Electronic Supplementary Material (ESI) for Soft Matter.

Supporting information

The influence of amino acid sequence on structure and morphology of polydiacetylene containing peptide fibres

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Protocol for Chlorine/TDM detection on TLC plates:

Three solution have been prepared:

A: Dissolve 2.5 g 4,4'-tetramethyldiaminodiphenylmethane in 10 mL acetic acid and dilute with 50 mL water (filtrate off any insolubles)

B: Dissolve 5 g KI in 100 mL water

C: Dissolve 300 mg ninhydrin in 100 mL n-butanol and add 3 mL glacial acetic acid

The staining solution is prepared by mixing solution A and B and subsequently adding 1.5 mL of solution C. The TLC dry plate is first exposed for 10 seconds to a chlorine atmosphere after which it is sprayed with or dipped in the staining solution. Amide (NH) containing compounds will give a blue stain.

This protocol is adapted from E. V. Arx, M. Faupel and M. Brugger, J. Chromatogr., **1976**, 120, 224-228.

Analysis PAs:

$C_{24}H_{41}C(O)$-Gly-Ala-Gly-Ala-Gly-OH (GGo):

TLC: R_f 0.33 (eluent: MeOH/ $CHCl_3$/ H_2O (25:65:4).

^{1}H-NMR [DMSO-d6]: δ 0.85 (t, 3H), 1.24 (m, 32H), 1.44 (m, 6H), 2.11 (t, 2H), 2.27 (t, 4H), 3.5 (m, 6H), 4.23 (m, 2H), 7.41 (s, 1H), 8.25 (d, 1H), 8.35 (m, 2H), 8.49 (t, 1H). Mass spectrometry: Calc for $[C_{37}H_{61}N_5O_7 + Na]^+$ 710.4469, found 710.4479.

$C_{24}H_{41}C(O)$-Gly-Ala-Gly-Ala-Gly-NH_2 (GGn):

TLC: R_f 0.50 (eluent: MeOH/ $CHCl_3$/ H_2O (25:65:4).

^{1}H-NMR [DMSO-d6]: δ 0.85 (t, 3H), 1.29 (m, 32H), 1.44 (m, 6H), 2.10 (t, 2H), 2.27 (t, 4H), 3.61 (m, 6H), 4.22 (dt, 2H), 7.06 (s, 1H), 7.16 (s, 1H), 7.99 (t, 2H), 8.09 (t, 2H), 8.20 (t, 1H). Mass spectrometry: Calc for $[C_{37}H_{62}N_6O_6 + Na]^+$ 709.4629, found 709.4615.

$C_{24}H_{41}C(O)$-Gly-Ala-Gly-Ala-Glu-OH (GEo):

TLC: R_f 0.12 (eluent: MeOH/ $CHCl_3$/ H_2O (25:65:4).

^{1}H-NMR [DMSO-d6]: δ 0.85 (t, 3H), 1.24 (m, 32H), 1.44 (m, 6H), 1.66 (m, 1H), 1.84 (m, 1H), 2.10 (t, 2H), 2.16 (t, 2H), 2.27 (t, 4H), 3.68 (m, 4H), 4.00 (m, 1H), 4.24 (m, 2H), 7.75 (d, 1H), 8.01 (d, 1H), 8.33 (m, 3H). Mass spectrometry: Calc for $[C_{40}H_{65}N_5O_9 + H]^+$ 760.4861, found 760.4866.

$C_{24}H_{41}C(O)$-Gly-Ala-Gly-Ala-Glu-NH_2 (GEn):

TLC: R_f 0.20 (eluent: MeOH/ $CHCl_3$/ H_2O (25:65:4).

^{1}H-NMR [DMSO-d6]: δ 0.85 (t, 3H), 1.24 (m, 32H), 1.44 (m, 6H), 1.80 (m, 2H), 2.10(t, 4H), 2.27 (t, 4H), 3.69 (m, 4H), 3.90 (m, 1H), 4.11 (m, 1H), 4.22 (m, 1H), 6.90 (s, 1H), 6.95 (s, 1H), 8.02 (d, 1H), 8.18 (t, 1H), 9.02 (s, 1H), 0.88 (s, 1H), 9.55 (s, 1H).

