Supporting Information

Flexible and luminescent fibers of a 1D Au(I)-thiophenolate coordination polymer and formation of gold nanoparticles-based composite materials for SERS

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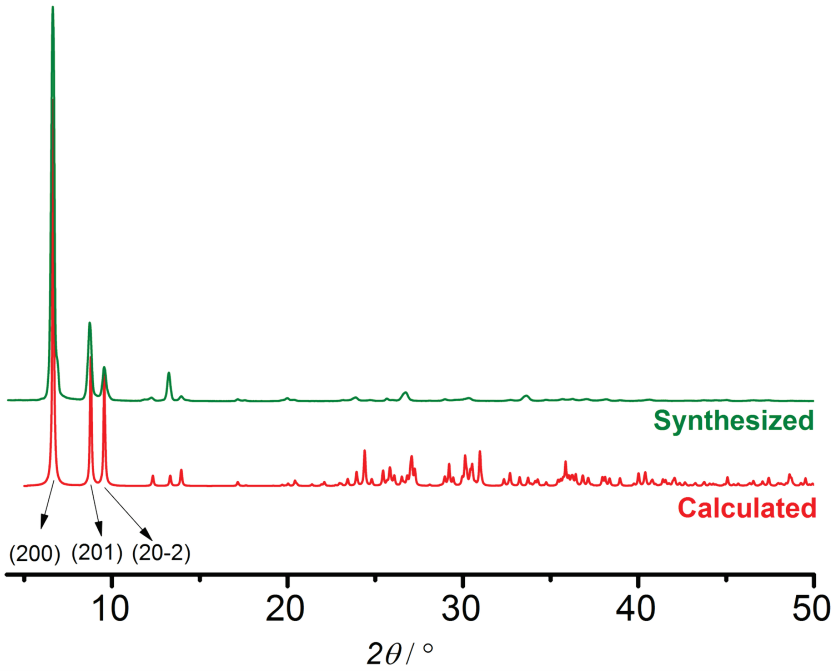


Figure S1. Powder X-Ray diffraction (PXRD) patterns of the obtained fibers compared to the calculated one of $[Au(SPh)]_n$.

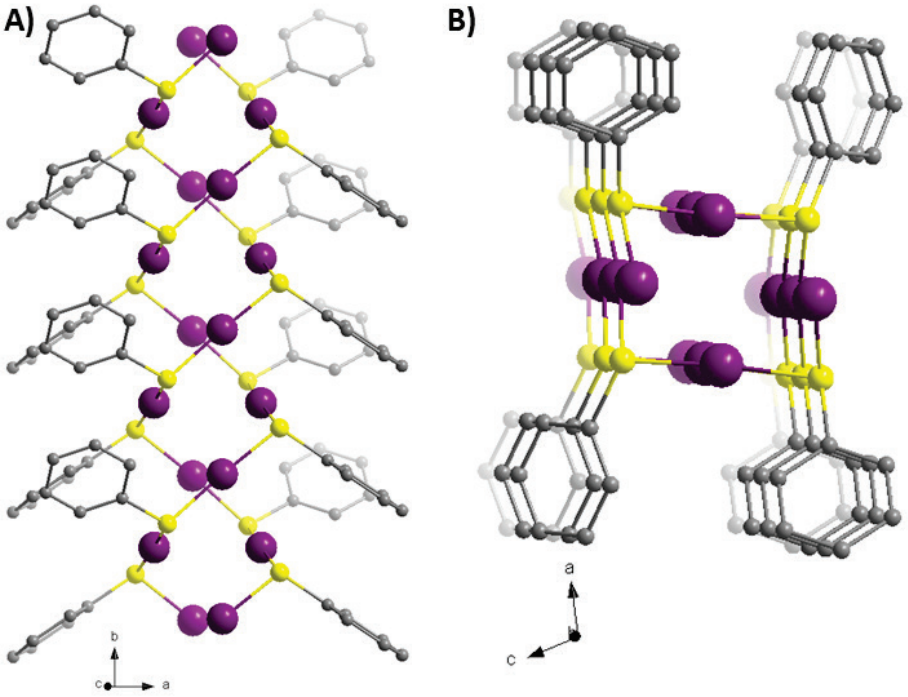


Figure S2. $[Au(SPh)]_n$ coordination polymer structure. View of the double helix along the A) b-axis and B) (ac) plane. Purple, Au(I); yellow, S; gray, C. Hydrogen atoms are omitted for clarity.

