

SUPPORTING INFORMATION AVAILABLE

Table 1. Analysis of the main components of the amide I' band for ADA2h variants.

WT								I23V							
Initial		t = 3 min		t = 8 min		t = 35 min		Initial		t = 3 min		t = 8 min		t = 35 min	
Position (cm ⁻¹)	Area (%)	Position (cm ⁻¹)	Area (%)	Position (cm ⁻¹)	Area (%)	Position (cm ⁻¹)	Area (%)	Position (cm ⁻¹)	Area (%)	Position (cm ⁻¹)	Area (%)	Position (cm ⁻¹)	Area (%)	Position (cm ⁻¹)	Area (%)
1646.4	30.3	1644.8	28.9	1644.0	24.3	1641.6	23.2	1644.5	24.1	1645.4	20.1	1644.5	21.4	1644.3	23.5
1632.2	27.0	1631.2	24.1	1629.0	17.5	1628.0	21.2	1630.2	27.9	1632.3	26.5	1631.1	22.5	1629.5	21.3
1619.3	14.3	1619.3	14.4	1617.3	18.1	1616.9	25.4	1617.8	18.6	1619.2	24.4	1617.8	21.5	1616.7	21.8
N58A								F65A							
Initial		t = 3 min		t = 8 min		t = 35 min		Initial		t = 3 min		t = 8 min		t = 35 min	
Position (cm ⁻¹)	Area (%)	Position (cm ⁻¹)	Area (%)	Position (cm ⁻¹)	Area (%)	Position (cm ⁻¹)	Area (%)	Position (cm ⁻¹)	Area (%)	Position (cm ⁻¹)	Area (%)	Position (cm ⁻¹)	Area (%)	Position (cm ⁻¹)	Area (%)
1646.5	23.4	1646.2	21.5	1644.1	19.8	1642.6	22.6	1642.3	23.8	1643.1	22.0	1643.2	19.8	1641.4	24.0
1632.7	29.0	1632.9	27.3	1630.8	23.0	1629.2	19.7	1628.2	29.4	1629.4	28.3	1628.8	27.4	1628.6	18.8
1619.6	20.3	1619.8	20.6	1617.9	25.3	1616.7	20.4	1617.8	18.6	1619.2	24.4	1617.4	24.0	1616.7	21.8

Changes in position and area of the main bands of the spectra of ADA2h variants at the most remarkable times of the amyloid fibril formation kinetics at pD 3. These bands are representative of the initial protein (1632 and 1647 cm⁻¹) and the fibrillated form (1619 main cm⁻¹). The main changes upon aggregation are associated with the 1619 cm⁻¹ band, which increases in area; whereas the bands associated with the native β -sheet and α -helices suffer a decrease in their area.

Table 2. Analysis of the minor components of the amide I' band for ADA2h variants.

WT								I23V							
Initial		t = 3 min		t = 8 min		t = 35 min		Initial		t = 3 min		t = 8 min		t = 35 min	
Position (cm ⁻¹)	Area (%)	Position (cm ⁻¹)	Area (%)	Position (cm ⁻¹)	Area (%)	Position (cm ⁻¹)	Area (%)	Position (cm ⁻¹)	Area (%)	Position (cm ⁻¹)	Area (%)	Position (cm ⁻¹)	Area (%)	Position (cm ⁻¹)	Area (%)
1682.4	5.0	1683.4	4.1	1682.1	7.8	1683.4	4.4	1684.3	3.2	1683.7	3.8	1683.4	6.4	1683.6	5.9
1671.2	8.2	1671.6	11.4	1670.3	9.2	1672.9	9.1	1671.3	10.6	1670.4	10.4	1670.0	10.9	1669.8	9.6
1660.1	15.2	1658.7	17.1	1659.8	18.5	1659.0	16.7	1658.7	15.6	1658.2	14.8	1658.2	17.0	1657.9	17.9
N58A								F65A							
Initial		t = 3 min		t = 8 min		t = 35 min		Initial		t = 3 min		t = 8 min		t = 35 min	
Position (cm ⁻¹)	Area (%)	Position (cm ⁻¹)	Area (%)	Position (cm ⁻¹)	Area (%)	Position (cm ⁻¹)	Area (%)	Position (cm ⁻¹)	Area (%)	Position (cm ⁻¹)	Area (%)	Position (cm ⁻¹)	Area (%)	Position (cm ⁻¹)	Area (%)
1681.0	5.3	1681.5	6.6	1683.5	4.7	1683.5	5.6	1682.6	1.2	1682.7	1.6	1683.3	3.4	1683.5	4.6
1669.6	8.6	1669.3	9.8	1670.9	11.3	1670.9	12.7	1672.2	9.9	1672.3	10.9	1671.6	10.6	1671.2	11.4
1658.9	13.4	1658.4	14.2	1658.3	15.6	1657.8	19.0	1657.6	16.9	1657.8	16.7	1658.2	16.9	1657.7	19.3

Changes in position and area of the high-frequency component of the aggregated β -sheet (1682 cm⁻¹) and the components related to β -turns (1660 and 1671 cm⁻¹) of the spectra of ADA2h variants at the most remarkable times of the amyloid fibril formation kinetics. The changes of the 1682 cm⁻¹ component prove to be related to the ones experimented by the 1619 cm⁻¹ component.

