

Supporting Information

Chemical Environment as Control Element in the Evolution of Shapes - 'Hexagons and Rods' from an 11-Helical $\alpha,\beta^{2,3}$ -hybrid Peptide

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Larger area SEM images:

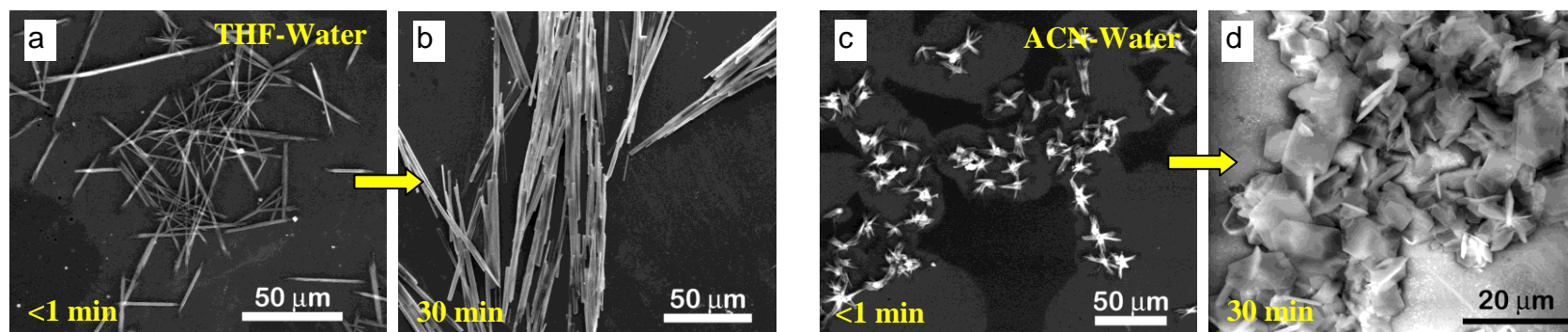


Figure S1. Larger area SEM images a-d) showing the time-dependent morphology changes in the samples of **1**.

