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Supplementary Information

Study of the BPP7a Peptide and its β-Cyclodextrin Complex: Physicochemical Characterization and Complete Sequence Specific NMR Assignments

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Table S1. ^{1}H NMR (600 MHz) spectral data for BPP7a, 5 °C (10% D_2O/H_2O)

Residue	δ NH	δ α–H	δ β–H	δ others	
p-Glu	7.74	4.03	β CH_2 2.13	γ CH_2	2.24-2.29 and 1.77-1.83
Asp[a]	8.51 (8.48) and (8.30)	4.54	2.67 and 2.51		–
Gly[a]	8.09 (8.06)	α CH_2 3.87 and 3.73	–		–
Pro[b]	–	4.10	1.53-1.59 and 1.91-1.99	γ CH_2 δ CH_2	2.02-2.12 and 1.55-1.65 3.31
Ile[a]	8.21 (7.74) (8.26) and (8.43)	4.14	1.58-1.53	γ CH_2 γ CH_3 δ CH_3	0.91 and 1.26 0.69 0.59
Pro[b]	–	4.38	1.74	γ CH_2 δ CH_2	1.69-1.73 3.68-3.62 and 3.34-3.43
Pro[b]	–	4.07	1.72	γ CH_2 δ CH_2	1.99-2.04 and 1.78-1.70 3.45-3.56 and 3.34-3.41

[a]Into brackets are presented chemical shifts of NH groups of other peptide conformations in solution; [b]signals can change; the attribution is based on NOE results.

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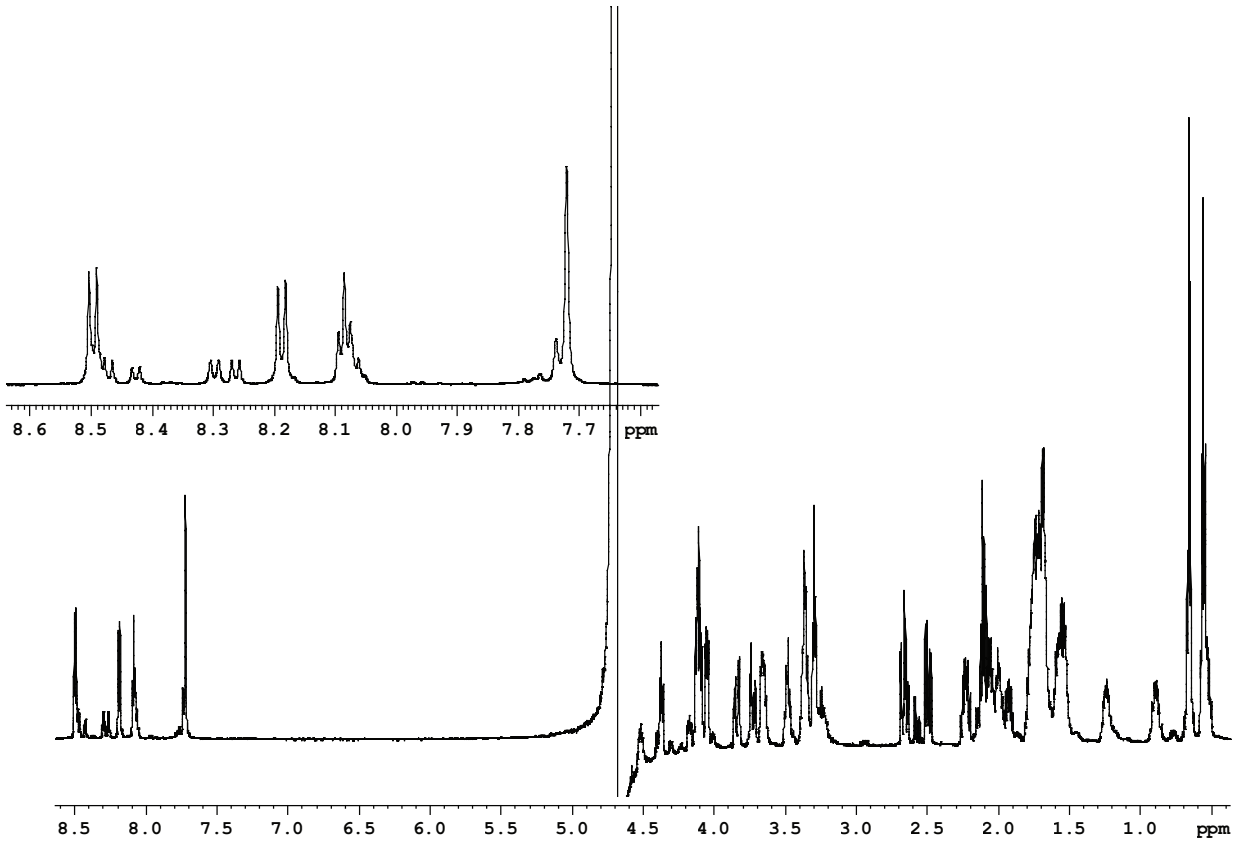

