGEOGROGPRG B: EOGPOGPEGEOGPEGPRGPRGROGROGPRG C: PEGPEGROGPRGROGPRGEOGPEGEOGEOG	–23	22	15	14
A: ROGPRGPRGROGROGPEGEOGPEGROGPRG B: PRGEOGPEGPEGEOGPRGPRGROGROGPRG C: PRGEOGPEGROGPRGROGPEGPEGEOGEOG	–25	22	13	17
A: PRGPRGPRGROGROGPRGEOGPEGEOGEOG B: EOGPRGPEGPEGPEGEOGPEGROGPRGROG C: PEGEOGPEGROGPRGPRGROGPRGEOGPEG	–21	22	15	15
A: PRGEOGPEGEOGPEGROGPRGROGPEGEOG B: EOGPEGPRGPRGROGROGEOGPEGEOGROG C: PEGROGPRGPEGPEGEOGPEGPRGROGEOG	–13	21	17	13

Table S2. Interaction scores using the structure-based model of all the species of peptides A, B, and C at pH 1.1.

Species	**Interaction Scores**
AAA	**0**
BBB	**10**
CCC	**8**
ABB	**2**
BAB	**8**
BBA	**4**
AAB	**0**
ABA	**2**
BAA	**2**
BCC	**4**
CBC	**4**
CCB	**4**
BBC	**2**
CBB	**2**
BCB	**6**
ACC	**4**
CAC	**2**
CCA	**4**
AAC	**2**
ACA	**2**
CAA	**2**
ABC	**2**
ACB	**0**
BAC	**4**
BCA	**2**
CAB	**2**
CBA	**2**