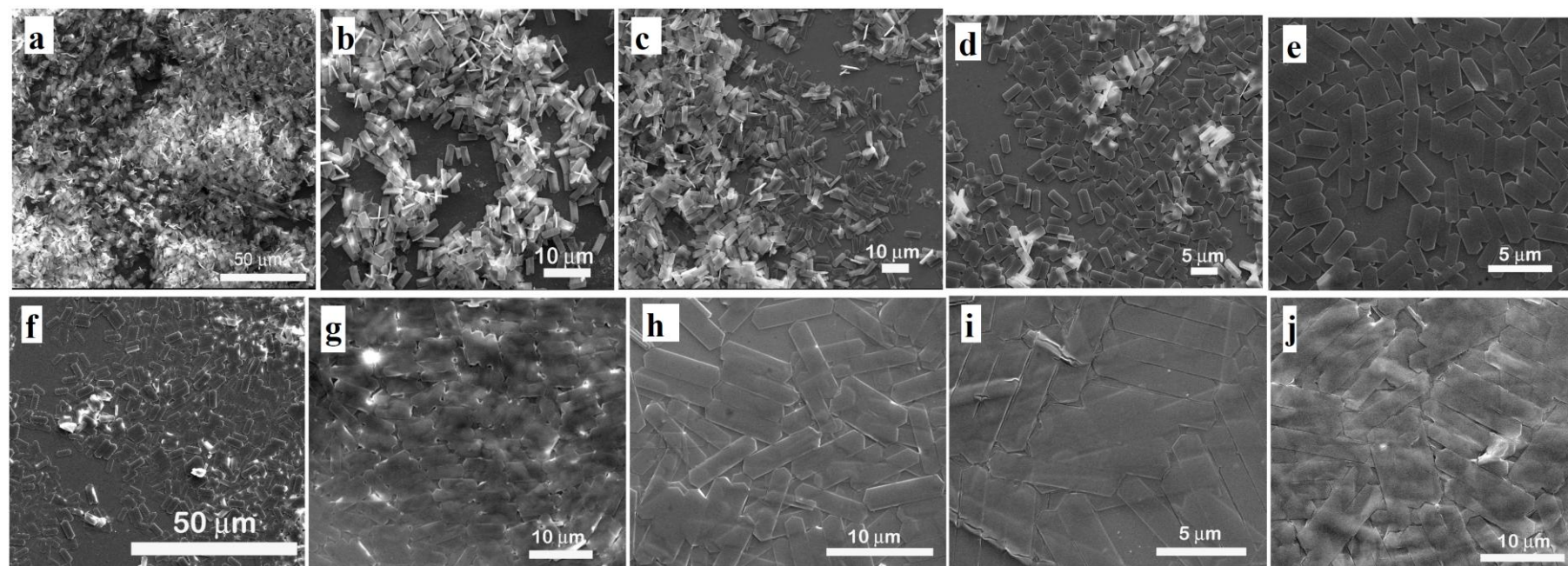


Figure S2. Larger area SEM images of samples of the tetrapeptide **1** formed by the addition of its 1 mg/mL solution in ACN (200 μL) to water containing various concentrations of P123: (a) 0.001, (b) 0.01, (c) 0.05, (d) 0.1, (e) 0.5, (f) 1.0, (g) 2.0, (h) 3.0, (i) 4.0, (j) 5.0 g/L.

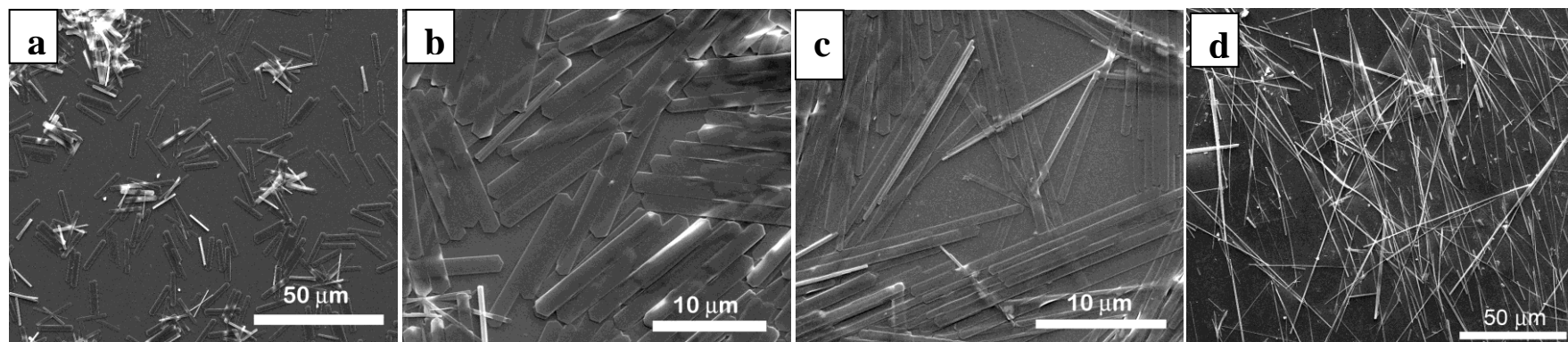


Figure S3. Larger area SEM images showing different morphologies of samples of **1** formed by addition of its 1 mg/mL solution in THF (200 μ L) to water containing various concentrations of P123: (a) 1.0, (b) 2.0, (c) 3.0, (d) 5.0 g/L.