Mass spectrometry: Calc for $[C_{40}H_{66}N_6O_8 + Na]^+$ 781.4840, found 781.4842.

$C_{24}H_{41}C(O)$-Glu-Ala-Gly-Ala-Gly-OH (EGo):

TLC: R_f 0.56 (eluent: MeOH/ $CHCl_3$/ H_2O (25:65:4).

^{1}H-NMR [DMSO-d6]: δ 0.85, 1.24, 1.44, 1.72, 1.86, 2.01, 2.10, 2.19, 2.27, 2.33, 2.64, 2.84, 3.03, 3.17, 3.51, 3.61, 3.67, 5.24, 6.69, 7.10, 7.16, 7.50, 7.69, 8.00, 8.10, 8.22, 9.4. Mass spectrometry: Calc for $[C_{40}H_{65}N_5O_9 + Na]^+$ 782.4680, found 782.4665.

$C_{24}H_{41}C(O)$-Glu-Ala-Gly-Ala-Gly-NH_2 (EGn):

TLC: R_f 0.14 (eluent: MeOH/ $CHCl_3$/ H_2O (25:65:4).

^{1}H-NMR [DMSO-d6]: δ 0.85 (t, 3H), 1.24 (m, 32H), 1.44 (m, 6H), 1.75 (m, 1H), 1.83 (m, 1H), 2.09 (m, 4H), 2.66 (t, 4H), 3.65 (m, 4H), 3.80 (m, 1H), 4.22 (m, 2H), 7.00 (s, 1H), 7.23 (s, 1H), 8.05 (d, 1H), 8.12 (d, 1H), 8.16 (d, 1H), 8.53 (s, 1H). Mass spectrometry: Calc for $[C_{40}H_{66}N_6O_8 + Na]^+$ 781.4840, found 781.4831.

$C_{24}H_{41}C(O)$-Gly-Ala-Gly-Ala-Lys-OH (GKo):

TLC: R_f 0.79 (eluent: MeOH/ $CHCl_3$/ H_2O (25:65:4).

^{1}H-NMR [DMSO-d6]: δ 0.85 (t, 3H), 1.24 (m, 34H), 1.44 (m, 9H), 1.69 (m, 1H), 2.11 (t, 2H), 2.27 (t, 4H), 2.75 (t, 2H), 3.70 (m, 3H), 4.02 (q, 1H), 4.13 (m, 1H) 4.22 (m, 2H), 7.77 (s,

2H), 7.88 (d, 1H), 8.02 (t, 1H), 8.11 (d, 1H), 8.13 (d, 1H), 8.21 (t, 1H). Mass spectrometry: Calc for $[C_{41}H_{70}N_6O_7 + H]^+$ 759.5384, found 759.5360.

$C_{24}H_{41}C(O)$-Gly-Ala-Gly-Ala-Lys-NH_2 (GKn):

TLC: R_f 0.34 (eluent: MeOH/ $CHCl_3$/ H_2O (25:65:4).

^{1}H-NMR [DMSO-d6]: δ 0.85 (t, 3H), 1.24 (m, 34H), 1.44 (m, 9H), 1.69 (m, 1H), 2.11 (t, 2H), 2.27 (t, 4H), 2.75 (t, 2H), 3.70 (m, 3H), 4.02 (q, 1H), 4.13 (m, 1H) 4.22 (m, 2H), 7.03 (s, 1H), 7.17 (s, 1H), 7.71 (s, 2H), 7.83 (d, 1H), 8.03 (t, 1H), 8.15 (d, 1H), 8.27 (t, 1H). Mass spectrometry: Calc for $[C_{41}H_{71}N_7O_6 + H]^+$ 758.5544, found 758.5522.

