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Supporting Information

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Self-assembled foldamer capsules: combining single and double helical segments in one aromatic amide sequence

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Table of contents

Page 2	Color version of Figure 1
Page 2	NMR binding studies
Page 5	^1H and ^{13}C NMR spectra of new compounds

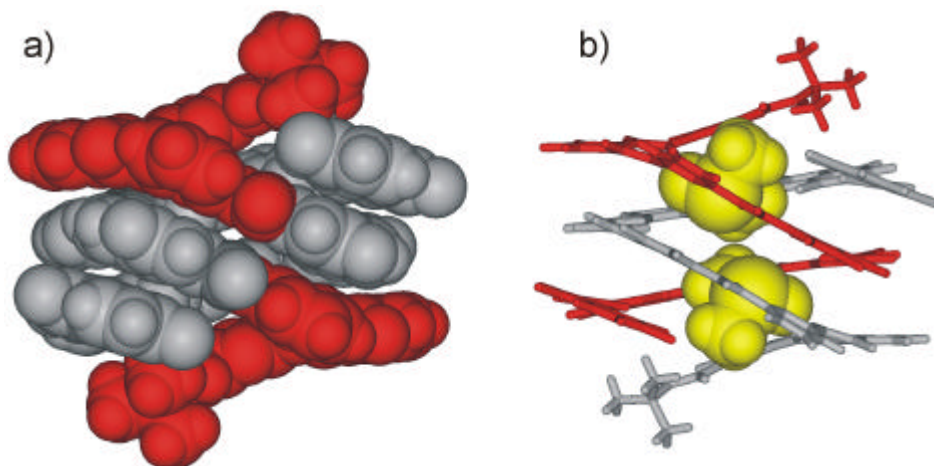


Figure 1. Structure of (1)₂ in the solid state. Isobutyl side chains, included solvent molecules, and hydrogen atoms have been omitted for clarity. In the CPK view shown in a), the nature of the monomers is color coded as follows: P in red and Q^F in grey. The red units belong to single helical-like (crescent) segments whereas the grey units belong to a double helix. In b), the two strands of the duplex are represented in tube representations in red and grey, respectively. Two included DMSO molecules are shown in yellow.

NMR binding studies

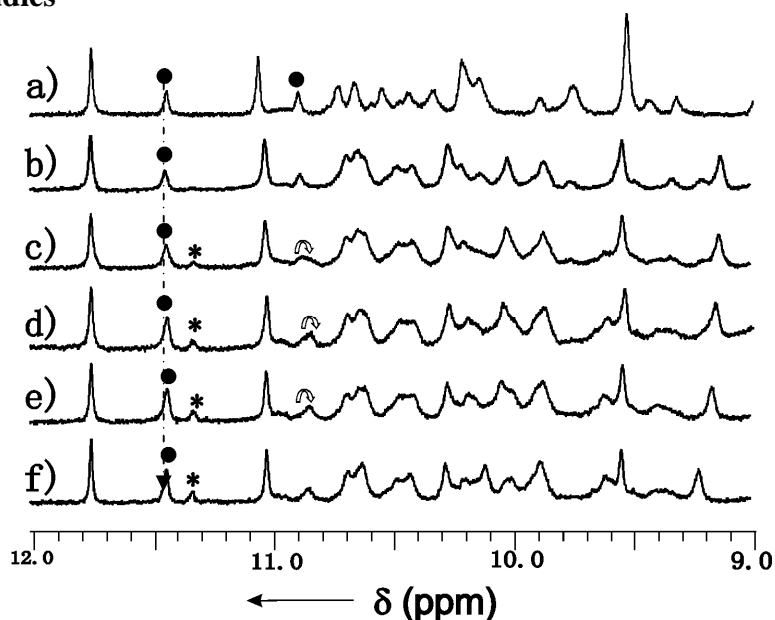


Figure S1. Part of the 300 MHz ^1H NMR spectra of 2 (2 mM in CDCl_3 at 25°C) in the presence of 1,9-nonanediol: a) 0 equiv.; b) 0.5 equiv.; c) 2.5 equiv.; d) 5.0 equiv.; e) 7.0 equiv.; f) 9.0 equiv. These spectra show an increase of the proportion of the double helix upon adding the guest. Black circles indicate signals of the double helical capsule. Arrows point to the conversion of the empty double helical capsule into a capsule-guest complex. Signals marked with a star are not identified.