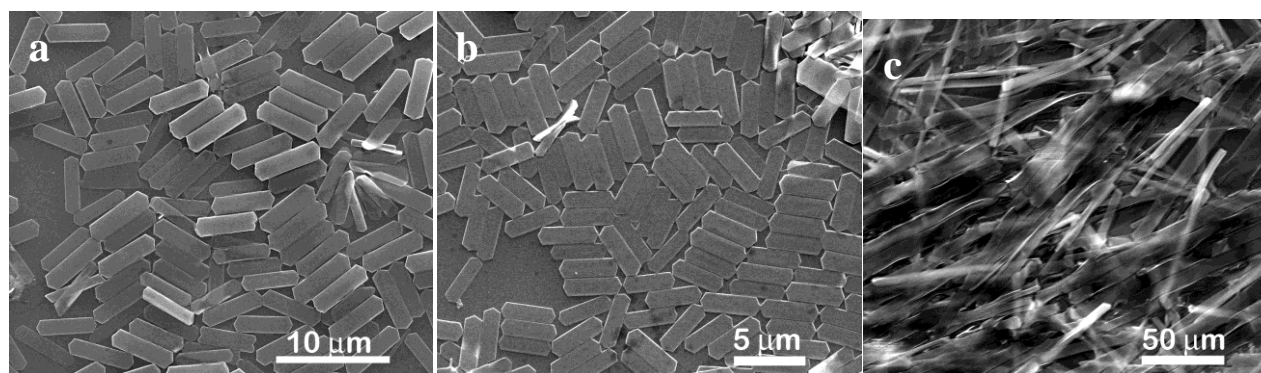


Figure S4. Figures showing the morphology control on sequential use of organic co-solvents during the initiation and propagation phases of aggregation. a) 100 μ L of a 2 mg/mL solution of **1** in ACN was added to 0.1 g/L P123-water (1 mL), and after stirring for 1 min, 100 μ L of THF was added; b) 100 μ L of a 2 mg/mL solution of **1** in THF was added to 0.1 g/L P123-water (1 mL) and after stirring for 1 min, 100 μ L of ACN was added; c) 200 μ L of a 1 mg/mL solution of **1** in 1:1 ACN-THF mixture was added to 0.1 g/L P123-water (1 mL).

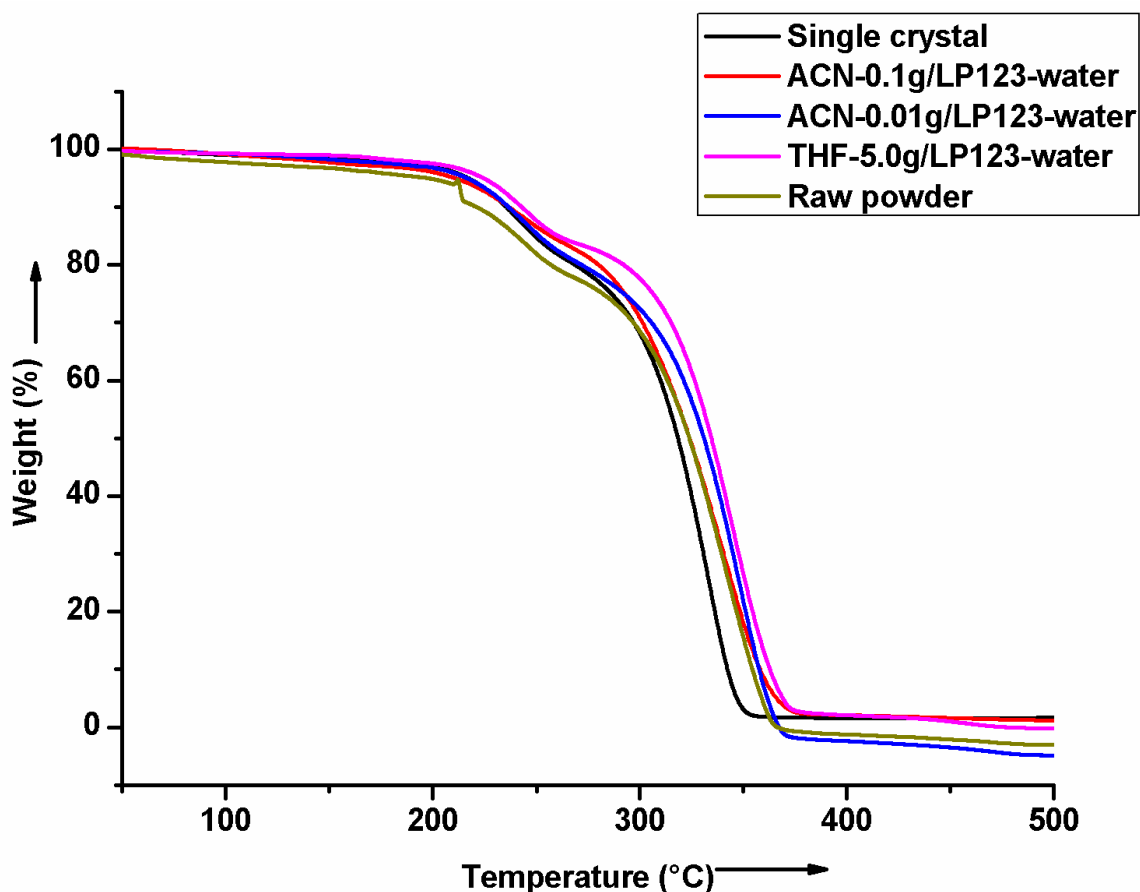


Figure S5. Thermogravimetric analysis (TGA) of aggregates formed from **1** under various conditions.