Figure S1. [1]H NMR spectrum of BPP7a peptide at 5 °C (presaturation, 600 MHz, 10% D_2O/H_2O), including expansion of amidic and aromatic region (upper portion).

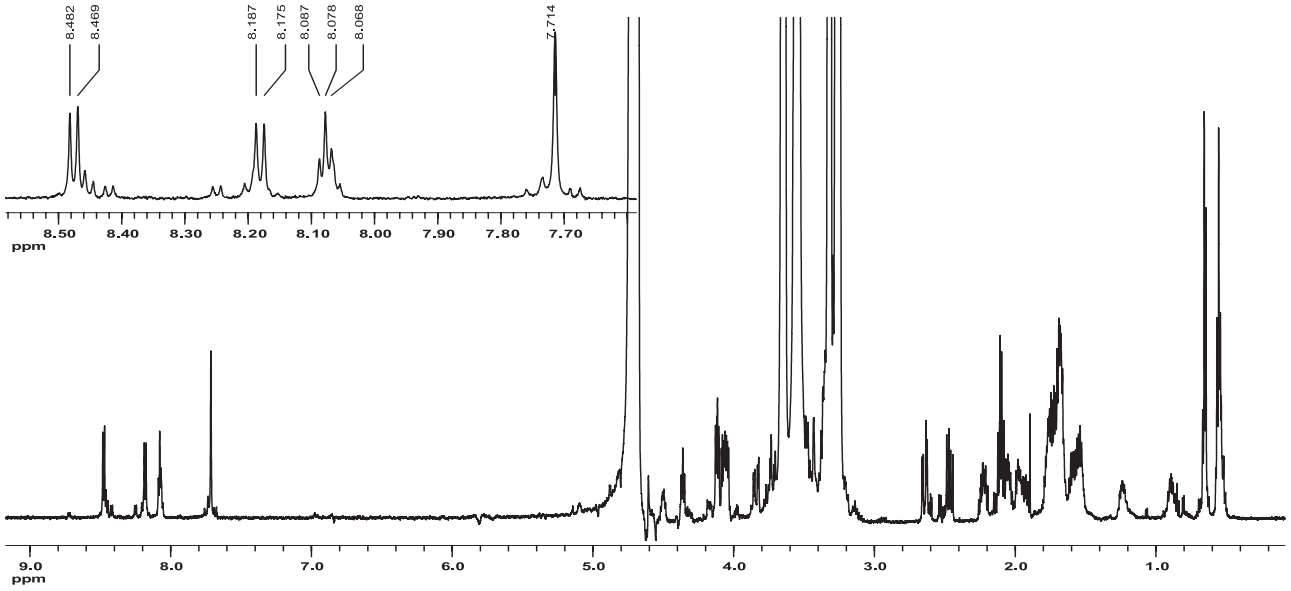

Figure S2. [1]H NMR spectrum of the BPP7a/β-cyclodextrin complex at 5 °C (presaturation, 600 MHz, 10% D_2O/H_2O), including expansion of amidic and aromatic region (upper portion).