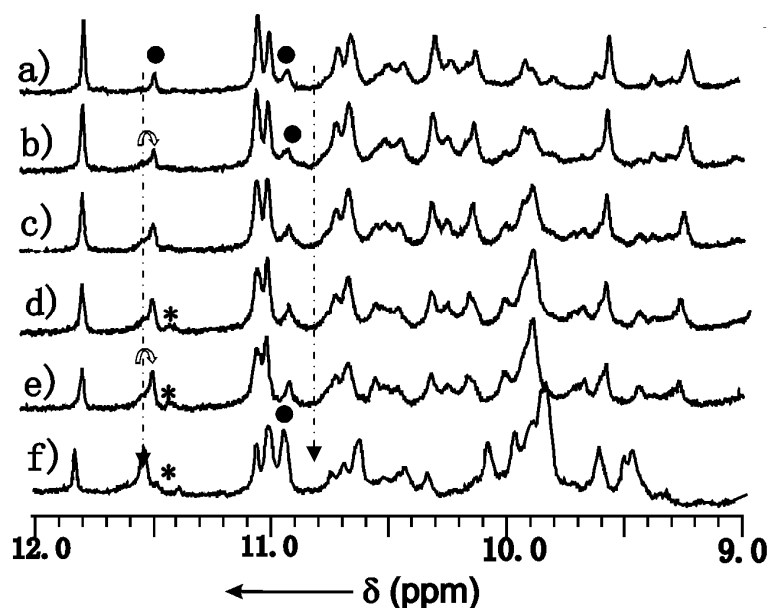


Figure S2. Part of the 300 MHz ^1H NMR spectra of **2** (2 mM in CDCl_3 at 25°C) in the presence of 1,10-decanediol: a) 0 equiv.; b) 0.5 equiv.; c) 2 equiv.; d) 4.5 equiv.; e) 9.0 equiv.; f) 9.0 equiv. at -20°C . These spectra show an increase of the proportion of the double helix upon adding the guest. Black circles indicate signals of the double helical capsule. Arrows point to the conversion of the empty double helical capsule into a capsule-guest complex. Signals marked with a star are not identified.

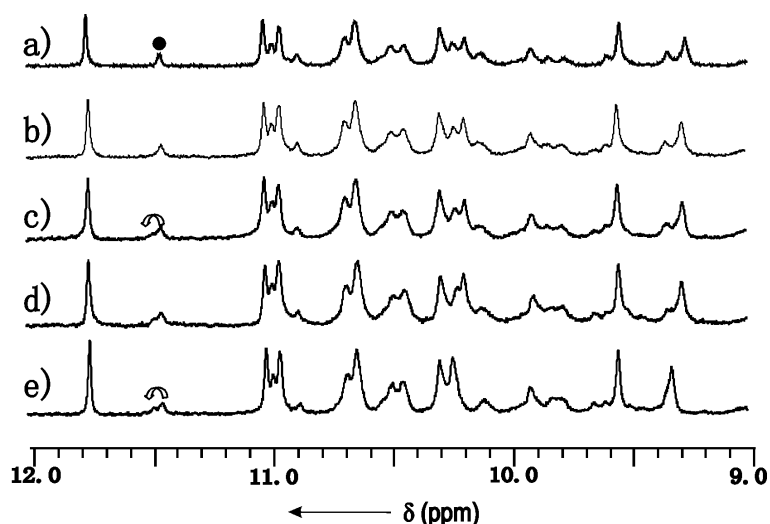


Figure S3. Part of the 300 MHz ^1H NMR spectra of **2** (2 mM in CDCl_3 at 25°C) in the presence of 1,11-undecanediol: a) 0 equiv.; b) 0.5 equiv.; c) 4.0 equiv.; d) 7.0 equiv.; e) 9.0 equiv. These spectra show no significant increase of the proportion of the double helix upon adding the guest during the conversion of the empty capsule into the capsule-guest complex. Black circles indicate signals of the double helical capsule. Arrows point to the conversion of the empty double helical capsule into a capsule-guest complex.

