

Supporting Information

Characterization of the spherical intermediates and fibril formation of hCT in HEPES solution using solid-state ^{13}C -NMR and transmission electron microscopy

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Table S1. ^{13}C chemical shifts (ppm from TMS) and assignment of Wt-hCT monomers and fibrils.

pH/ sample		Labeling positions							
		C=O				CH ₃			
		Gly10		Phe22 ^d		Ala26		Ala31 ^d	
5.6	monomer ^a	171.8	α -helix			16.9	random coil		
	fibril ^b	169.6	β -sheet			19.2	β -sheet ^e		
						16.9	random coil		
						19.4	β -sheet		
7.5 ^c	monomer ^a					16.9	random coil	17.2	random coil
	fibril ^b	169.1	β -sheet	168.8	β -sheet	18.7	β -sheet	17.0	random coil
				171.5	random coil ^e			18.8	β -sheet ^e
4.1 ^f	monomer ^a	171.8	α -helix	171.4	random coil	16.9	random coil	17.2	random coil
	fibril ^b	169.4	β -sheet	171.4	random coil	16.9	random coil	17.2	random coil
		171.8	α -helix			19.1	β -sheet		
~ 3.3 ^c	monomer ^a	171.8	α -helix	171.4	random coil	16.9	random coil	17.2	random coil
	fibril ^b	169.9	β -sheet	170.1	β -sheet	16.9	random coil	17.3	random coil ^e
						19.3	β -sheet	19.7	β -sheet
						21.3	β -sheet		
Standard		171.6	α -helix	175.2	α -helix	14.9	α -helix		
		170.9	random coil	173.2	random coil	16.9	random coil		
		168.5	β -sheet	169.0	β -sheet	20.3	β -sheet		

^a: Observed in DD-MAS spectra.

^b: Observed in CP-MAS spectra.

^c: Reference 20.

^d: Assigned taking neighboring Pro into consideration (see text).

^e: Shoulder or minor peaks.

^f: Reference 22.

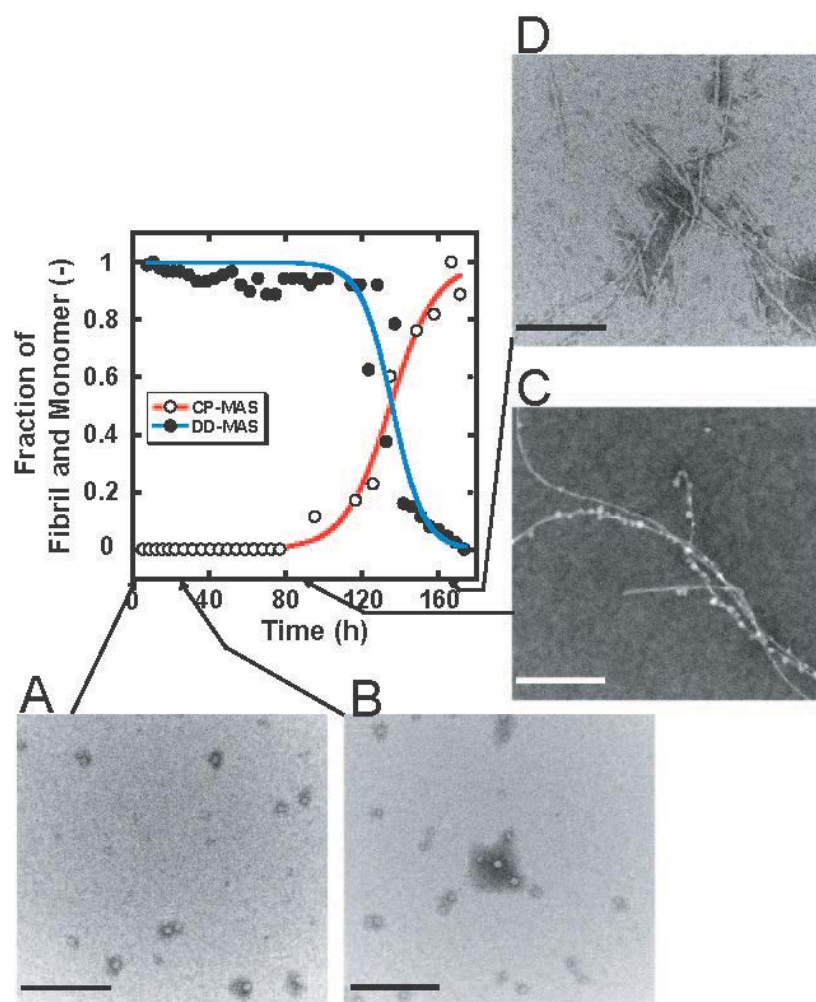


Figure S1. Change in CP-MAS and DD-MAS ^{13}C -NMR signal intensities over time and TEM images taken at (A) 0, (B) 24, (C) 91, and (D) 163 h. The scale bars represent 100 nm. hCT fibrils of 40 mg/ml were grown at pH 5.6 in 20 mM HEPES solution (20 °C).

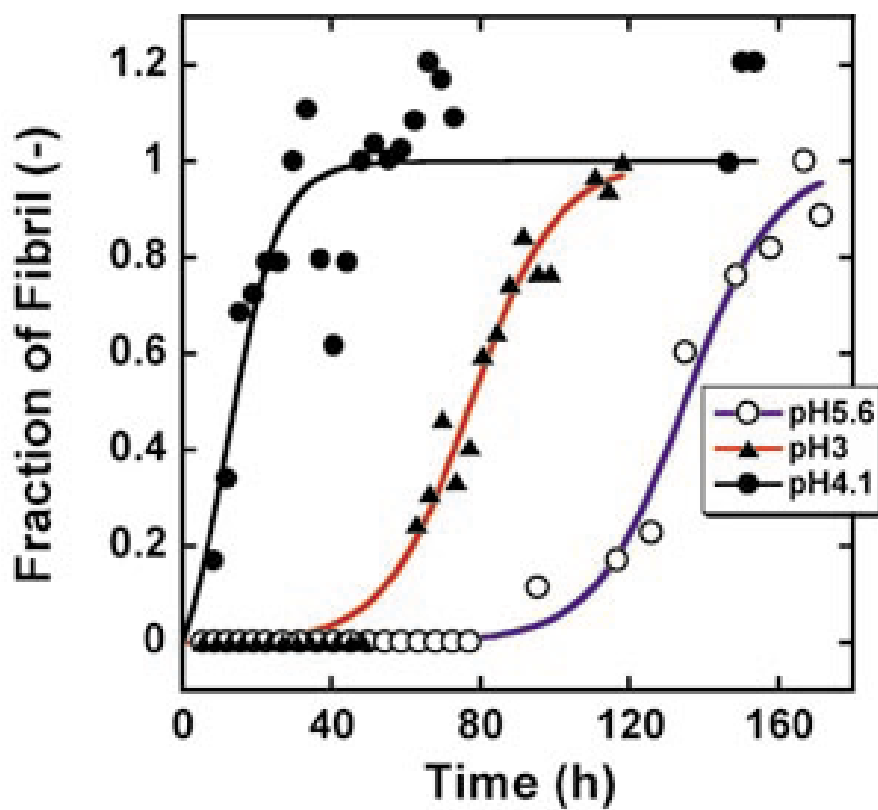


Figure S2. Formation of hCT fibrils over time in acidic solutions (pH 4.1²² and pH 3²⁰) and in HEPES solution at pH 5.6.