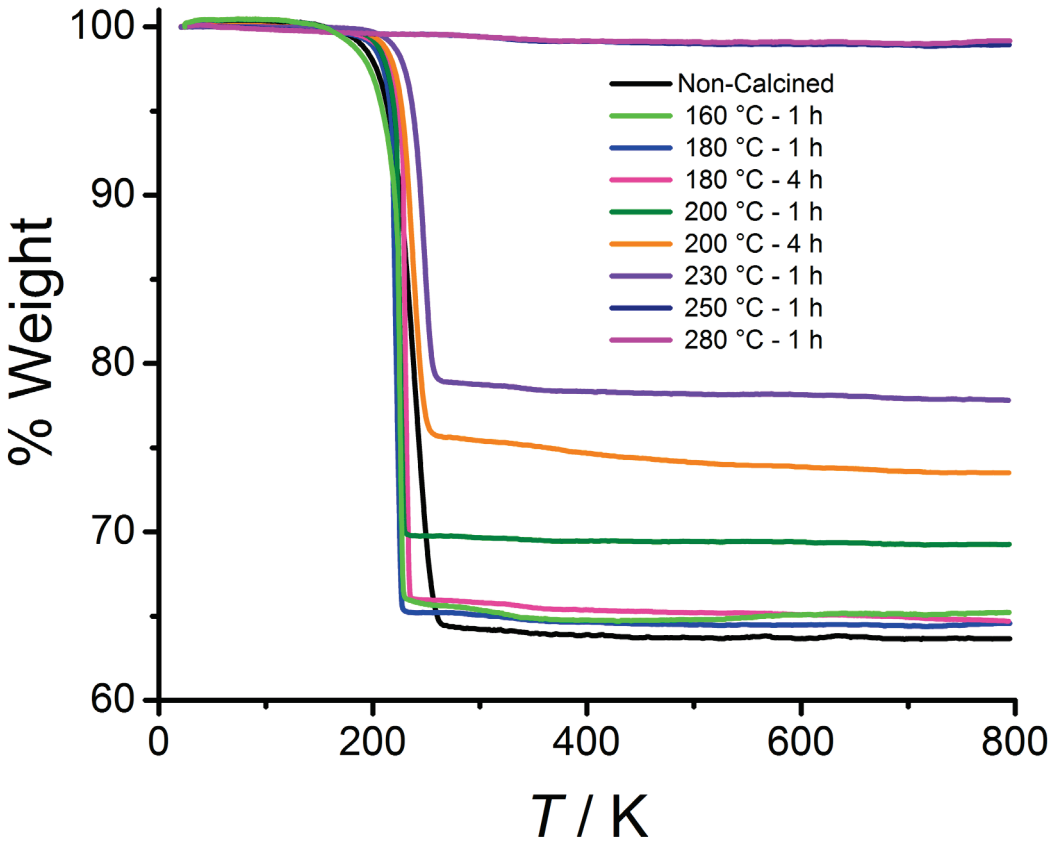


Figure S3. TGA (carried out under air) of $[Au(SPh)]_n$ CP and the composite materials obtained after different temperatures and times of calcination.

Table S1. Ligand and gold contents and the percentage of CP in the composite material obtained from TGA experiments.