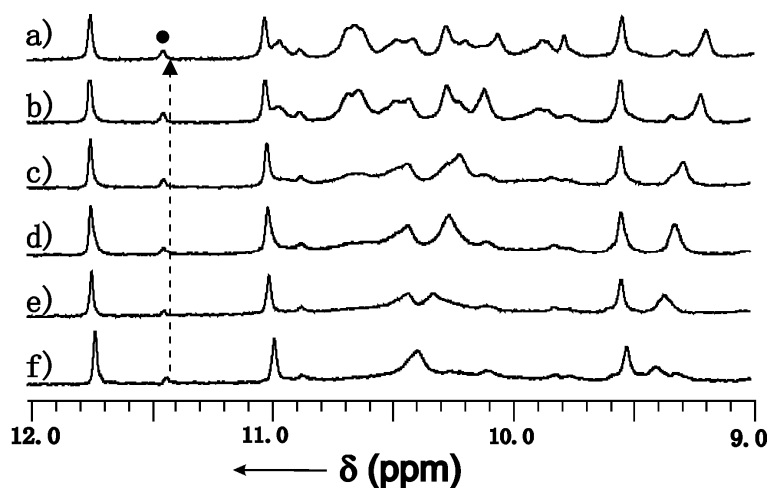


Figure S4: Part of the 300 MHz ^1H NMR spectra of **2** (2 mM in CDCl_3 at 25°C) in the presence of *ter*-Bu-CO₂(CH₂)₆-NH₂: a) 0 equiv.; b) 1.0 equiv.; c) 5.0 equiv.; d) 15.0 equiv.; e) 35.0 equiv.; f) 100 equiv. These spectra show little change of the proportion of single and double helix upon guest addition, along with a broadening of most of the single helix signals. Black circles indicate signals of the double helical capsule.

