## **Supporting Information**

# Influence of End-Capping on the Self-Assembly of Model Amyloid Peptide Fragments

Valeria Castelletto, Ian W. Hamley,\* Çelen Cenker, Ulf Olsson, Jozef Adamcik, Raffaele Mezzenga, Juan F. Miravet,\* Beatriu Escuder, Francisco Rodríguez-Llansola

#### **SI Table 1.** NOE correlations for **F** at two concentrations

### a) 2.6 wt%

	Е	С	В	Α	D	N	Hb Ha	Hc	14	20	24	3	7	9 13	12 10	8	6	2	22 23	11	19 5	18 21	4	1	
1					х		х	х																0	1
4									х														0		4
18 21																						0			18 21
19 5		х								x				x							0				9 15
11															х					0					11
22 23											x								0						22 23
2												х						0						х	2
6			х	х					X				х				0								6
8				х					х					х		0									8
10 12						x		х	х						0										10 12
9 13								х	х					0											9 13
7			х	х					х				0												7
3	х				х							0												х	3
24		х	х								0														24
20		х			х					0															20
14									0														х	х	14
Hc								0	х																Hc
Hb Ha							0		x																Hb Ha
N						0																			N
D					0																				D
Α				0																					Α
В			0																						В
С		0							х																С
Е	0																								Е
	Е	С	В	A	D	N	Hb Ha	Hc	14	20	24	3	7	9 13	12 10	8	6	2	22 23	11	9 15	18 21	4	1	

## b) 0.4 wt%

			, ,				,																		
	С	В	E	А	D	N	Hb Ha	Hc	14	20	24	3	7	9 13	12 10	8	6	2	22 23	11	19 5	18 21	4	1	
1																		х						0	1
4																							0		4
18 21																						0			18 21
19 5																					0				9 15
11																				0					11
22 23																			0						22 23
2																		0						х	2
6													х				0								6
8														х		0									8
10 12															0										10 12
9 13														0		х									9 13
7													0												7
3												0					х								3
24											0														24
20					x					0															20
14									0																14
Hc								0						х	х										Hc
Hb Ha							0																		Hb Ha
N						0																			N
D					0							х													D
Α				0									x			x									Α
Е			0									x													В
В		0									х						x								С
С	0										х														Е
	Е	С	В	A	D	N	Hb Ha	Hc	14	20	24	3	7	9 13	12 10	8	6	2	22 23	11	9 15	18 21	4	1	

SI Table 2. NOESY contacts for FF (1.8 wt% solution). All the contacts correspond to negative NOE effects.  $^{11}$ 

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	
1	0						х	х								Х	х			х	х	х	х	1
2	1	0	х	х	х													х	х	х	х	х	х	2
3		1	0	х	Х												Į.	х					х	3
4				0														х	х			х	x	4
5				-	0	х												Х						5
6						0												x		10				6
7		8					0									х	х						х	7
8	- 3						-	0								х				ó		х	x	8
9									0						х	х								9
10		3							-	0										х	х	х	х	10
11											0									Х	Х	х	х	11
12												0					2						V.	12
13													0							х	х	х	x	13
14														0						X	х	х	X	14
15															0	-							9	15
16		8													0	0				ĵ.		х	х	16
17																	0	X			X	X	X	17
18																		0						18
19	1		C P		1					2					9		1		0	2			х	19
20																				0		х	х	20
21					-										7						0	- "		21
22																				0		0	171	22
23																							0	23