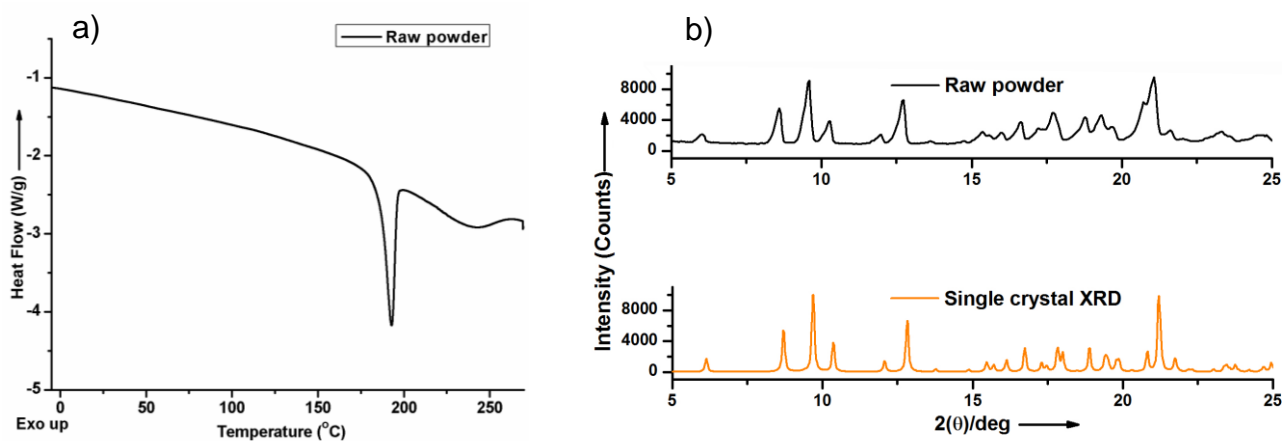


Figure S6. a) DSC profile of the raw powder; b) Powder XRD patterns of the raw powder and single crystal (simulated from single crystal X-ray data).