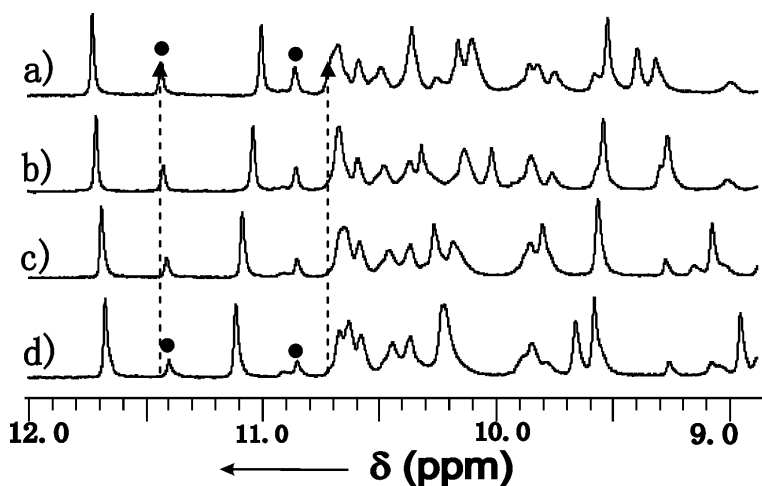
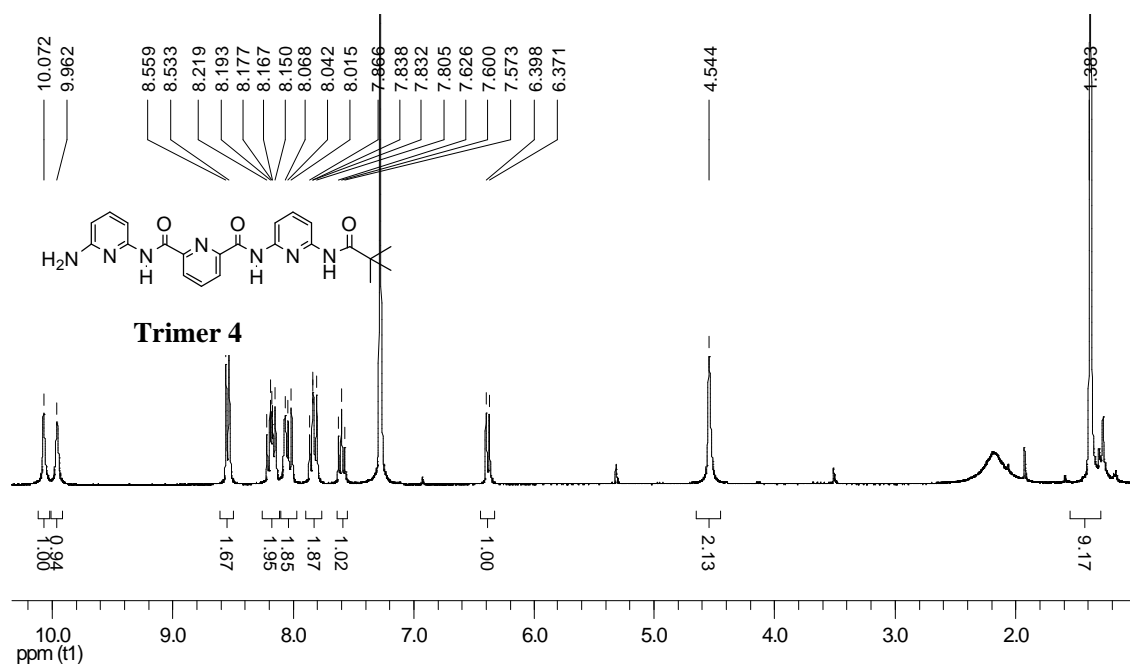
