Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Study of the effect of polymorphism on the self-assembly and catalytic performance of an L-proline based molecular hydrogelator

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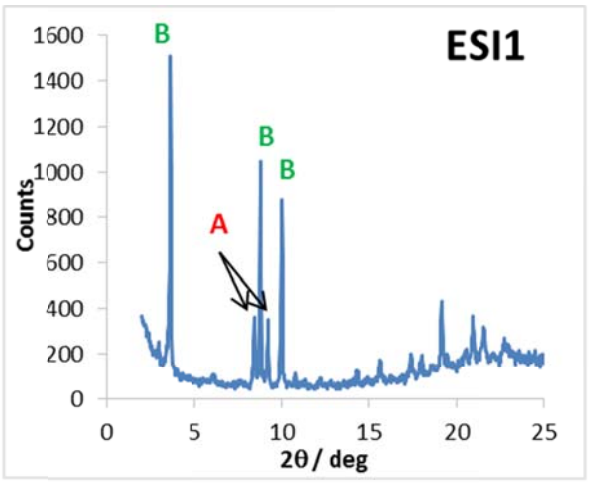
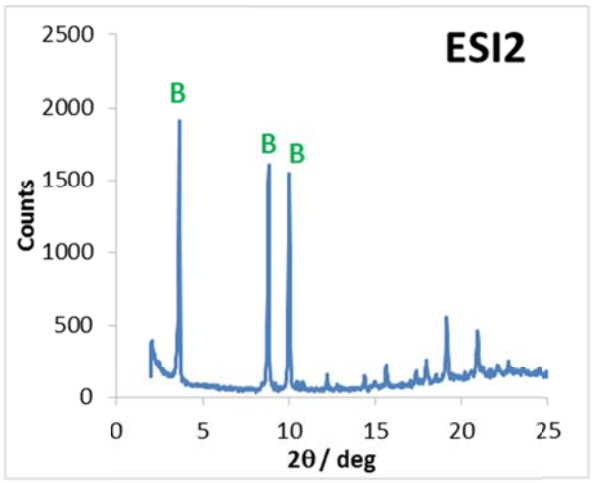
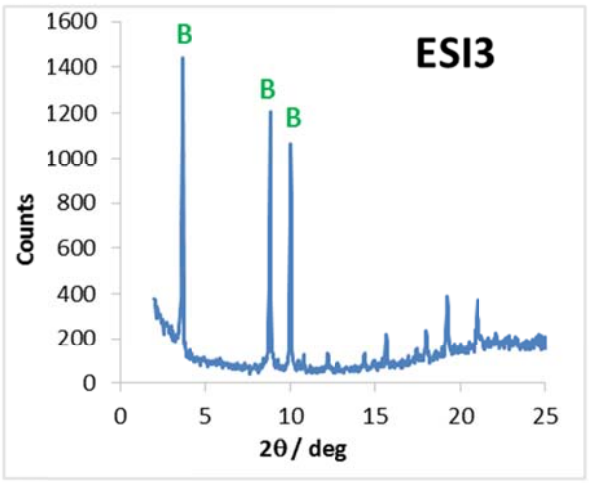
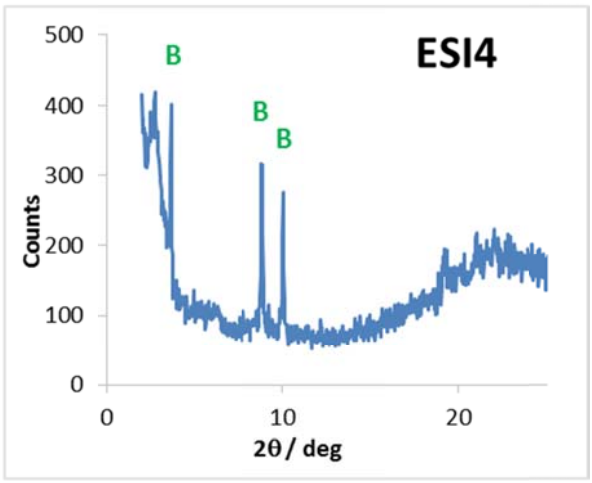
Electronic Supporting Information