$C_{24}H_{41}C(O)$-Lys-Ala-Gly-Ala-Gly-OH (KGo):

TLC: R_f 0.55 (eluent: MeOH/ $CHCl_3$/ H_2O (25:65:4).

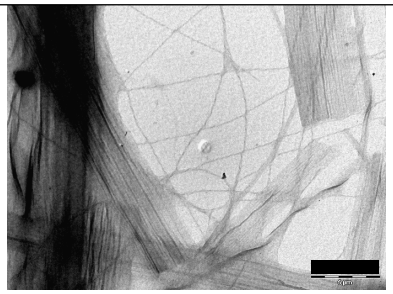
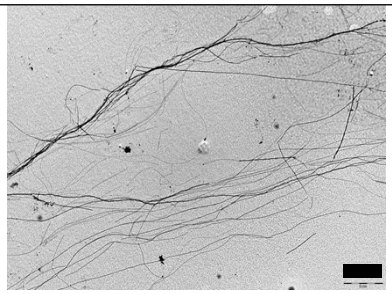
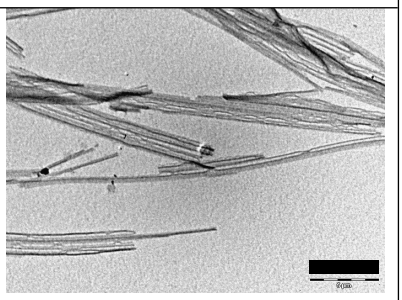
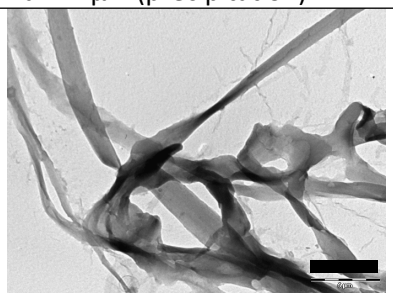
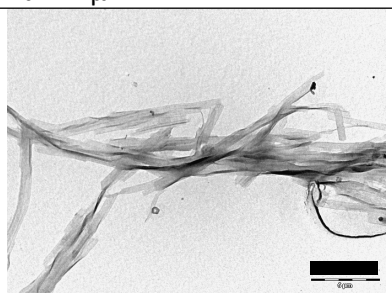
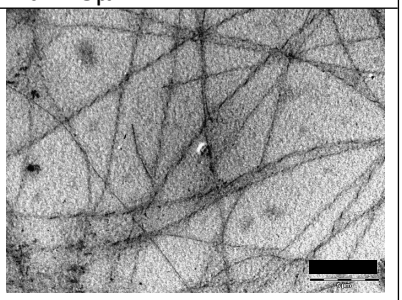
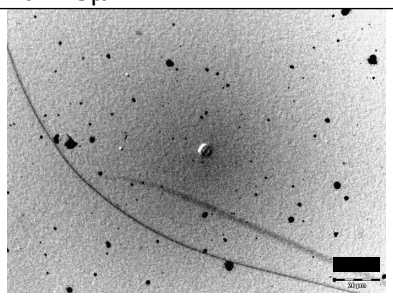
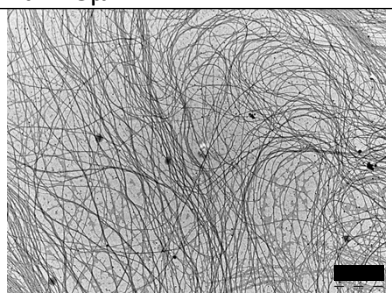
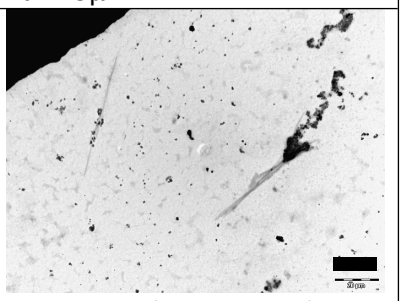
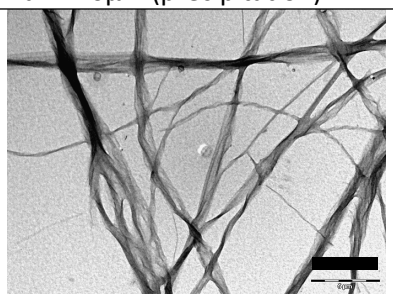