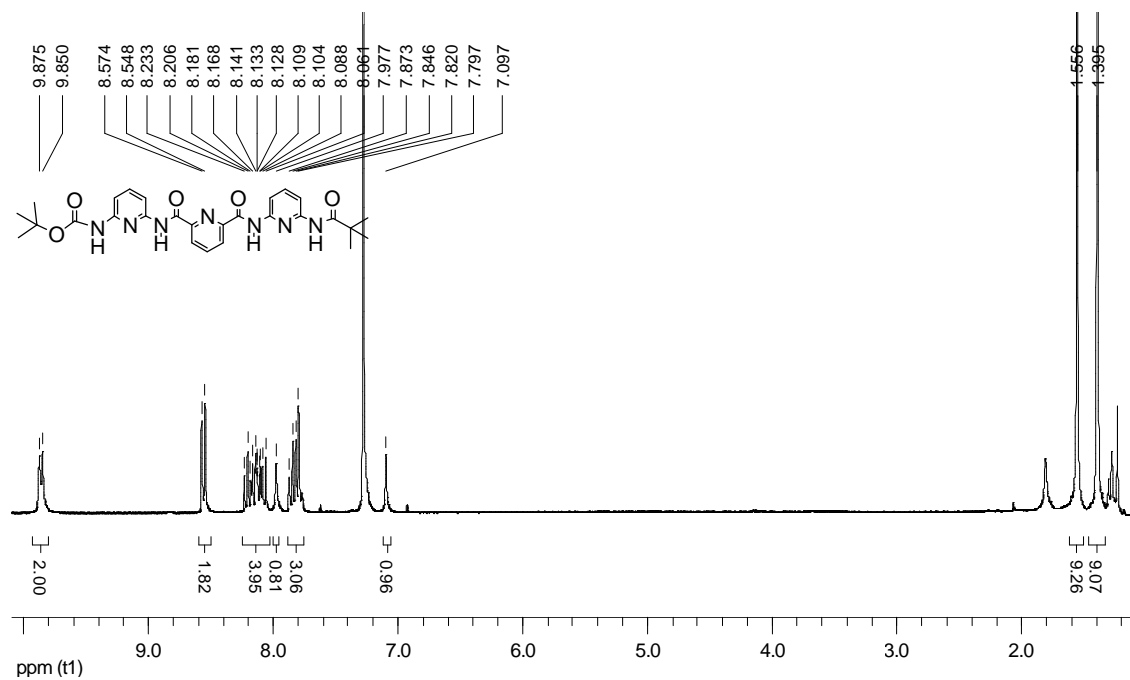
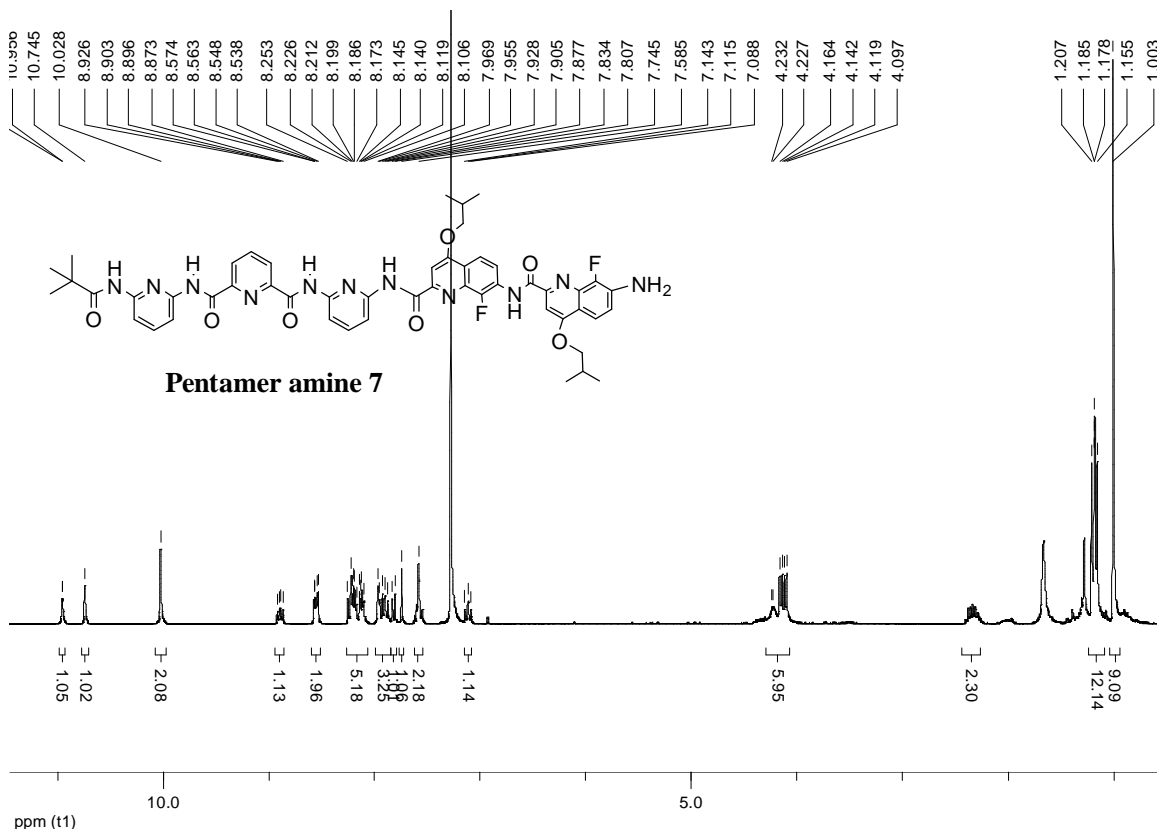
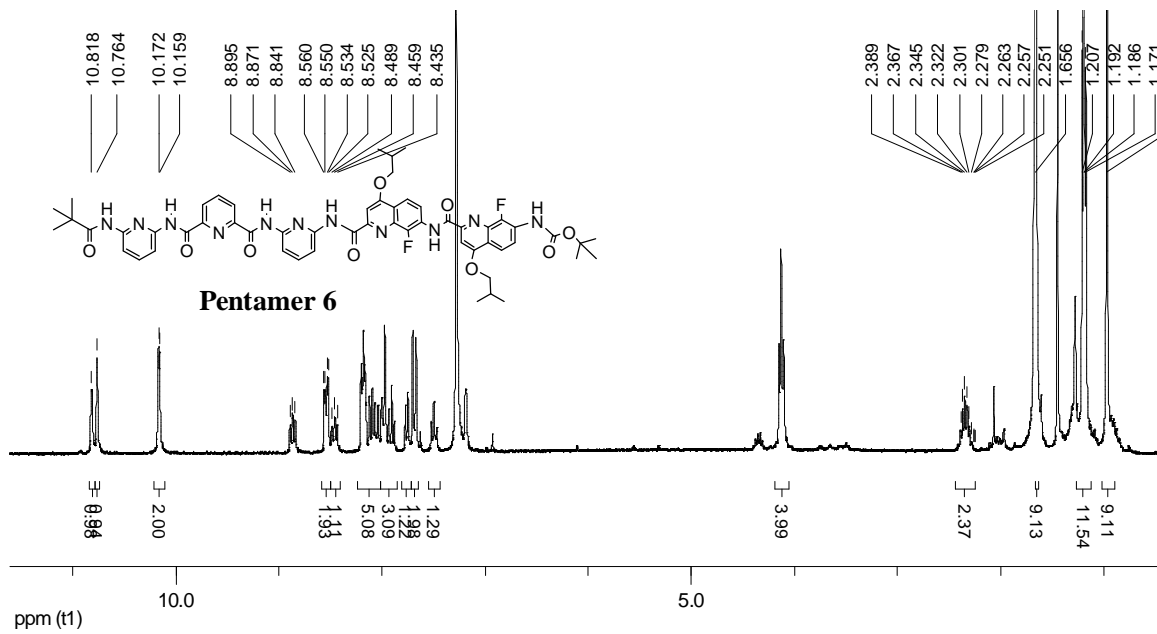