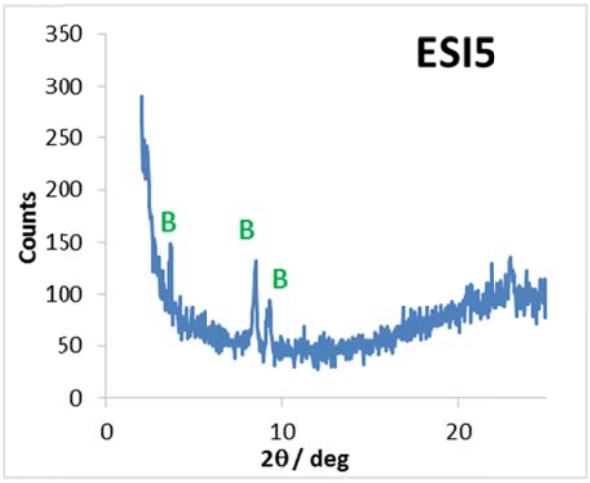
Figures ESI1-ESI19. WAXD patterns corresponding to Table 1, Entries 1-19**.**

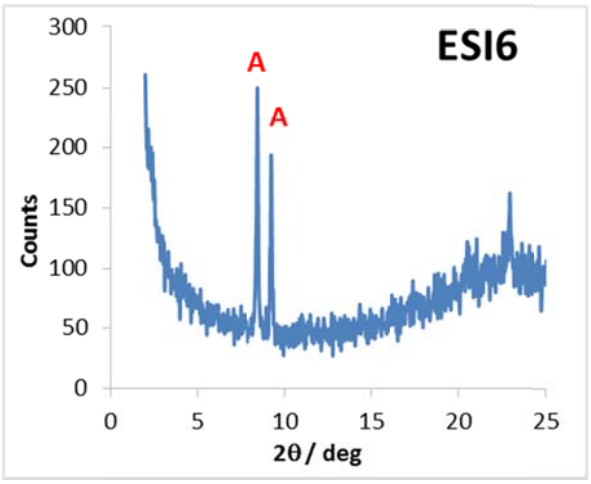


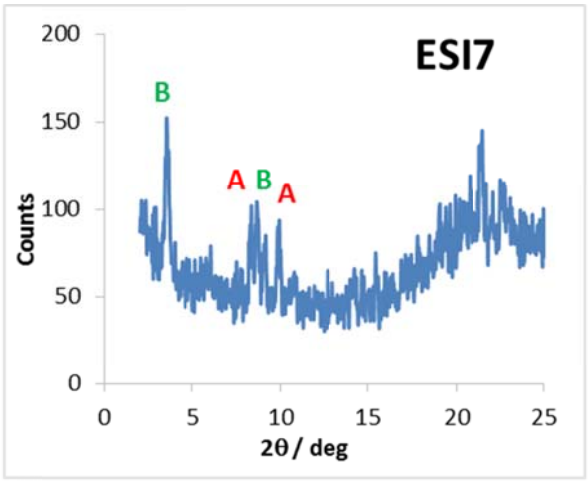


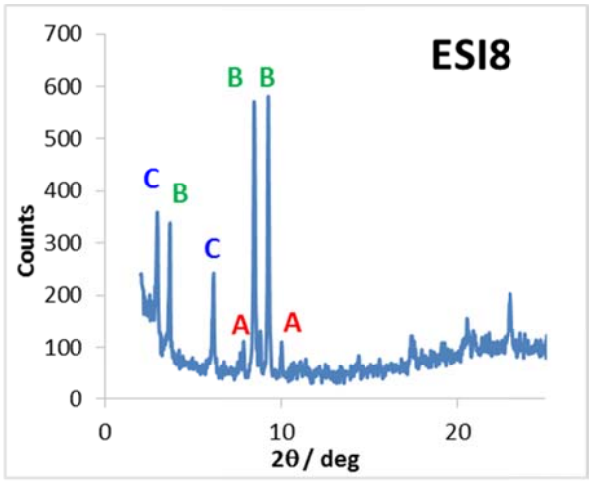


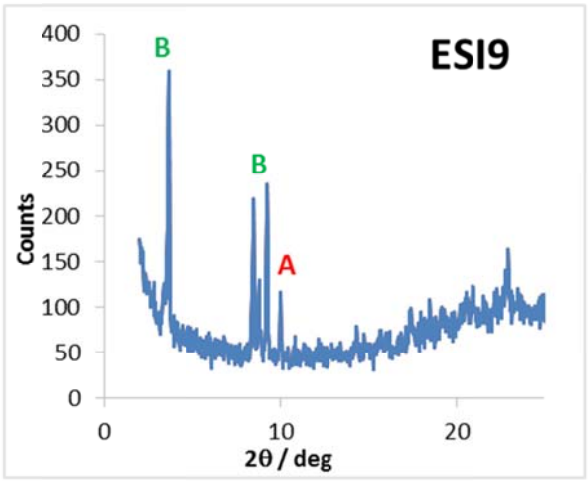


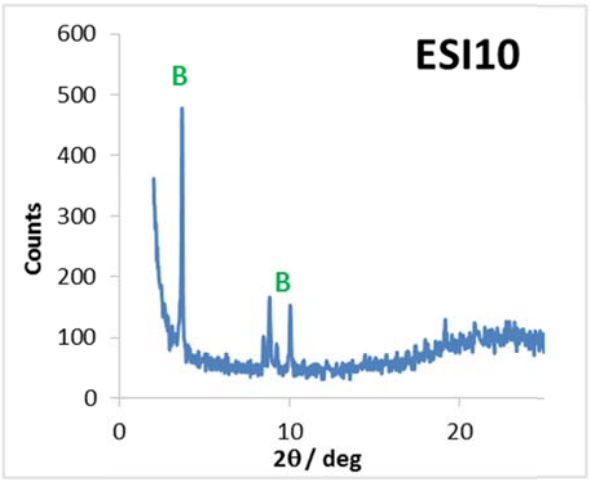


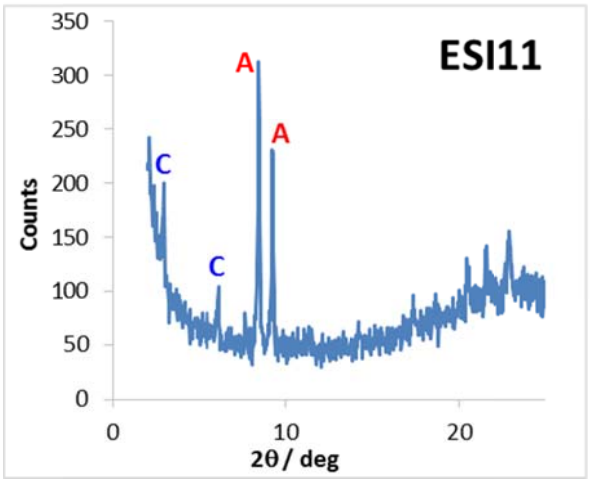


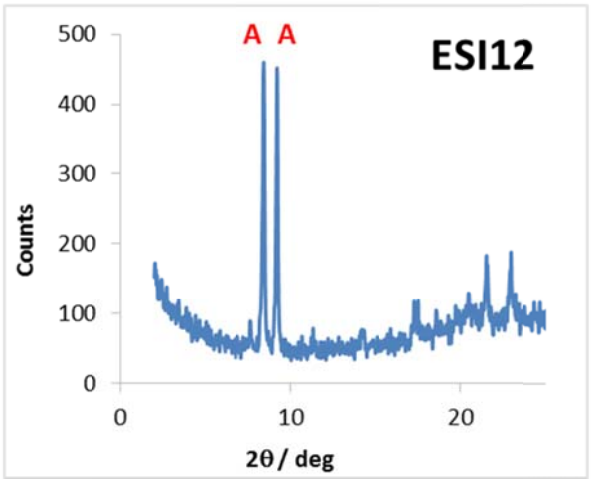