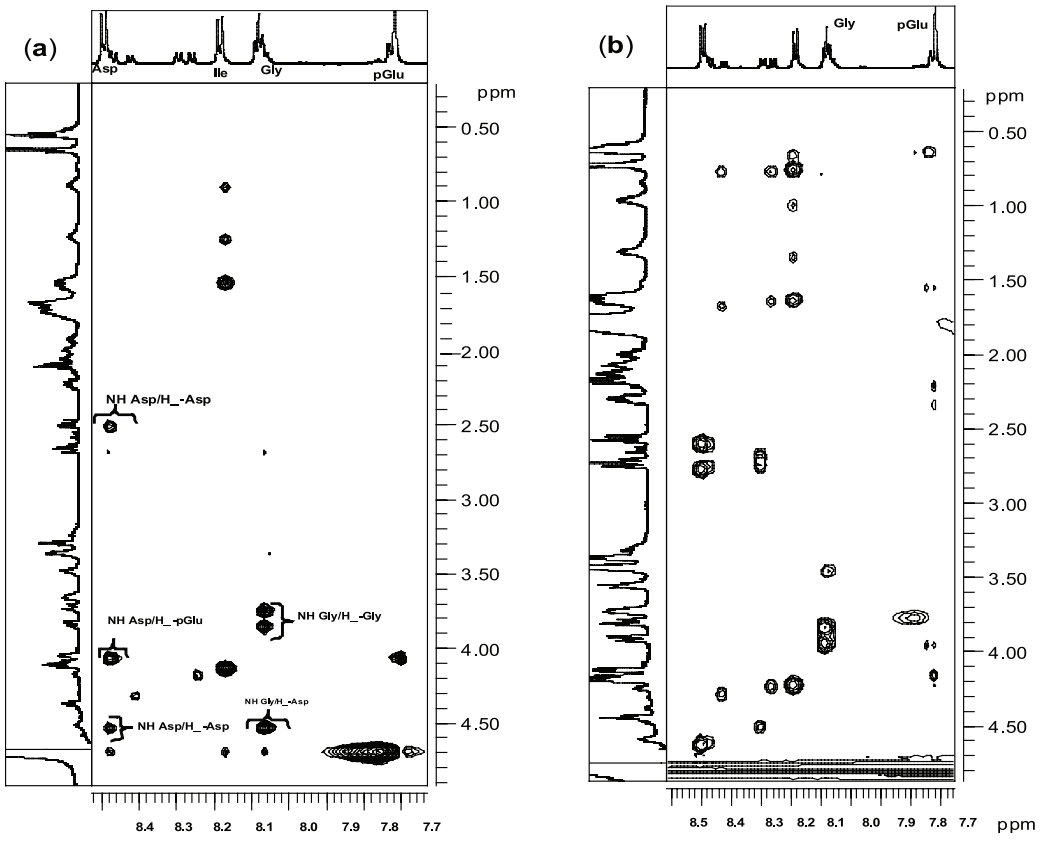

Figure S3. Amide region of ^{1}H NMR spectra of the BPP7a peptide at 5 °C (600 MHz, 10% D_2O/H_2O) (a) NOESY contour map of the amidic region, with a mixing time of 230 ms and (b) TOCSY contour map of amidic region, with a mixing time of 85 ms.