Fibers	Ligand content, %	Gold content, %	Content of CP in composite material, %
Non-calcined	36.0	64.0	100
160 °C – 1 h	35.3	64.7	98.9
180 °C – 1 h	35.3	64.7	98.9
180 °C – 4 h	35.3	64.7	98.9
180 °C – 12 h	35.1	64.9	98.3
200 °C – 1 h	30.7	69.3	86.0
200 °C – 4 h	26.5	73.5	74.2
200 °C – 12 h	21.0	79.0	58.8
230 °C – 1 h	23.0	77.0	64.4
250 °C – 1 h	1.0	99.0	2.8
280 °C – 1 h	1.0	99.0	2.8

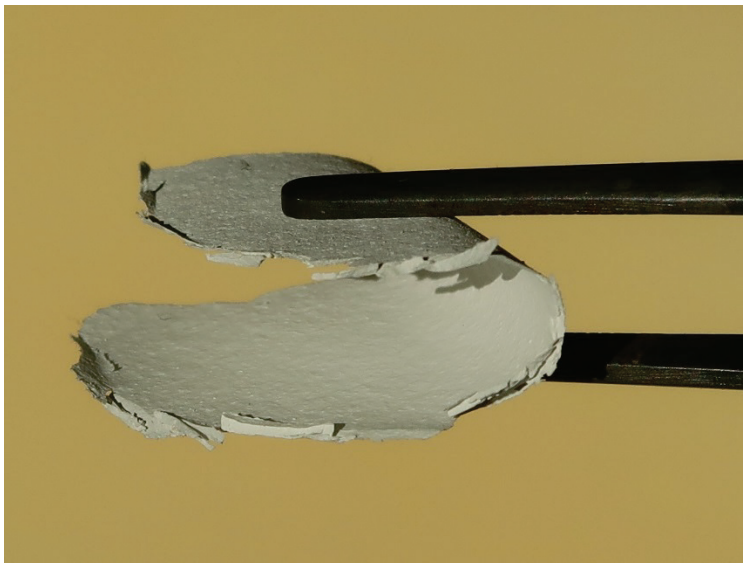


Figure S4. Photograph showing the flexibility of the fibers.

