Electronic Supplementary Material (ESI) for Soft Matter

Supporting Information

Conductance of Amyloid β Based Peptide Filaments: Structure-Function Relations

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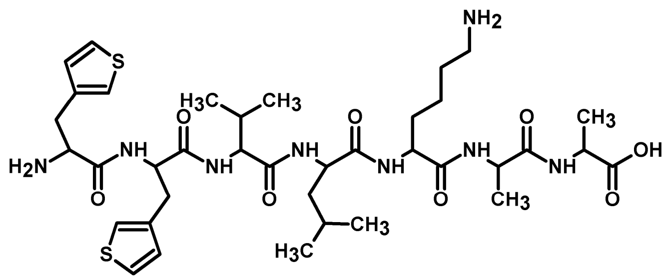
Synthesis of (3-Thi)(3-Thi)VLKAA

Fmoc-alanine-OH, Fmoc-lysine(Boc)-OH, Fmoc-leucine-OH and Fmoc-valine-OH, Fmoc-alanine−Wang resin (0.72 mmol g^{-1} substitution) , HBTU (2-(1H-benzotriazol-1-yl)-1,1,3,3-tetramethyluronium hexafluorophosphate) were purchased from Novabiochem (UK). Fmoc-L-3-Thienylalanine-OH, trifluoroacetic acid (TFA), piperidine and triisopropylsilane were purchased from Sigma-Aldrich. HOBt/DMF (a mixture of 1-hydroxybenzotriazole and dimethylformamide), DIEA/NMP (a mixture of diisopropylethylamine and N-methylpyrrolidone), and NMP were obtained from Applied Biosystems(UK). Water (HPLC grade), acetonitrile (HPLC grade) and diethyl ether were purchased from Fisher Scientific (UK).

The peptide (3-Thi)(3-Thi)VLKAA (Scheme 1) was synthesized by solid phase methods using standard FastMoc chemistry [Fmoc (9-fluorenylmethyloxycarbonyl) protecting group and activation by HBTU /HOBt] on a 0.25 mmol scale with a fully automated peptide synthesizer (433A Applied Biosystems), which allowed for direct conductivity monitoring of Fmoc deprotection. The crude peptide was purified with reverse phase HPLC (Perkin Elemer 200 with a Macherey-Nagel C18 semi-preparative column and a Perkin Elemer Series 200 UV/VIS Detector), followed by lyophilization to give a white solid. ESIMS m/z for $C_{37}H_{58}N_8O_8S_2$ $[M+H]^+$calcd 807.38, found $[M+H]^+$, 807.39; $[M+2H]^{2+}/2$ calcd 404.20, found 404.20.^{1}H NMR (700 MHz methanol-d_4, ppm): 0.96(d, J = 7.0 Hz, 3H), 0.99 (t, J = 7.0 Hz, 9H), 1.42 (dd, J = 19.6 Hz, 7.7 Hz, 6H), 1.49 (m, 2H), 1.58-1.75 (m, 6H), 1.85 (m, 1H), 2.06 (sep, J = 7.0 Hz, 1H), 2.95 (t, J = 7.0 Hz, 2H), 3.03 (dd, J = 14.7 Hz, 8.6 Hz, 1H), 3.14 (dd, J = 14.4 Hz, 7.7 Hz, 1H), 3.18 (dd, J = 14.4 Hz, 5.6 Hz, 1H), 3.28 (dd, J = 15 Hz, 4.2 Hz, 1H), 4.10 (dd, J = 7.7 Hz, 4.9 Hz, 1H), 4.21 (t, J = 7 Hz, 1H), 4.37 (ABq, J_{AB} = 7 Hz, 3H), 4.43 (ABq, J_{AB} = 5.6 Hz, 1H), 4.76 (m, 1H), 7.04 (t, J = 4.2 Hz, 2H), 7.17 (d, J = 2.2 Hz, 1H), 7.27 (d, J = 2.2 Hz, 1H), 7.34 (dd, J = 4.9 Hz, 3.5 Hz, 1H), 7.43 (dd, J = 4.9 Hz, 3.5 Hz, 1H), 8.14, 8.19, and 8.26-8.59(NH, NH_2 10 H).