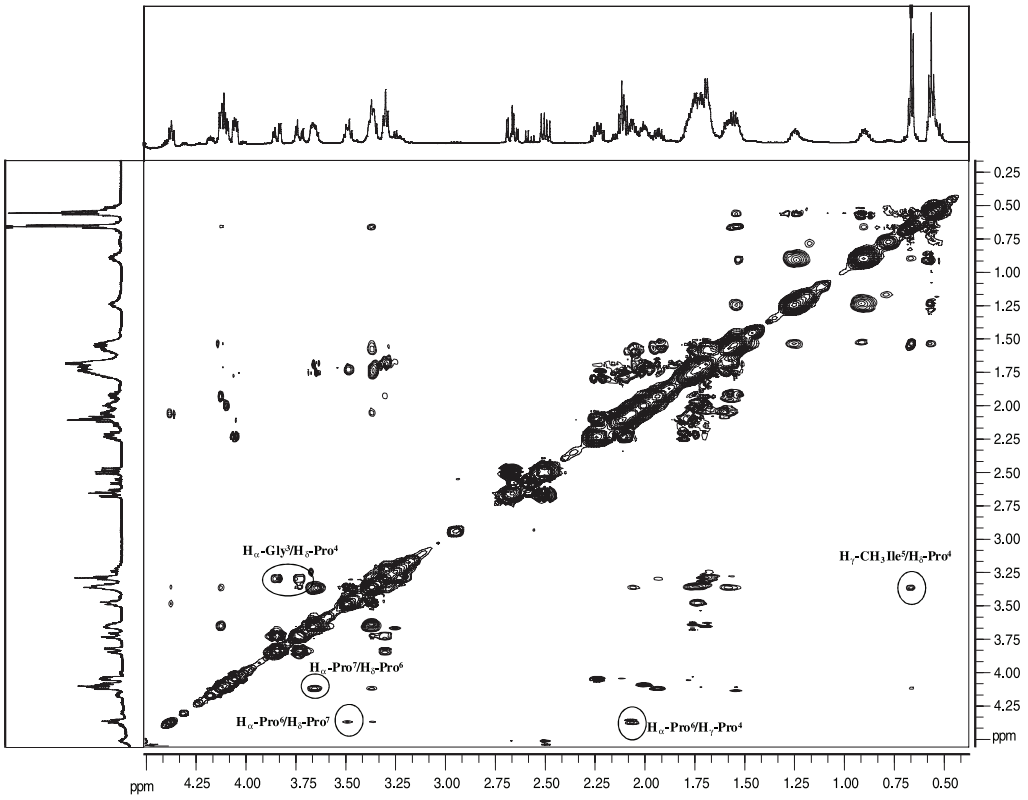

Figure S4. NOESY contour map of BPP7a at 5 °C (600 MHz, 10% D_2O/H_2O). For clarity, NOE correlations of Pro residues are indicated.

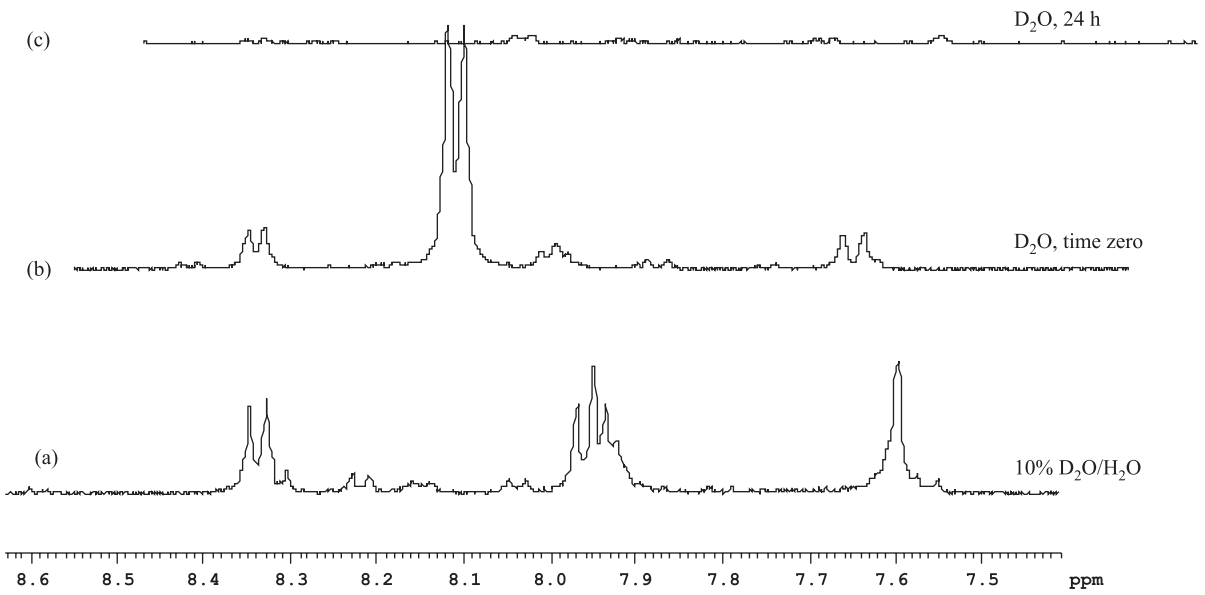

Figure S5. Amide region of ^{1}H NMR spectra of the BPP7a peptide at 5 °C, 400 MHz (a) 10% D_2O/H_2O, (b) D_2O, freshly prepared solution and (c) D_2O, 24 h after solution preparation.