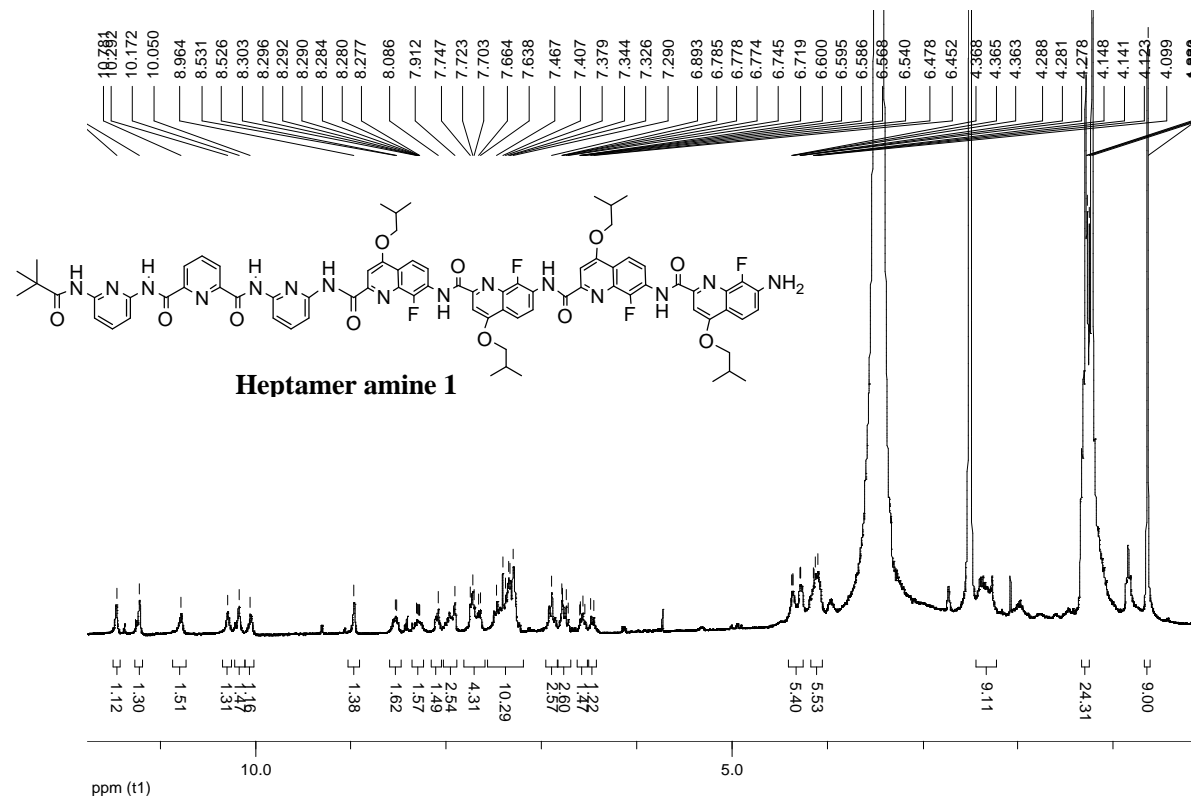
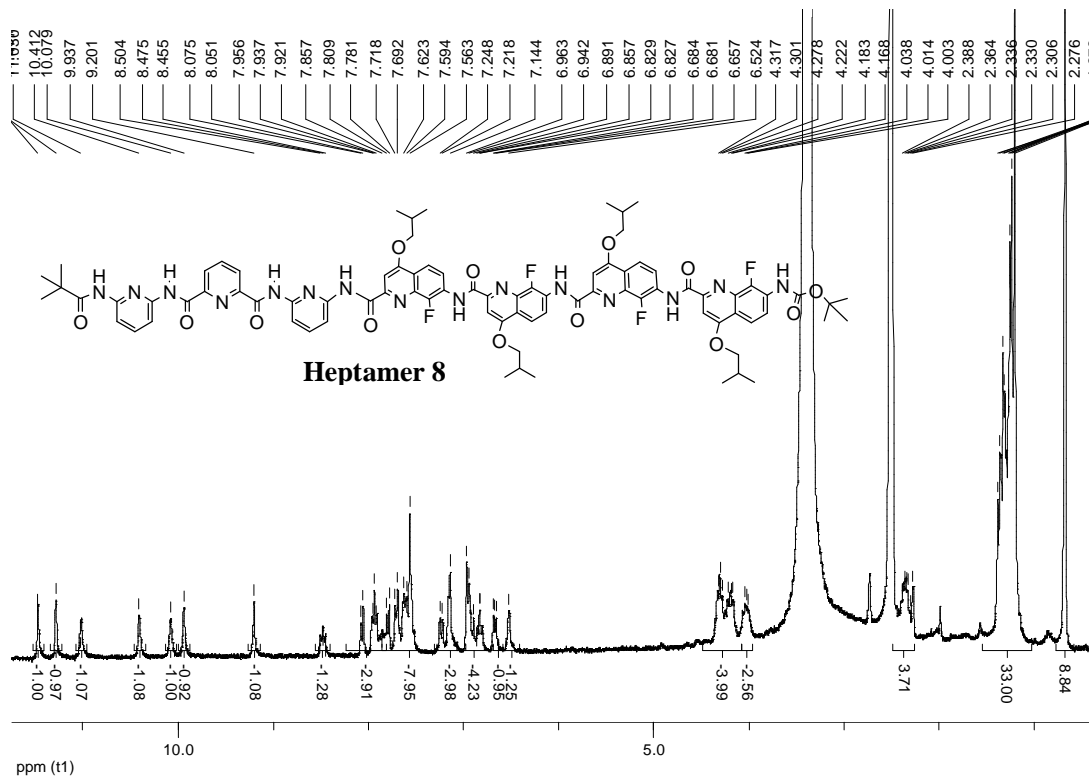