ESI7
Counts
2θ / deg
B
A B A

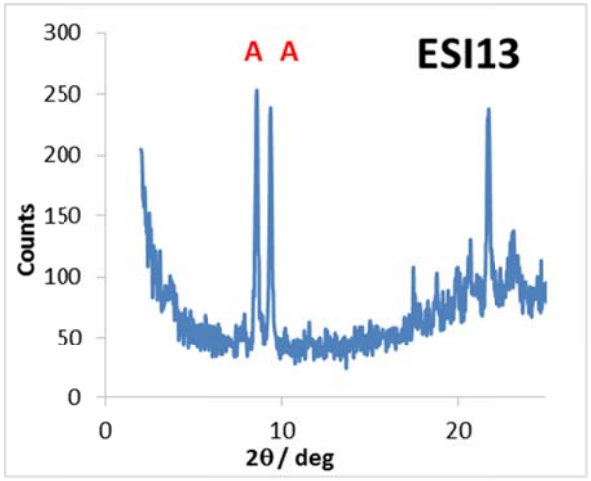

ESI8
Counts
2θ / deg
C B
B B
C
A
A

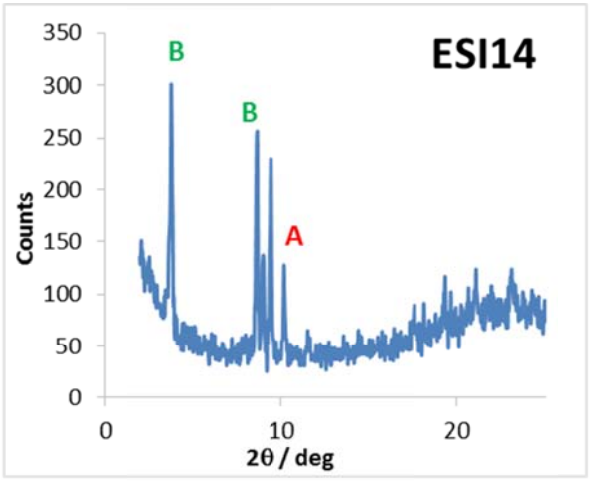

ESI9
Counts
2θ / deg
B
B
A

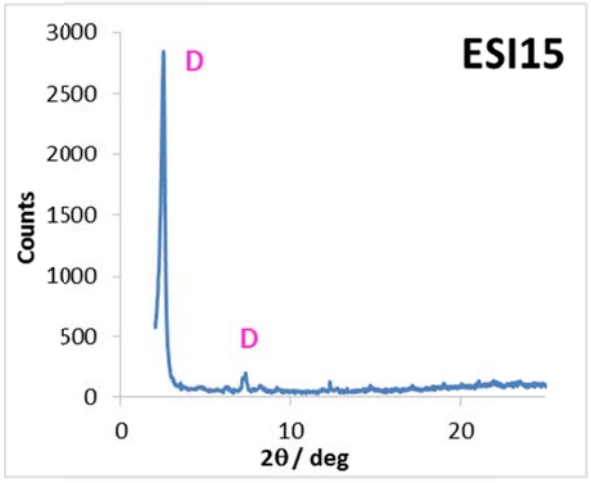

ESI10
Counts
2θ / deg
B
B

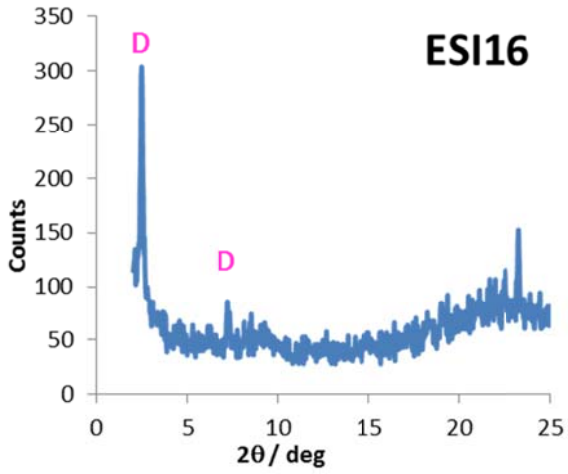

ESI11
Counts
2θ / deg
A
A
C
C

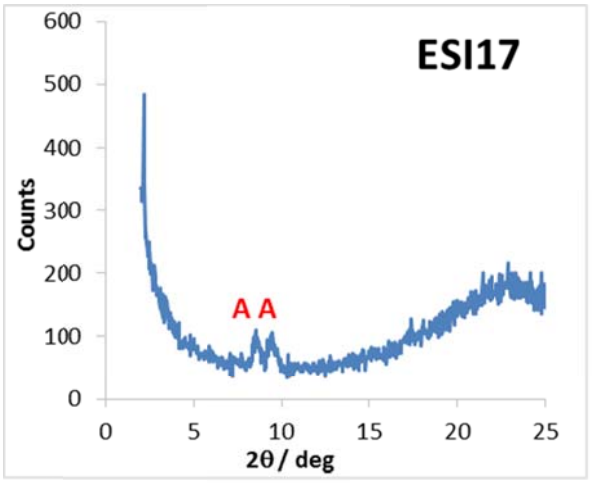

ESI12
Counts
2θ / deg
A A