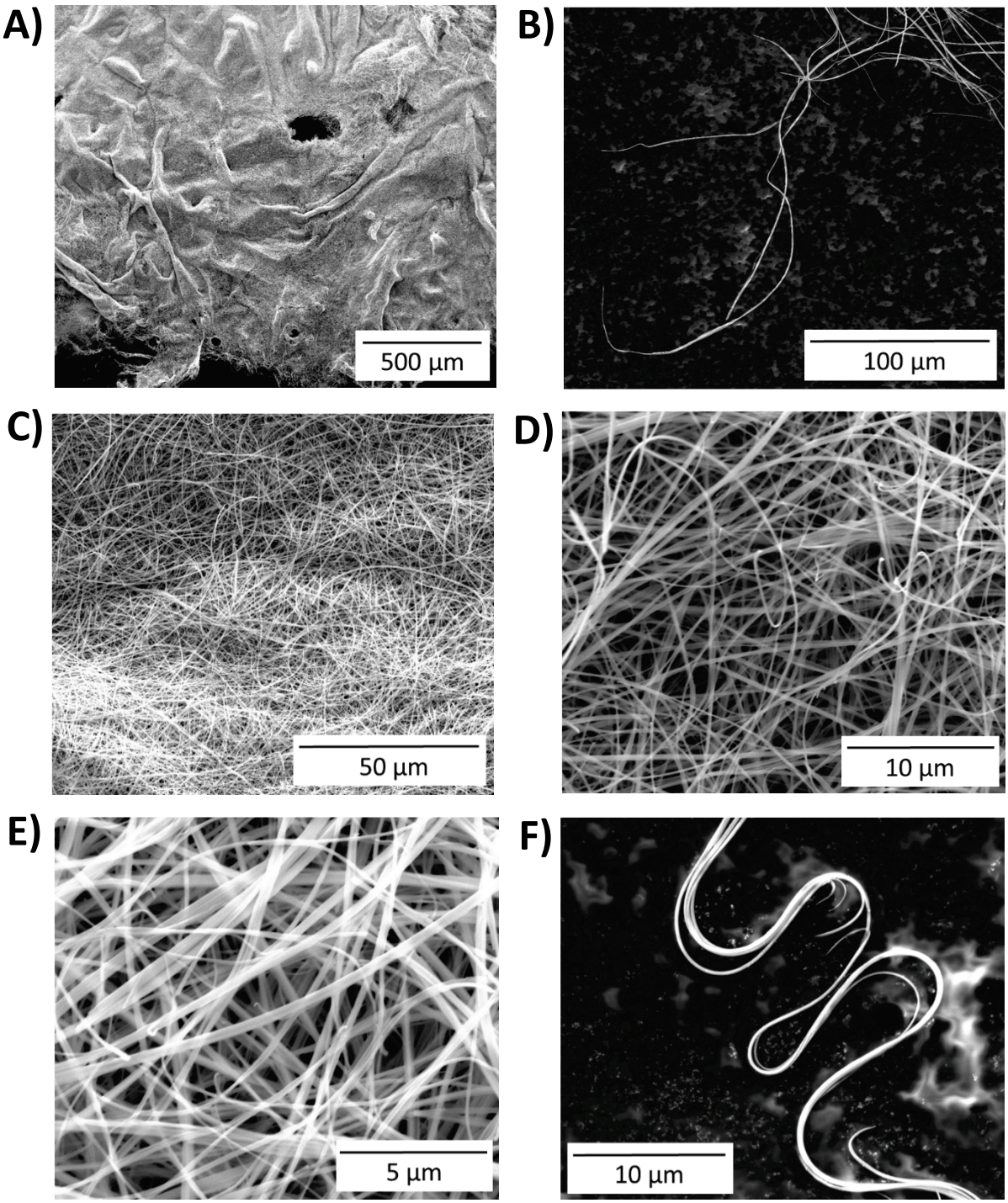


Figure S5. A-D) SEM images of the $[Au(SPh)]_n$ fibers at various magnification levels.

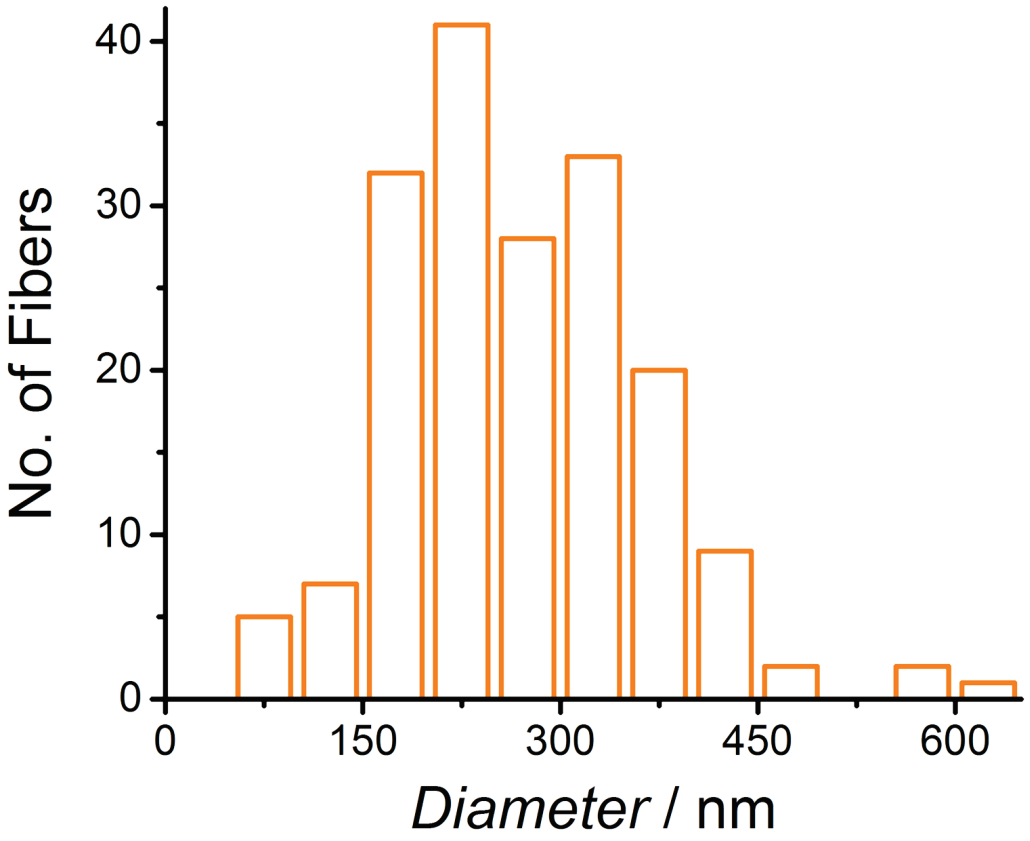


Figure S6. Histogram of the diameter distribution of the $[Au(SPh)]_n$ fibers measured by SEM.