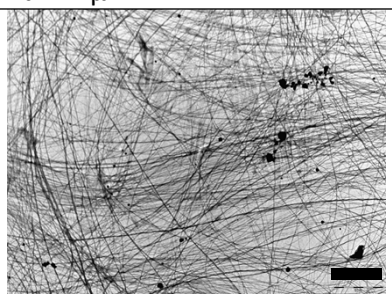
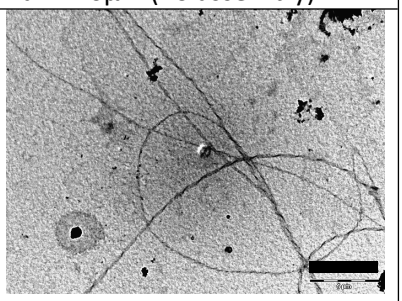
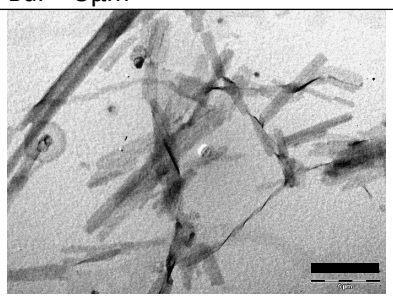
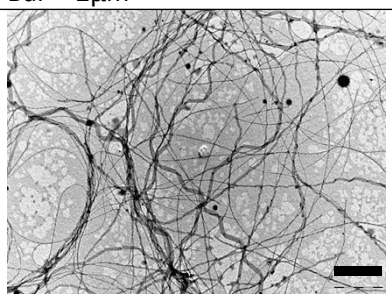
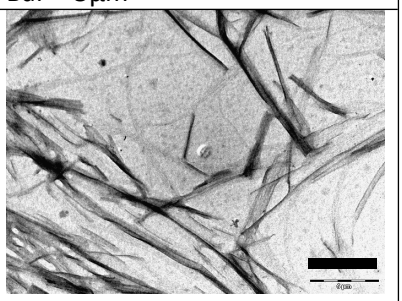
^{1}H-NMR [DMSO-d6]: δ 0.85 (t, 3H), 1.24 (m, 34H), 1.44 (m, 9H), 1.64 (m, 1H), 2.10 (t, 2H), 2.27 (t, 4H), 2.74 (t, 2H), 3.66 (m, 1H), 3.82 (m, 1H), 4.25 (m, 3H), 6.64 (s, 1H), 7.20 (s, 1H), 7.40 (s, 1H) 7.82 (s, 1H), 7.95 (d, 1H), 8.22 (d, 1H), 8.30 (d, 1H). Mass spectrometry: Calc for $[C_{41}H_{70}N_6O_7 + H]^+$ 759.5384, found 759.5378.