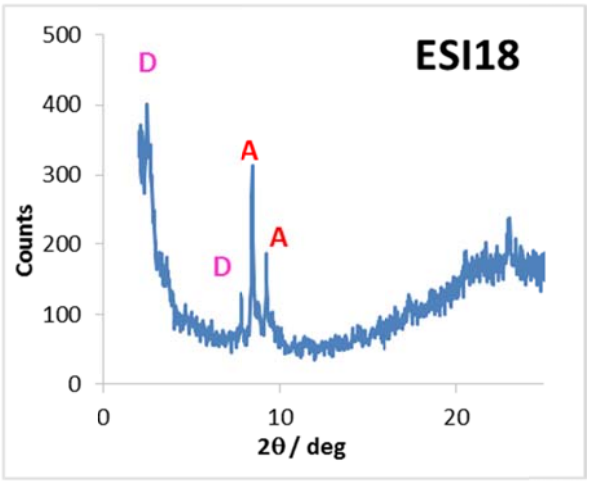

ESI13
A A
Counts
2θ / deg
0
50
100
150
200
250
300
0
10
20

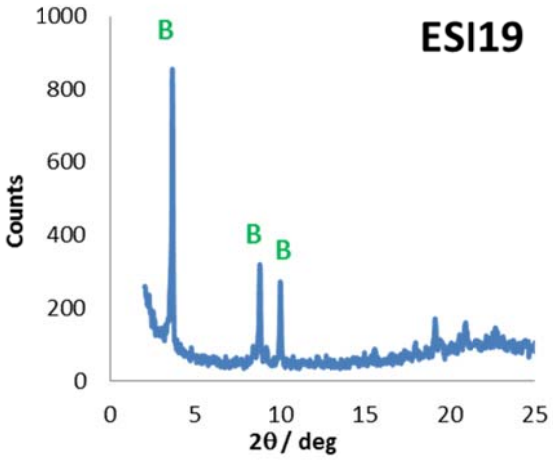

ESI14
B
B
A
Counts
2θ / deg
0
50
100
150
200
250
300
350
0
10
20


ESI15
D
D
Counts
2θ / deg
0
500
1000
1500
2000
2500
3000
0
10
20


ESI16
D
D
Counts
2θ / deg
0
50
100
150
200
250
300
350
0
5
10
15
20
25


ESI17
Counts
2θ / deg
A A


ESI18
Counts
2θ / deg
D
A
D
A