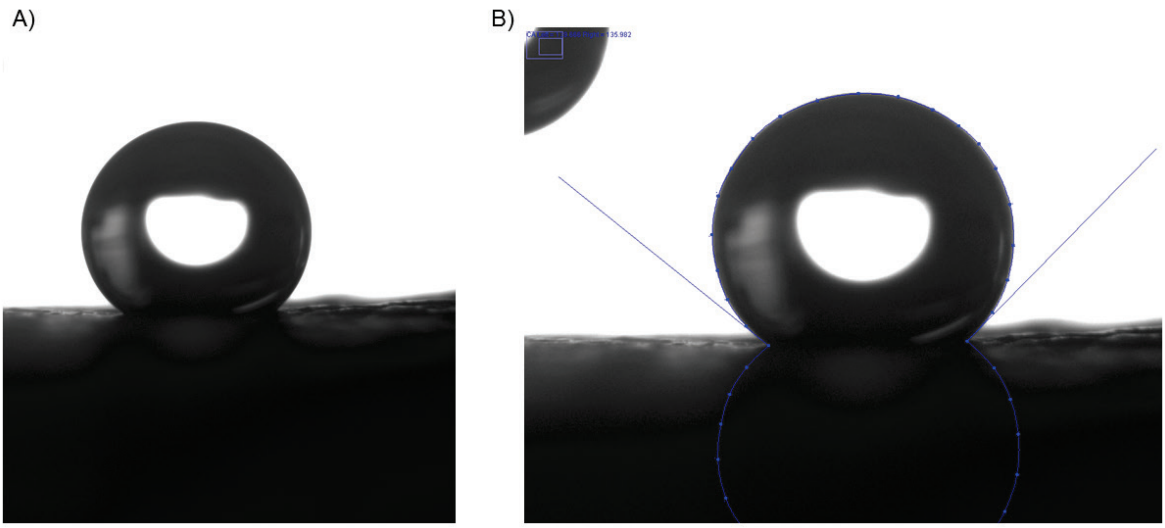


Figure S7. Contact angle measurement: A) and B) a droplet of water on a $[Au(SPh)]_n$ fibers film.

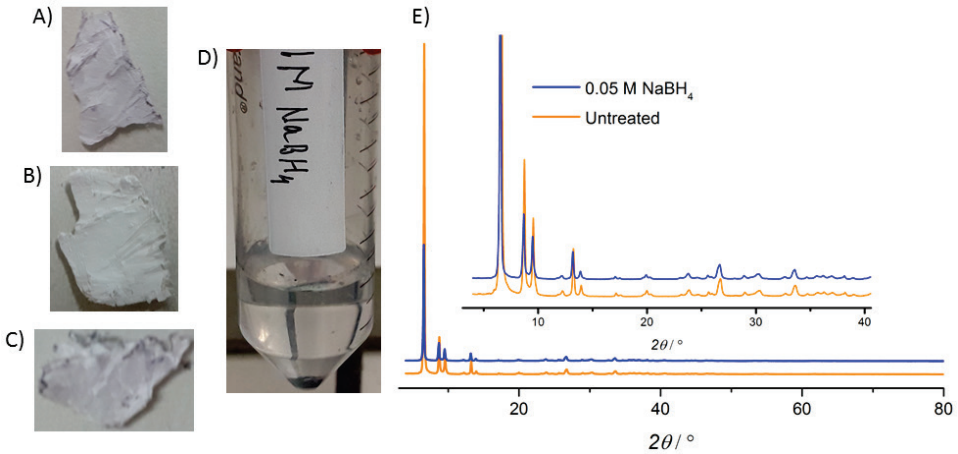


Figure S8. Pictures of the fibers treated with A) 10 M HCl, B) 5 M NaOH, C) 0.05 M $NaBH_4$ and D) 1 M $NaBH_4$, resulting in the formation of a black precipitate. E) PXRD of the fibers treated with 0.05 M $NaBH_4$.