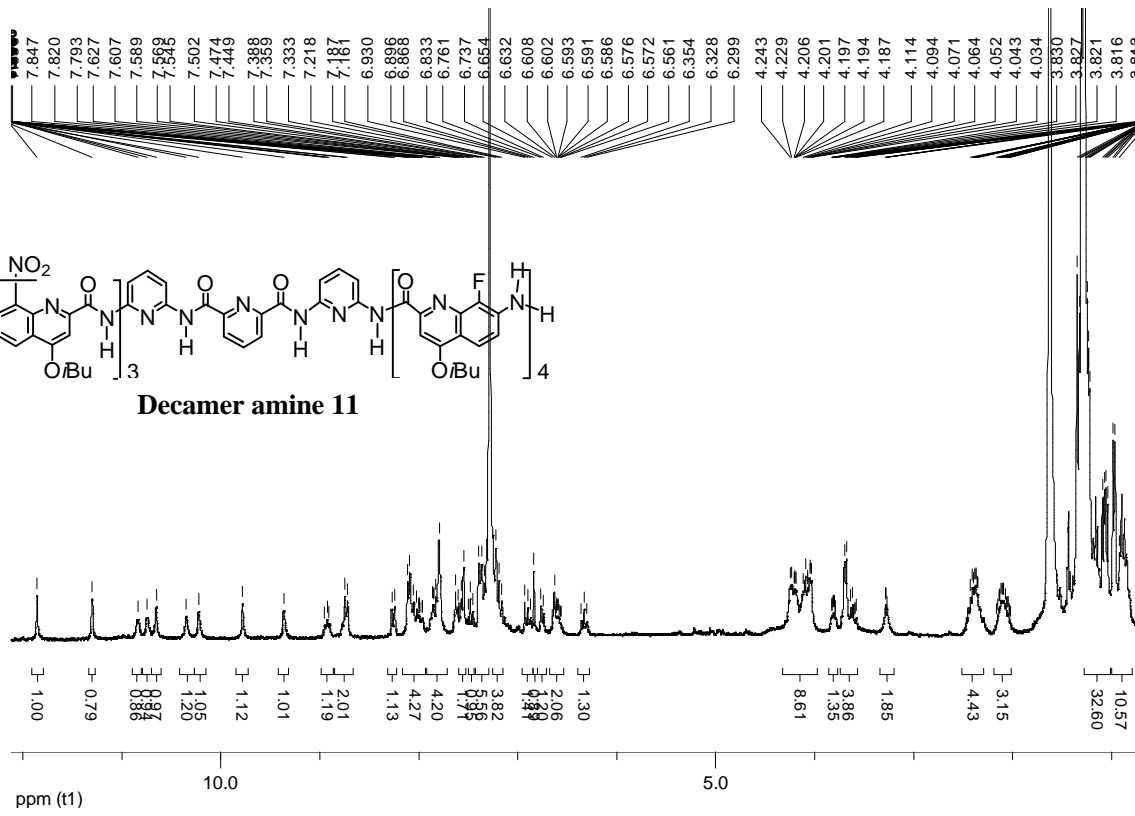
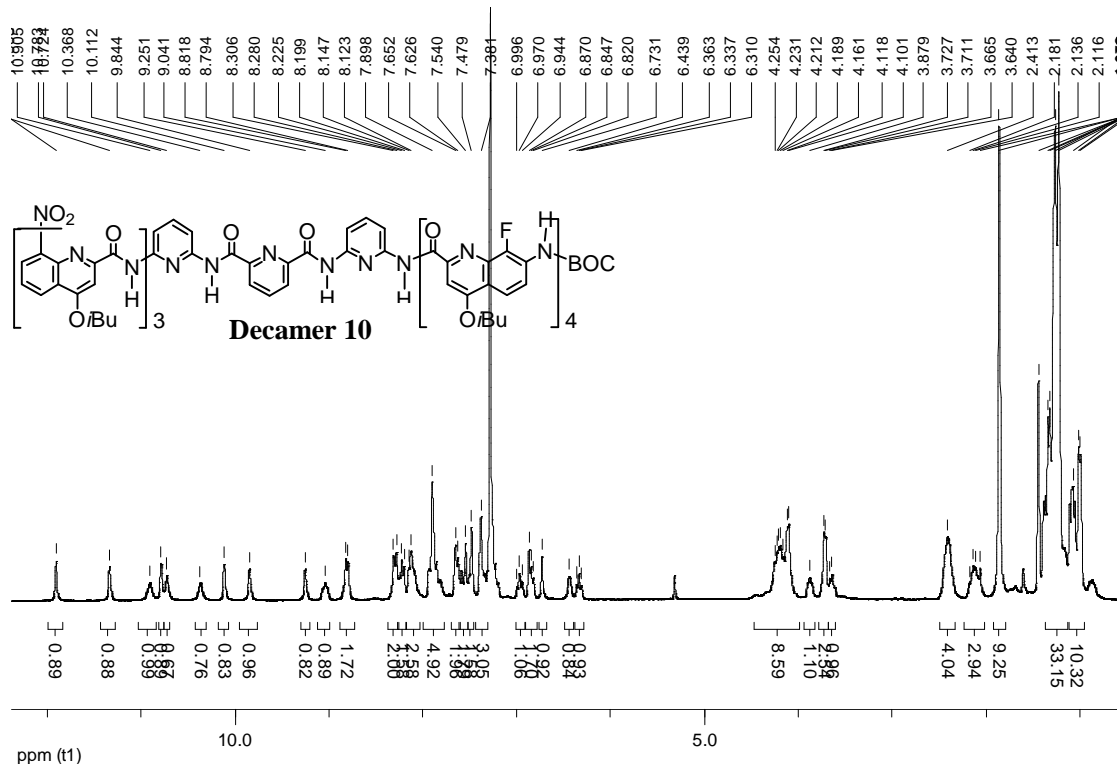
Figure S5. Part of the 300 MHz ^1H NMR spectra of **2** (5 mM in CDCl_3) at different temperatures: a) 25°C ; b) 35°C ; c) 50°C ; d) at 60°C . The black circle indicates signals assigned to the double helical capsule. The proportion of double helical capsule decreases upon increasing temperature.