Figure 1. Kinetics of the formation of amyloid fibrils by 4 variants of ADA2h followed by FT-IR. 3-D plots of the evolution of the deconvolved amide I' spectra of ADA2h WT (A) and the mutants I23V (B), N58A (C) and F65A (D) at acidic pH, using heat as the inductor.

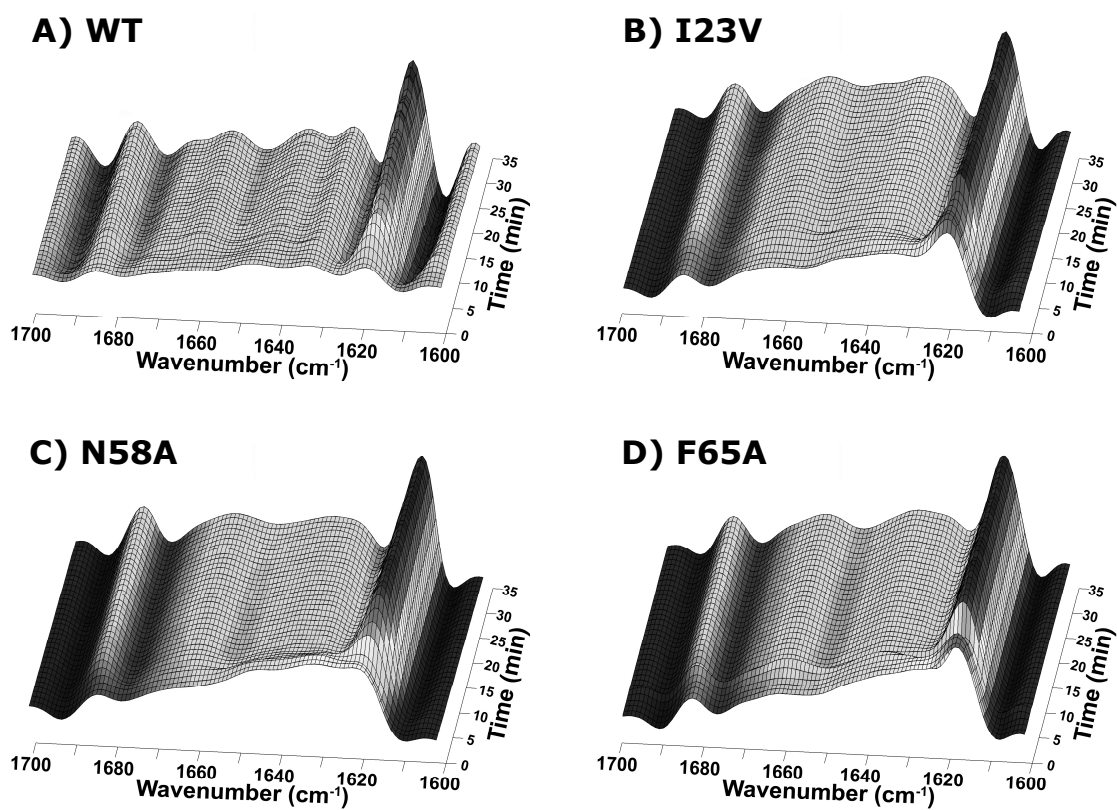


Figure 2. Plots showing variations in position and area of the main bands in amyloid-formation kinetics at acidic pD. The changes in position of the most significant bands, 1619 cm^{-1} (A), 1632 cm^{-1} (C) and 1647 cm^{-1} (E), are plotted against time for each mutant. The changes in area of these bands; 1619 cm^{-1} (B), 1632 cm^{-1} (D) and 1647 cm^{-1} (F) are also represented along the kinetics. Although the bands do change their position along time, they have been named only with the most relevant wavenumber for the sake of clarity. See Table 1 in the Supplementary material for further information regarding positions and areas of these bands. The changes in position and area of the 1619 cm^{-1} band are highlighted for the WT protein. A two-step transition in the area of the 1619 cm^{-1} band can be observed.