$C_{24}H_{41}C(O)$-Lys-Ala-Gly-Ala-Gly-NH_2 (KGn):

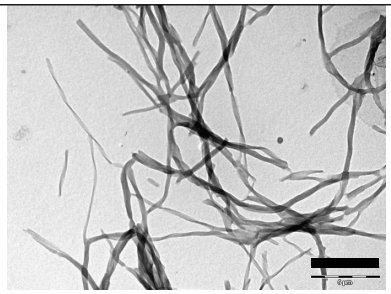
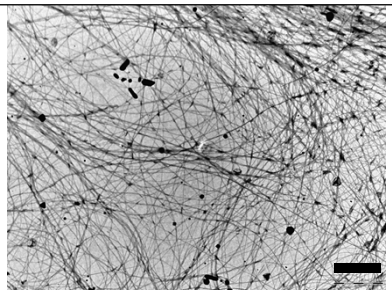
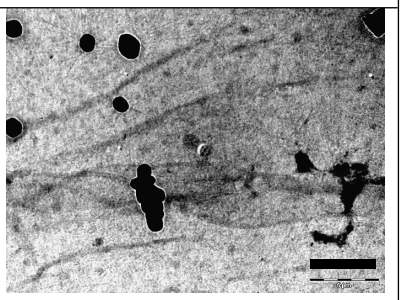
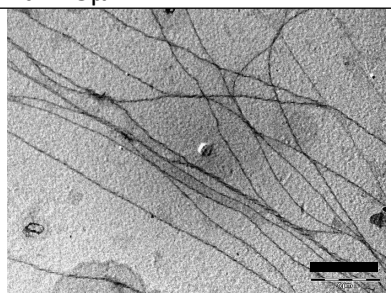
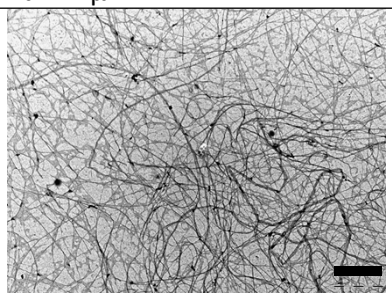
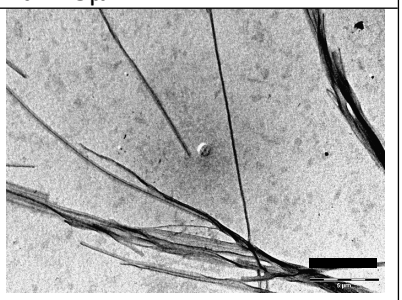
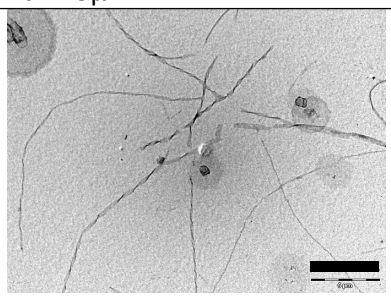
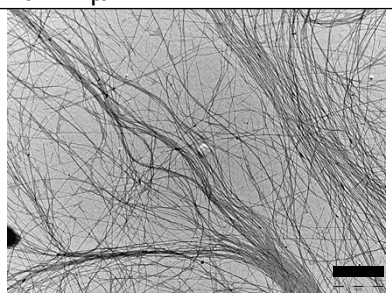
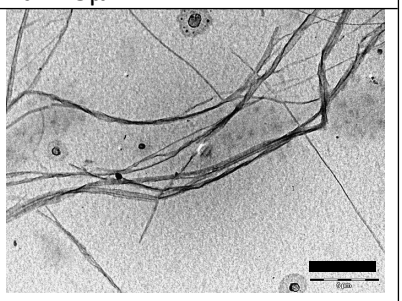
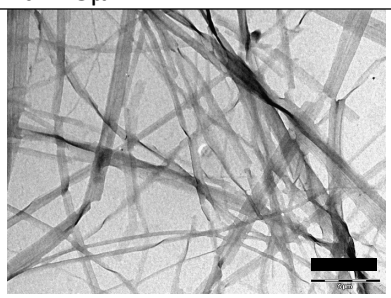
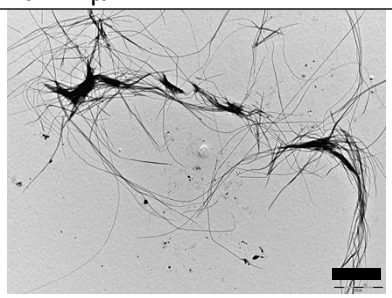
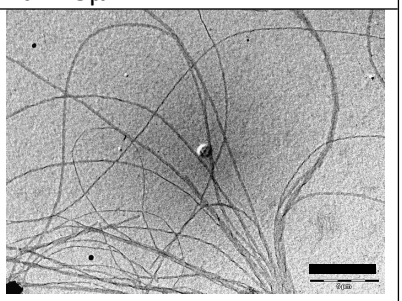
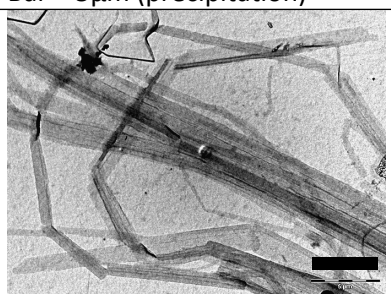
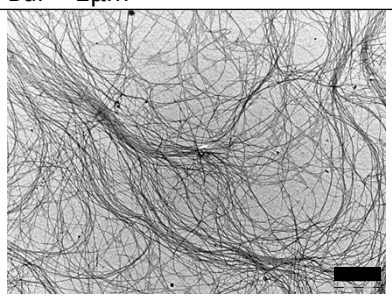
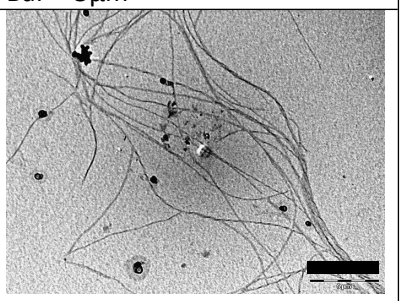
TLC: R_f 0.45 (eluent: MeOH/ $CHCl_3$/ H_2O (25:65:4).