(3-Thi)(3-Thi)VLKAA

Supporting figures

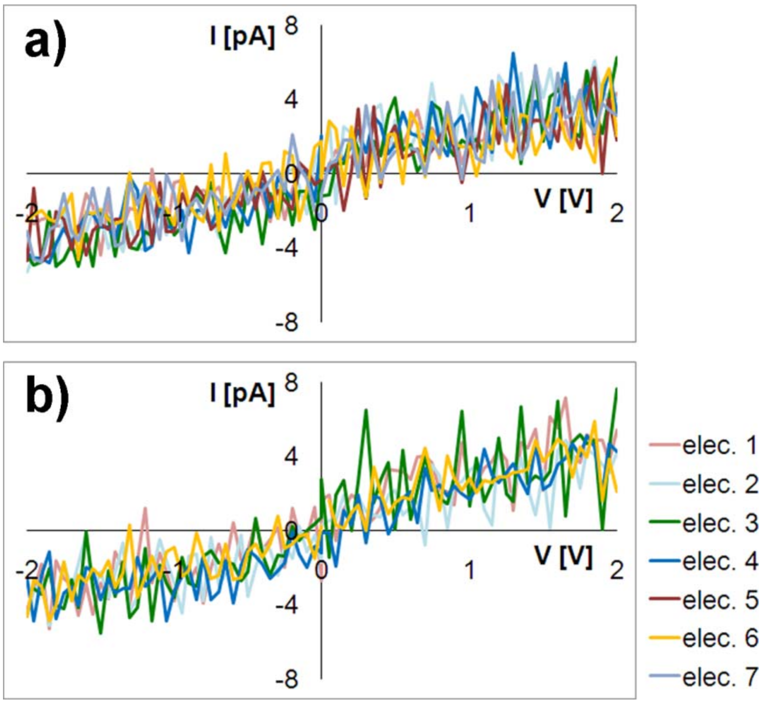
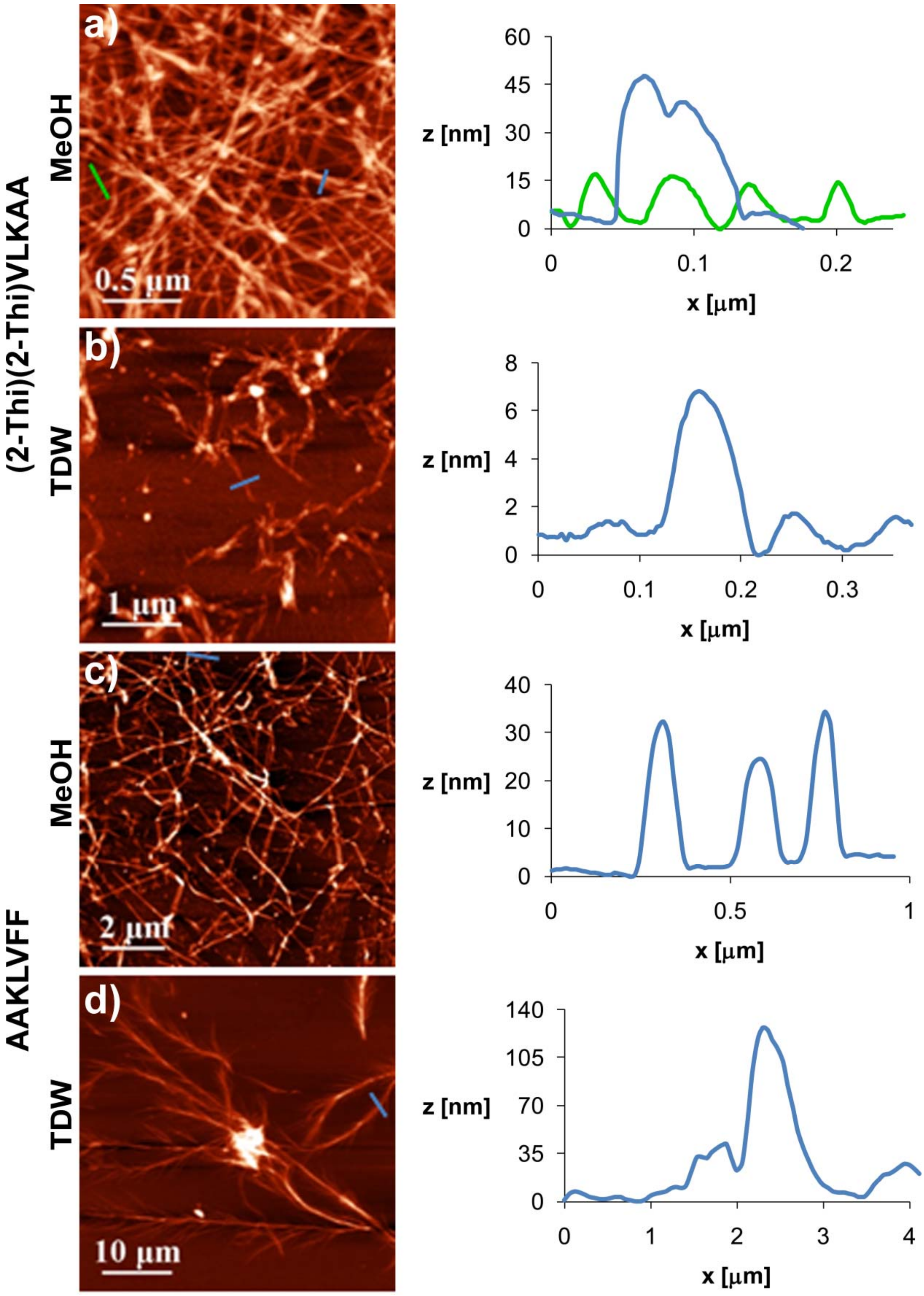


Figure S1. I-V curves of 0.03%wt (2-Thi)(2-Thi)VLKAA assembled in MeOH carried out on **a)** chip 1 and **b)** chip 2 under pressure of 10^{-3} mbar.