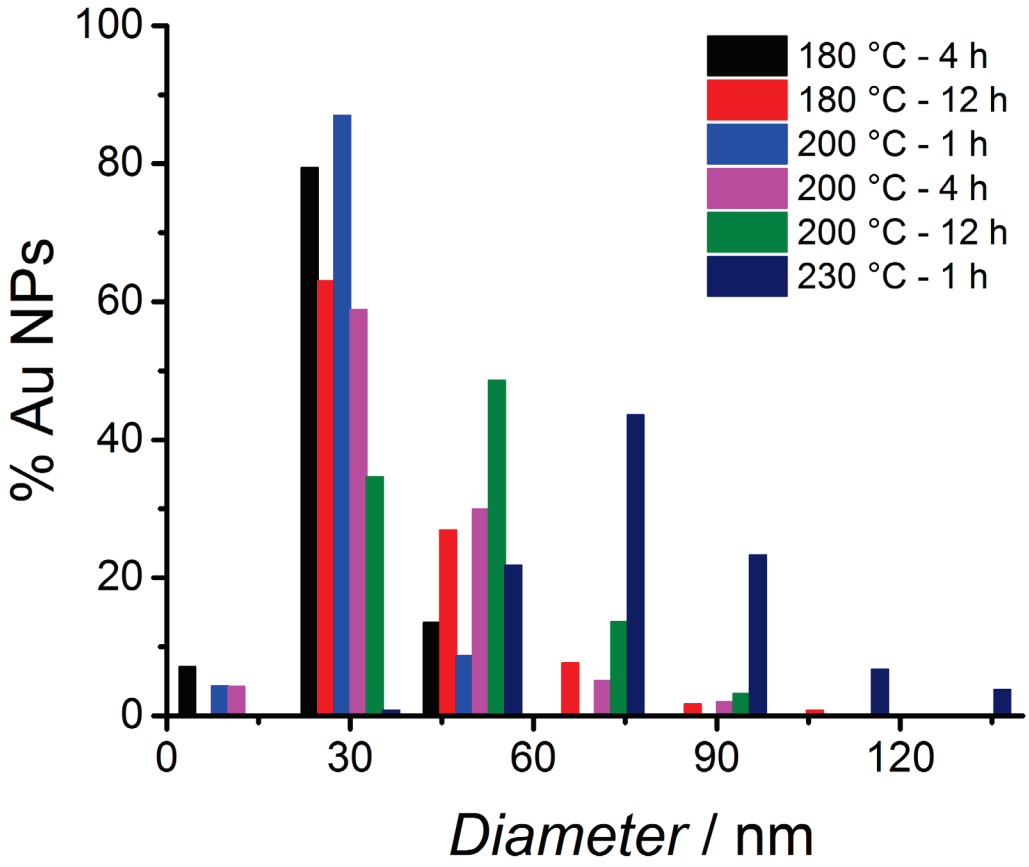


Figure S9. Histograms of the size distribution of the AuNPs formed on the $[Au(SPh)]_n$ fibers at various temperatures and times of calcination. The diameters are measured from SEM images.