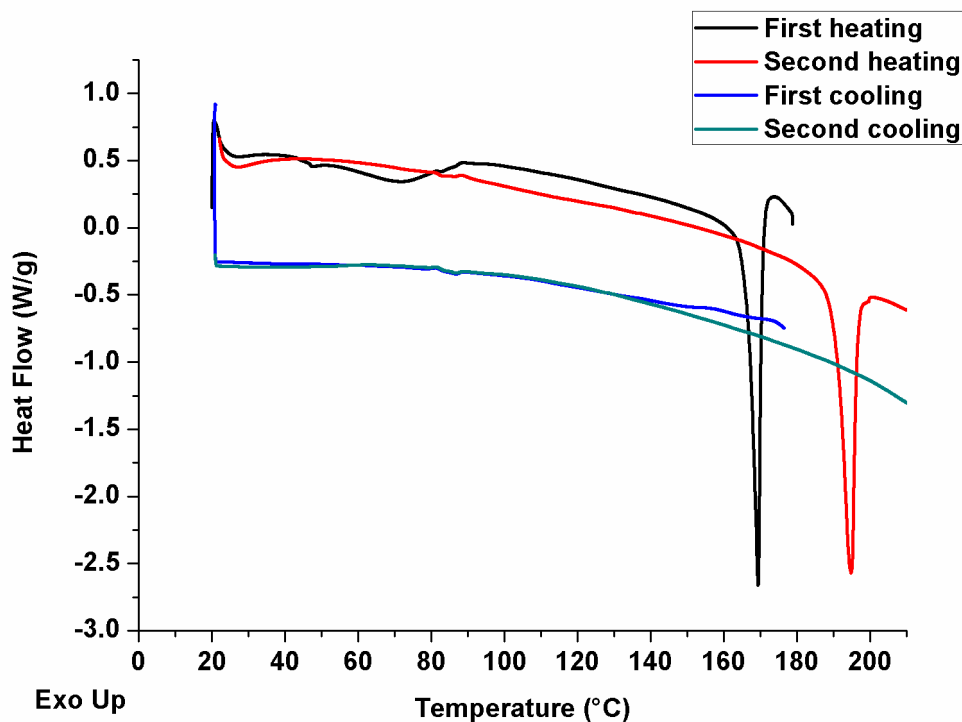


Figure S7. Detailed DSC analysis of the sample (edge distorted hexagons) from peptide **1** prepared under ACN-0.01g/L P123-water, to see the reversibility of phase transitions. The experiment was conducted in two runs. The *First heating* was carried out from RT to 180°C which gave sharp endothermic peak at 169°C. The sample was then cooled to RT (*First cooling*). The absence of exothermic peak showed that the phase change at 169°C is irreversible. During the *Second heating* cycle we did not see the endothermic peak at 169°C as expected, but the peak at 195°C corresponding to melting point of the crystalline sample was present. Cooling of this sample (*Second cooling*) back to the RT did not involve any exothermic heat change at 195°C, indicating that the melting is accompanied by decomposition.

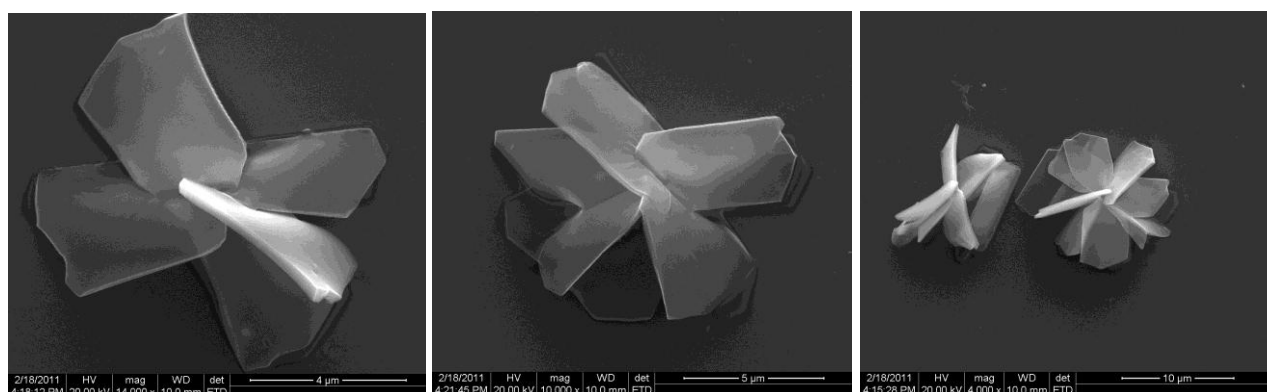


Figure S8. Development of hexagons from dendritic aggregates. Samples prepared under ACN-0.01g/LP123-water (Immediately after addition of ACN solution of peptide **1**, an aliquot was withdrawn from the stirring mixture and analysed through SEM)