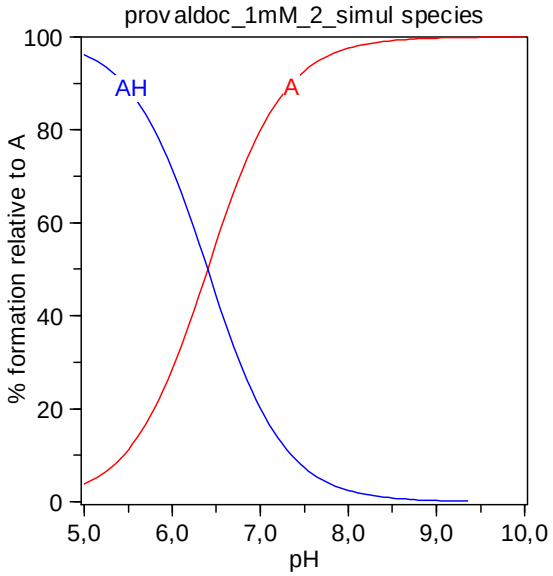

ESI19
Counts
2θ / deg
B
B
B

pKa determination. Compound **1** was dissolved in an excess of aqueous HCl (0.01M) and then titrated with aqueous NaOH (0.01M). The pH was monitored potentiometrically with a glass pH electrode and the data analysed with HYPERQUAD2013 to afford the acidity constants. The pKa was determined for two concentrations of **1**, as shown below.

