Supplementary Material for Organic & Biomolecular Chemistry

Supplementary data

De Novo Design of a Stable N-Terminal Helical Foldamer

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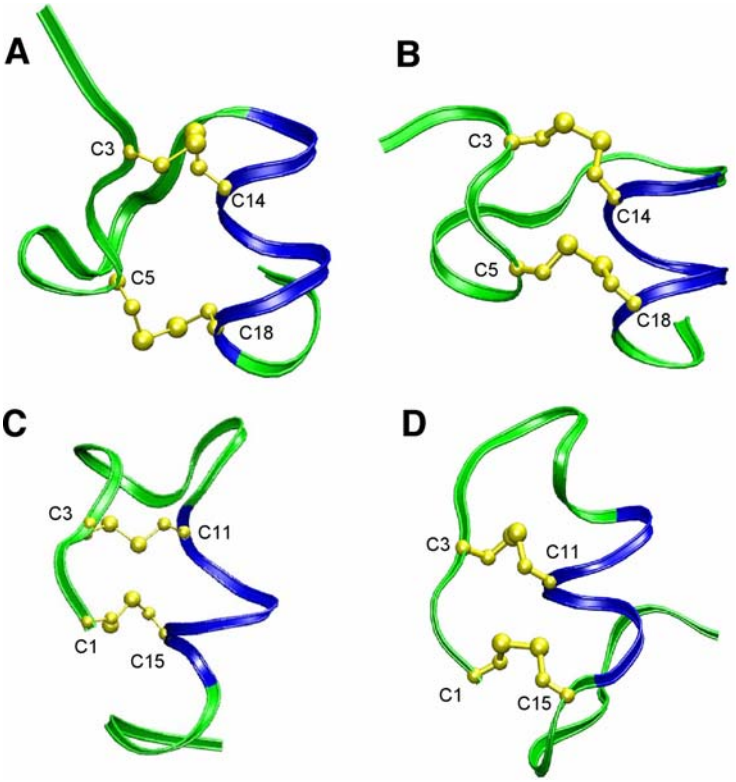

Figure S1: Validation of the modelling procedures using the known structures of tertiapin and endothelin. The structures of tertiapin (**A**) and endothelin (**C**) obtained using the modelling procedures described here are shown next to the experimentally determined structures of these peptides. The NMR-structure of tertiapin [1] is shown in panel **B**, while panel **D** depicts the crystal structure of endothelin. [2]. All structures were displayed using VMD.

Table S1 Summary of conformational constraints and statistics for the accepted 20 structures of NTH-18.

Unambiguous NOE distance restraints	96
Intra-residual (|i-j| = 0)	22
Sequential (|i-j| = 1)	47
Medium range (|i-j| < 5)	18
Long range (|i-j| > 4)	9
Ambiguous NOE distance restraints	12
RMSD from distance restraints (Å) [3, 4]	0.027 +/ -0.003
RMSD from covalent geometry [3, 4]	
Bond lengths (Å)	0.0019 ± 0.0001
Angles (deg)	0.415 ± 0.016
Impropers (deg)	0.290 ± 0.025
Ramachandran plot (%)[5]	
Most allowed regions (residues 2-8)	35.8
Disallowed regions (residues 2-8)	0
Most allowed regions (residues 2-8)	30.7
Disallowed regions (residues 2-8)	5
Most allowed regions (residues 1-18)	29.3
Disallowed regions (residues 1-18)	6.4
RMSD of the NMR ensemble[6]	
Mean backbone (residues 3-8)	0.13 ± 0.05
Mean heavy atoms (residues 3-8)	0.81 ± 0.20
Mean backbone (residues 2-8)	0.25 ± 0.10
Mean heavy atoms (residues 2-8)	1.00 ± 0.20
Mean backbone (residues 1-18)	1.33 ± 0.49
Mean heavy atoms (residues 1-18)	2.35 ± 0.70

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