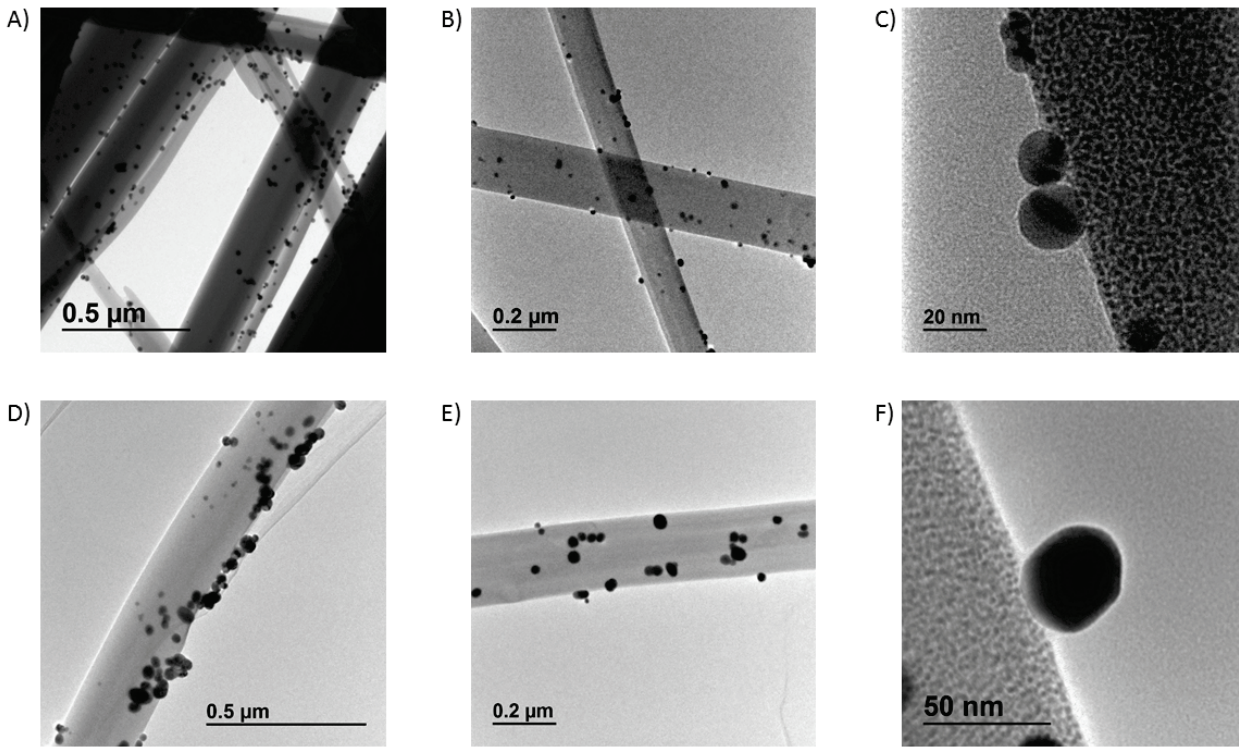


Figure S10. TEM images of the $[Au(SPh)]_n$ fibers calcined at A-C) 180 °C – 1 h and D-F) 200 °C – 1 h at various magnification levels.

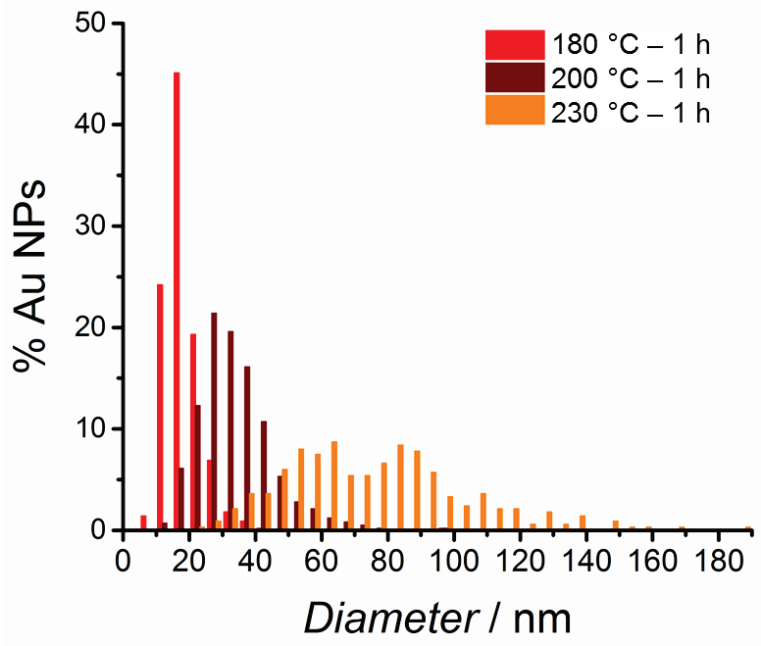


Figure S11. Histogram of the size distribution of the AuNPs formed on the $[Au(SPh)]_n$ fibers at 180 °C, 200 °C and 230 °C for 1 h. The diameters are measured from TEM images.