(2-Thi)(2-Thi)VLKAA
AAKLVFF
MeOH
TDW
a)
b)
c)
d)
0.5 µm
1 µm
2 µm
10 µm
z [nm]
x [µm]

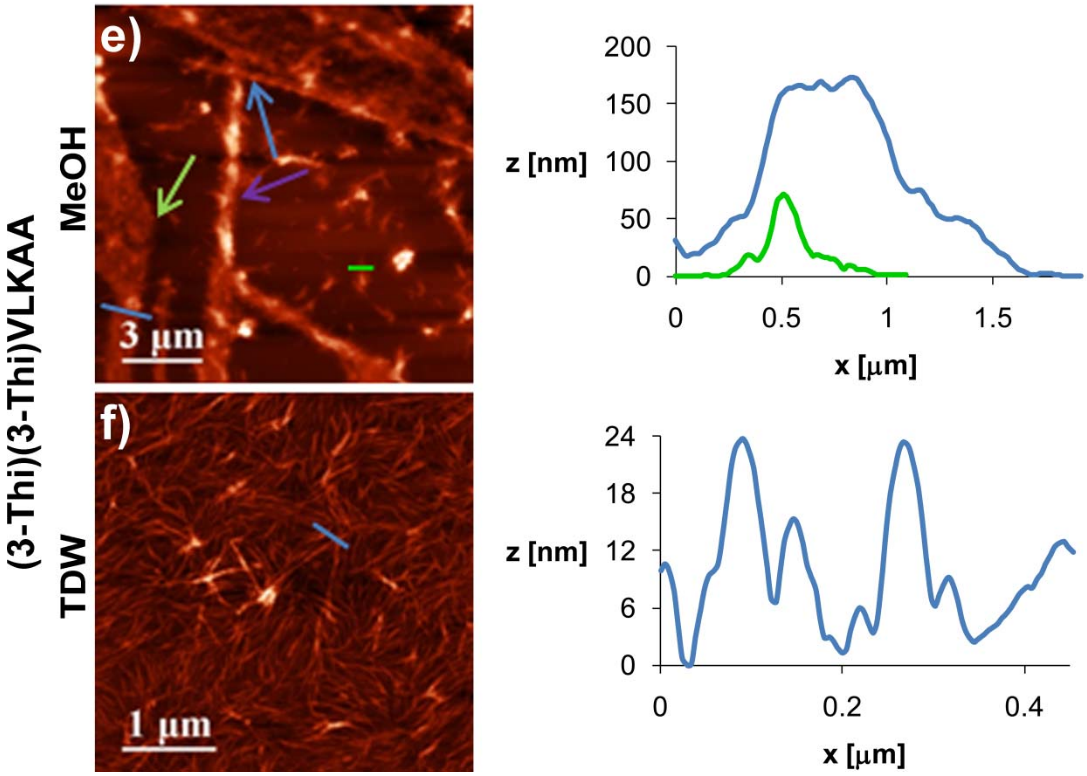


Figure S2. a) AFM height (z scale 88 nm) and the corresponding cross-sections across the blue and green lines of 0.03%wt (2-Thi)(2-Thi)VLKAA assembled in MeOH, showing fibers with diameter of ~45 nm and ~13 nm, respectively. **b)** AFM height (z scale 33 nm) and the corresponding cross-section across the blue line of 0.03%wt (2-Thi)(2-Thi)VLKAA assembled in TDW, showing bundled fibers with diameter of ~6 nm. **c)** AFM height (z scale 86 nm) and the corresponding cross-section across the blue line of 0.03%wt AAKLVFF assembled in MeOH, showing fibers with diameter of ~30 nm. **d)** AFM height (z scale 330 nm) and the corresponding cross-section across the blue line of 0.03%wt AAKLVFF assembled in TDW, showing branched fibers with diameter of ~120 nm. **e)** AFM height (z scale 460 nm) and the corresponding cross-sections across the blue and green lines of 0.03%wt (3-Thi)(3-Thi)VLKAA assembled in MeOH, showing wide tapes with height of ~150 nm (blue line), either folded or twisted (green and purple arrows, respectively), and bundled fibers (blue arrow) with diameter of ~70 nm (green line). **f)** AFM height (z scale 58 nm) and the corresponding cross-section across the blue line of 0.03%wt (3-Thi)(3-Thi)VLKAA assembled in TDW, showing twisted fibers with diameter of ~23 nm.