^{1}H-NMR [DMSO-d6]: δ 0.85 (t, 3H), 1.24 (m, 34H), 1.44 (m, 9H), 1.64 (m, 1H), 2.10 (t, 2H), 2.27 (t, 4H), 2.74 (t, 2H), 3.70 (m, 4H), 4.24 (m, 3H), 7.07 (s, 1H), 7.18 (s, 1H), 7.73 (s, 2H), 7.92 (d, 1H), 8.05 (d, 1H), 8.08 (d, 1H), 8.14 (q, 2H). Mass spectrometry: Calc for $[C_{41}H_{71}N_7O_6 + H]^+$ 758.5544, found 758.5515.

Representative TEM picture of PAs at acidic, neutral and basic pH

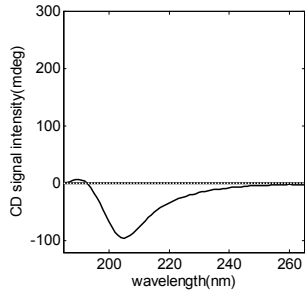
	acidic	Neutral	basic
GGo	 Bar = 4µm (precipitation)	 Bar = 2µm	 Bar = 5µm
GGn	 Bar = 5µm	 Bar = 5µm	 Bar = 5µm
GEo	 Bar = 20µm (precipitation)	 Bar = 2µm	 Bar = 20µm (no assembly)
GEn	 Bar = 5µm	 Bar = 2µm	 Bar = 5µm
EGo	 Bar = 5µm (precipitation)	 Bar = 2µm	 Bar = 5µm

Representative TEM pictures of PAs at acidic, neutral and basic pH

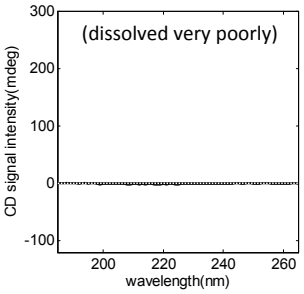
	acidic	Neutral	basic
EGn	 Bar = 5µm	 Bar = 2µm	 Bar = 5µm
GKo	 Bar = 5µm	 Bar = 2µm	 Bar = 5µm
GKn	 Bar = 5µm	 Bar = 2µm	 Bar = 5µm
KGo	 Bar = 5µm (precipitation)	 Bar = 2µm	 Bar = 5µm
KGn	 Bar = 5µm	 Bar = 2µm	 Bar = 5µm

CD spectra:

