Supporting Information

Spectroscopic in situ detection of amyloid fibrils at acidic pH by the fluorophore NIAD-4

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1. Identification of designed polypeptides by ESI-TOF mass spectrometry

All products were identified by high resolution mass spectra recorded on the Agilent 6210 ESI-TOF mass spectrometer (Agilent Technologies, Santa Clara, CA, USA). For the measurements the samples were dissolved in acetonitrile/water (1/1) containing 0.1% TFA and injected directly into the spray chamber by using a syringe pump with flow rates of 10 to 50 μ L/min. The spray voltage was 4000 V. The flow rate pressure of the drying nitrogen gas was set to 1 psi.

Table	S 1	Identification	ofsi	inthesized	nol	vne	ntides	h٦	FSLTOF	mass s	nectrometry	v
I able	S 1.	Identification	01 5	Innesizeu	por	ype	plues	Uy	LOI-IOF	mass s	pectrometri	y

	Observed		Calculated		
Model Peptides	[M+3H]3+	[M+4H]4+	[M+3H]3+	[M+4H]4+	
VW19	1075.9990	807.2511	1075.9863	807.2417	
RR01	1076.6289	807.7241	1076.6180	807.7155	

2. HPLC spectra of pure RR01 and VW19



Figure S1 HPLC chromatogram of peptide VW19 performed at 220 nm using a linear gradient of water/acetontitril/0.1% trifluoroacetic acid (5% to 70% acetonitril) and a C8 (10 μ m) Phenomenex® LUNATM column (Phenomenex Inc. Torrance, CA, USA).



Figure S2 HPLC chromatogram of peptide RR01 performed at 220 nm using a linear gradient of water/acetontitril/0.1% trifluoroacetic acid (5% to70% acetonitril) and a C8 (10 μ m) Phenomenex® LUNATM column (Phenomenex Inc. Torrance, CA, USA).

3. CD and ThT and NIAD-4 fluorescence spectra of RR01



Figure S3 (a) Change of emission spectra of a 10 μ M ThT solution in phosphate buffer (10 mM, pH 7.4, 0.1% NaN₃) in the presence of 200 μ M peptide 2 with the time of incubation. (b) Change of emission spectra of a 10 μ M NIAD-4 solution in phosphate buffer (10 mM, pH 7.4, 0.1% NaN₃) in the presence of 200 μ M peptide 2 with the time of incubation. (c) Change of CD spectra of a 200 μ M peptide 2 solution in phosphate buffer (10 mM, pH 7.4, 0.1% NaN₃) with the time of incubation.