[1] $_{initial}$	**pKa**
1 mM	6.4 ± 0.1
5 mM	6.0 ± 0.1

Figure ESI20. Species distribution diagram as a function of pH for compound **1**.

1 mM



5 mM

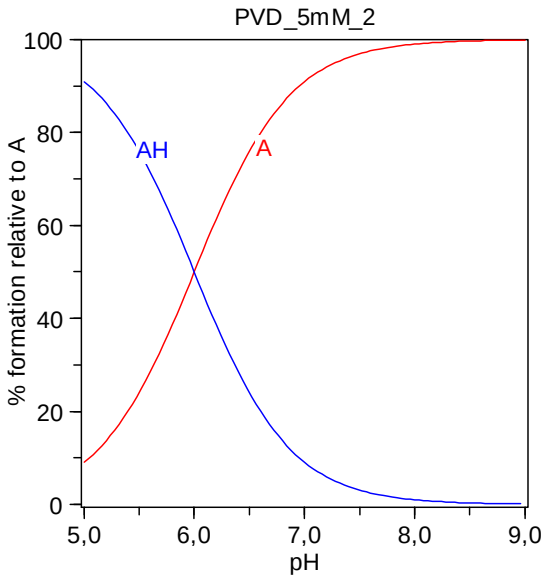


Figure ESI21. WAXD patterns of compound **1**·HCl·2H_2O simulated from single crystal data.[10]

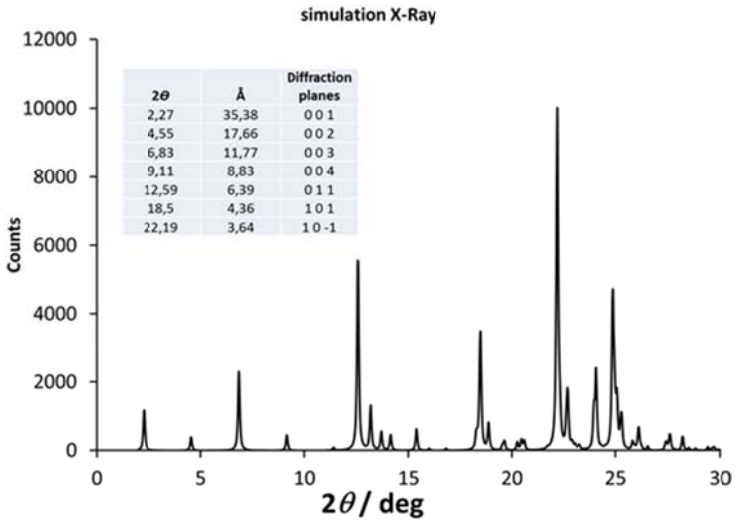


Figure ESI22. Macroscopic aspect of samples with polymorphs **A**, **B**, and **D**.