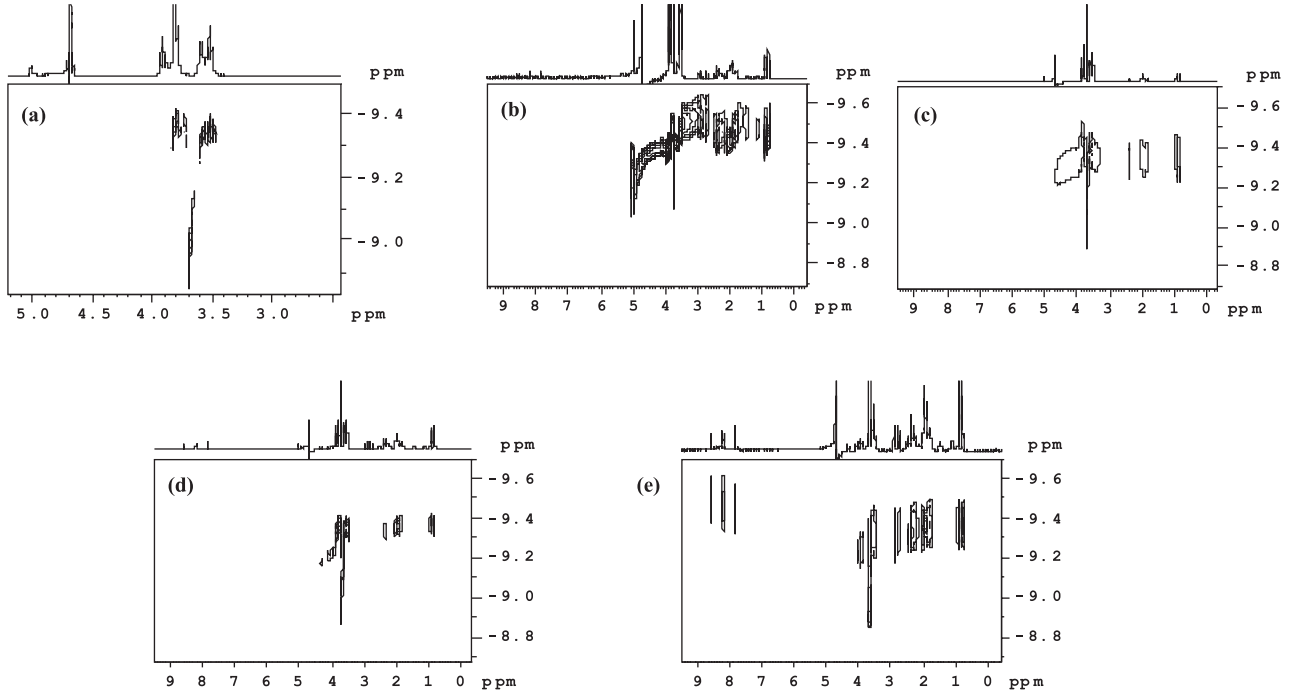

Figure S6. DOSY plots at 400 MHz in D_2O/H_2O for the supramolecular system BPP7a/β-cyclodextrin: (a) BPP7a/β-cyclodextrin [8 mmol L^{-1}], (b) BPP7a/β-cyclodextrin [2:6 mmol L^{-1}], (**c**) BPP7a/β-cyclodextrin [4:4 mmol L^{-1}], (d) BPP7a/β-cyclodextrin [6:2 mmol L^{-1}] and (e) BPP7a [8 mmol L^{-1}]. Experimental conditions: 10% D_2O/H_2O, 27 °C, 400 MHz.