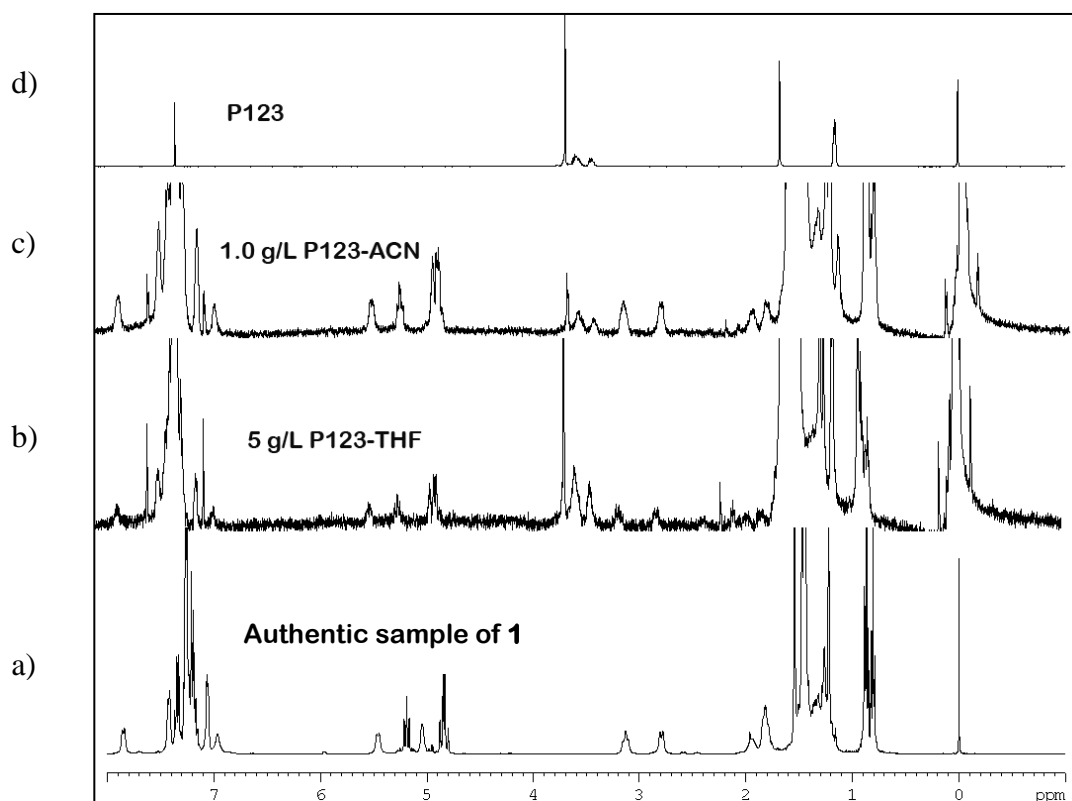


Figure S9. Comparison of the ^1H NMR (400 MHz, CDCl_3) spectrum of authentic sample of **1** (a) with that of the samples prepared under 5g/L P123-THF (b), 1 g/L P123-ACN (c) and P123 alone (d); signals corresponding to traces of P123 can be seen in the spectra of microcrystalline aggregates.

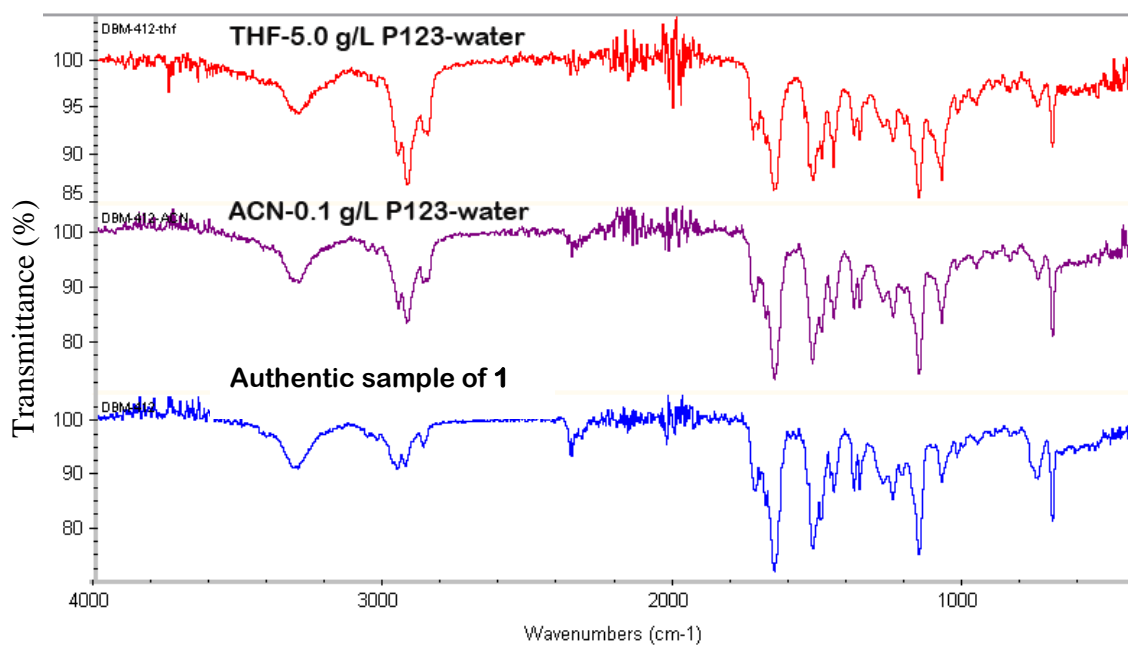


Figure S10. Comparison of the FT-IR spectrum of the authentic sample of **1** with that of its microcrystalline aggregates.