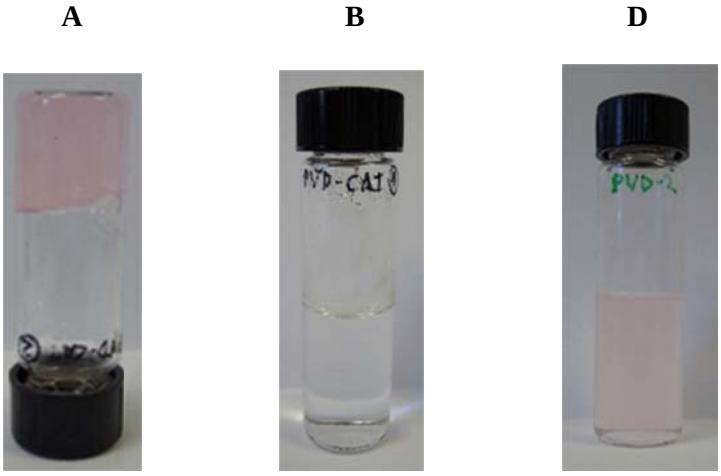
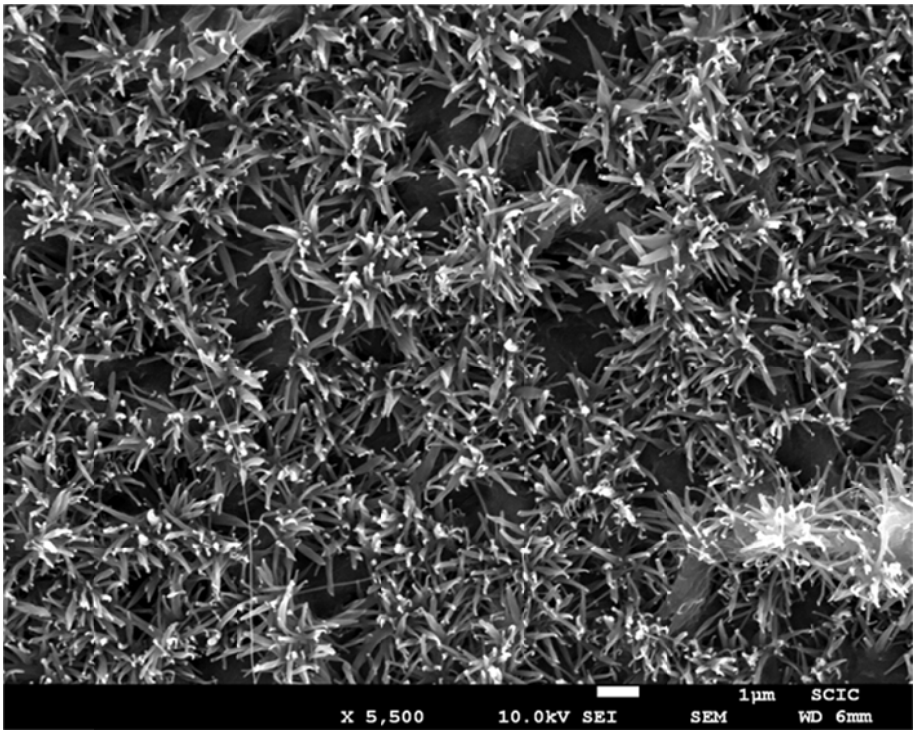


Figure ESI23. Additional FESEM (top) and TEM (bottom) of samples with polymorph **A**.



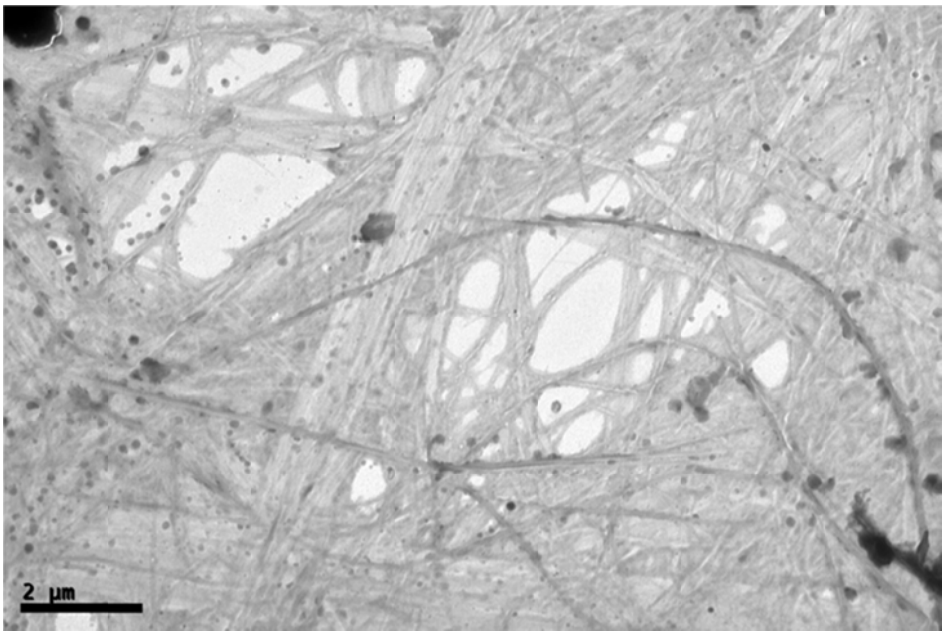
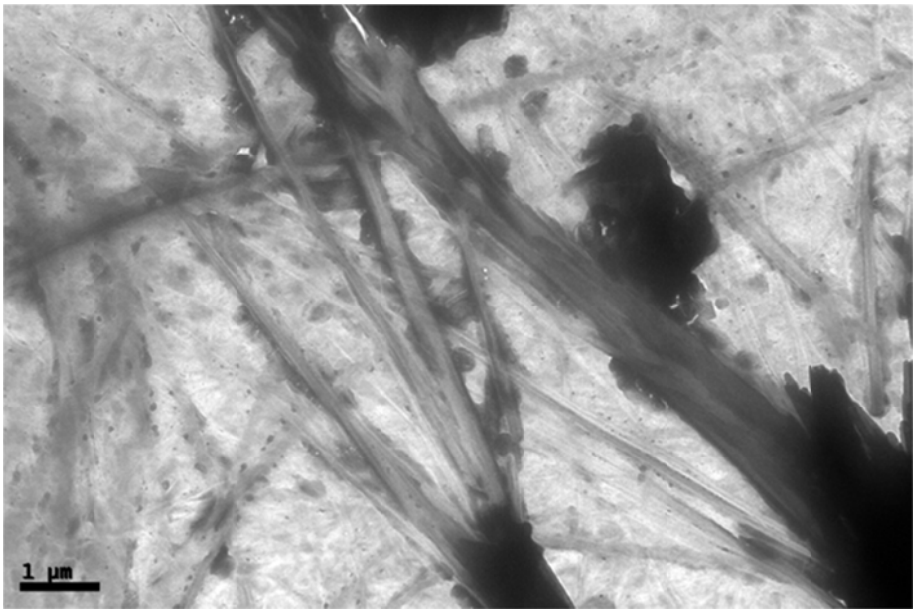