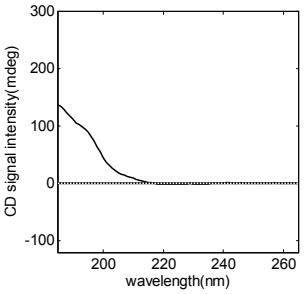
GGo



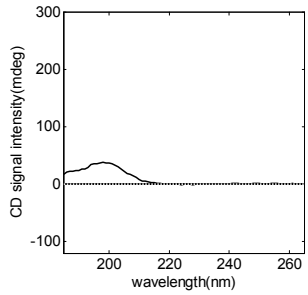
GGn



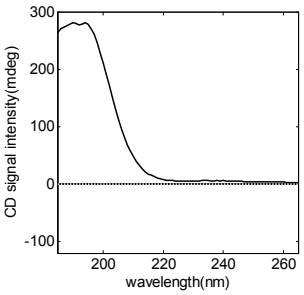
GEo



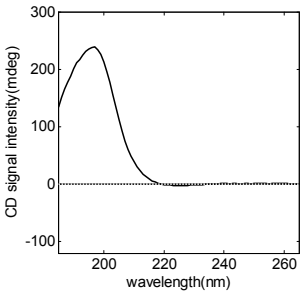
GEn



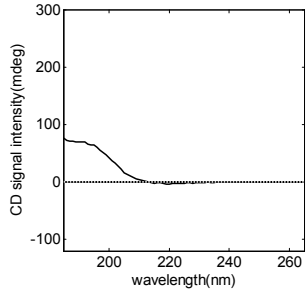
EGo



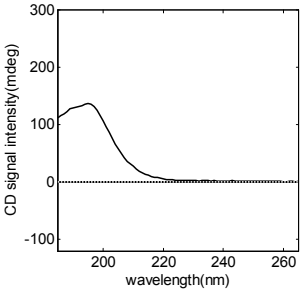
EGn



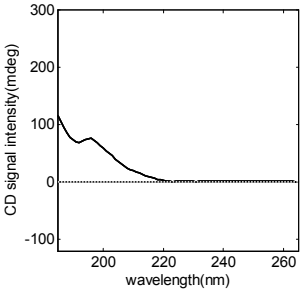
GKo



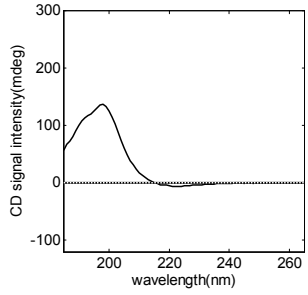
GKn



KGo



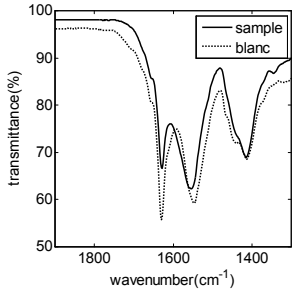
KGn



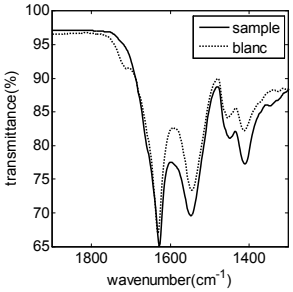
IR spectra:

Sample (solid lines) means lyophilised from water, blanc (dotted lines) means lyophilised from acetic acid.

GGo



GEo



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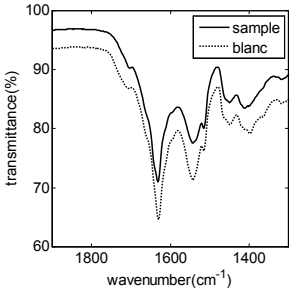

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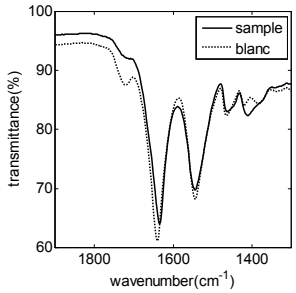

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