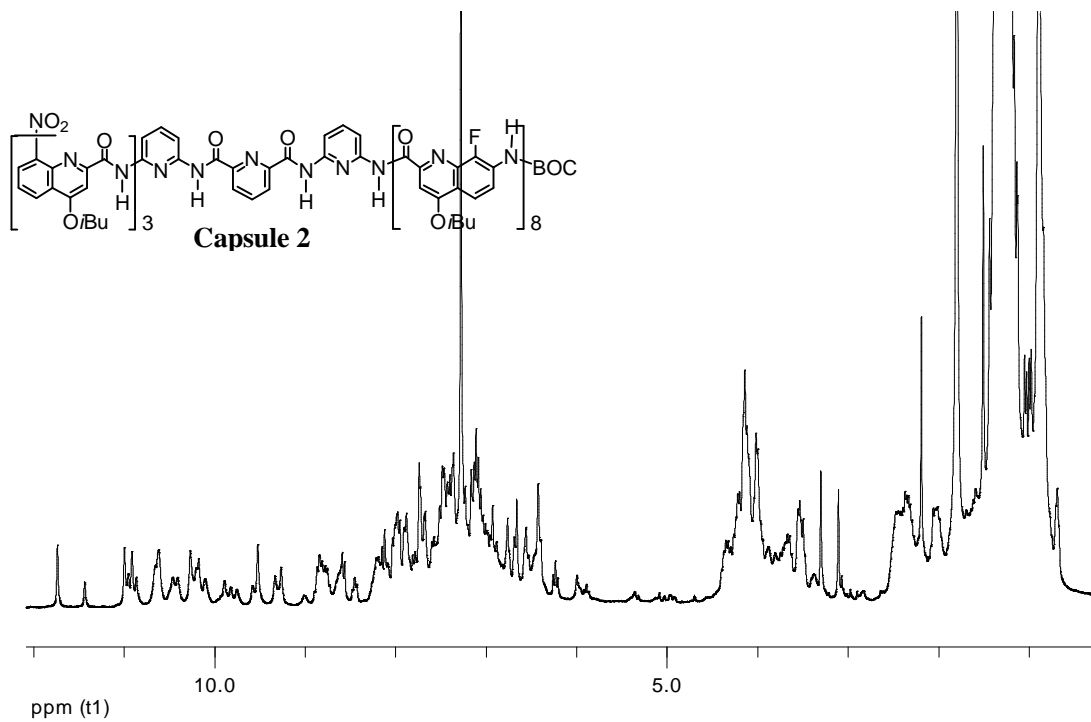
¹H NMR spectra of relevant synthetic intermediates and title compounds.











¹³C NMR spectra of relevant synthetic intermediates and title compounds.