Figure ESI24. Additional FESEM (top) and TEM (bottom) of samples with polymorph **B**.



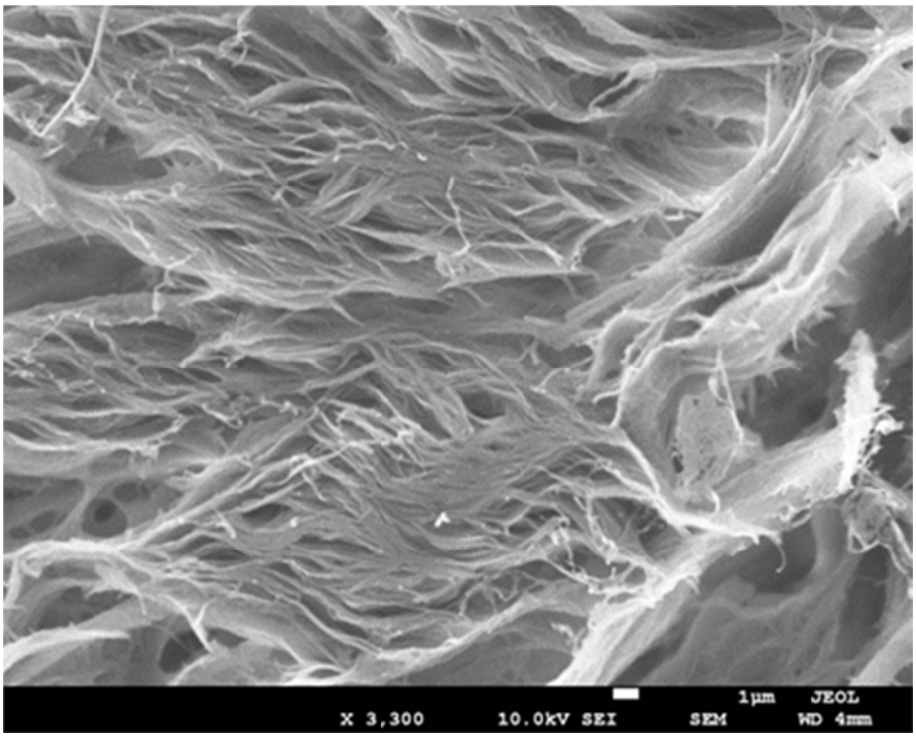


Figure ESI 25. Additional TEM images of samples with polymorph **D**.