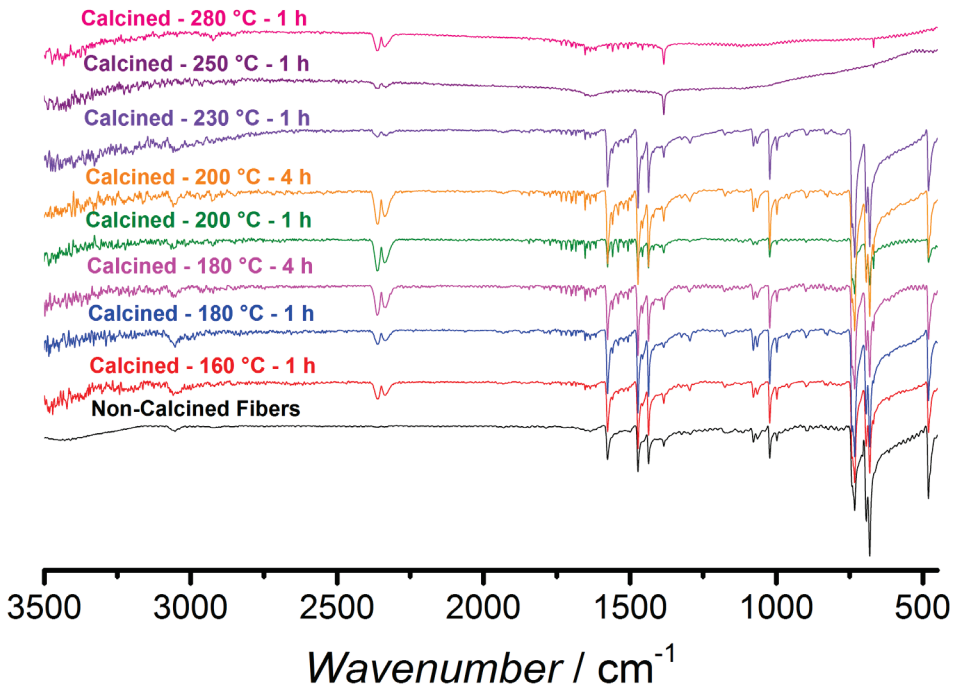


Figure S12. FTIR of the $[Au(SPh)]_n$ fibers calcined at different temperatures.

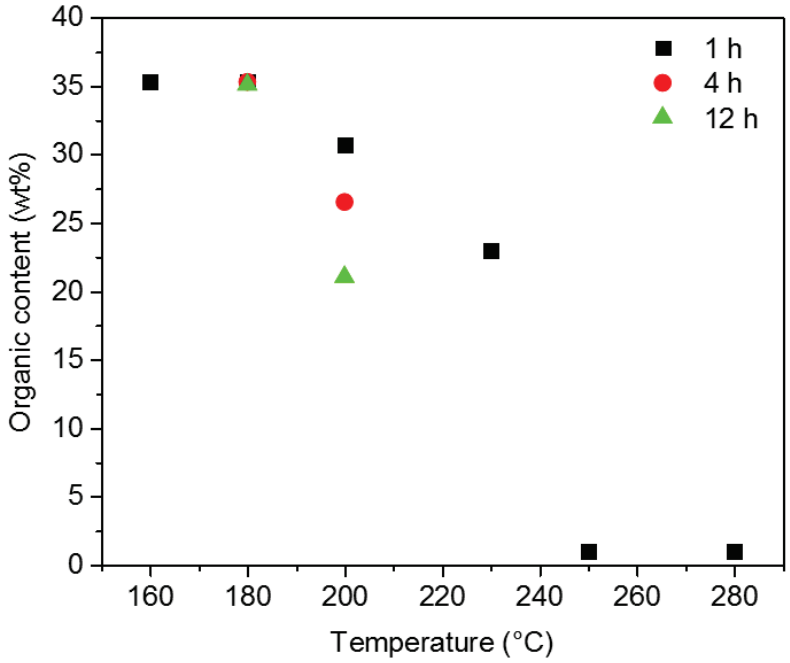
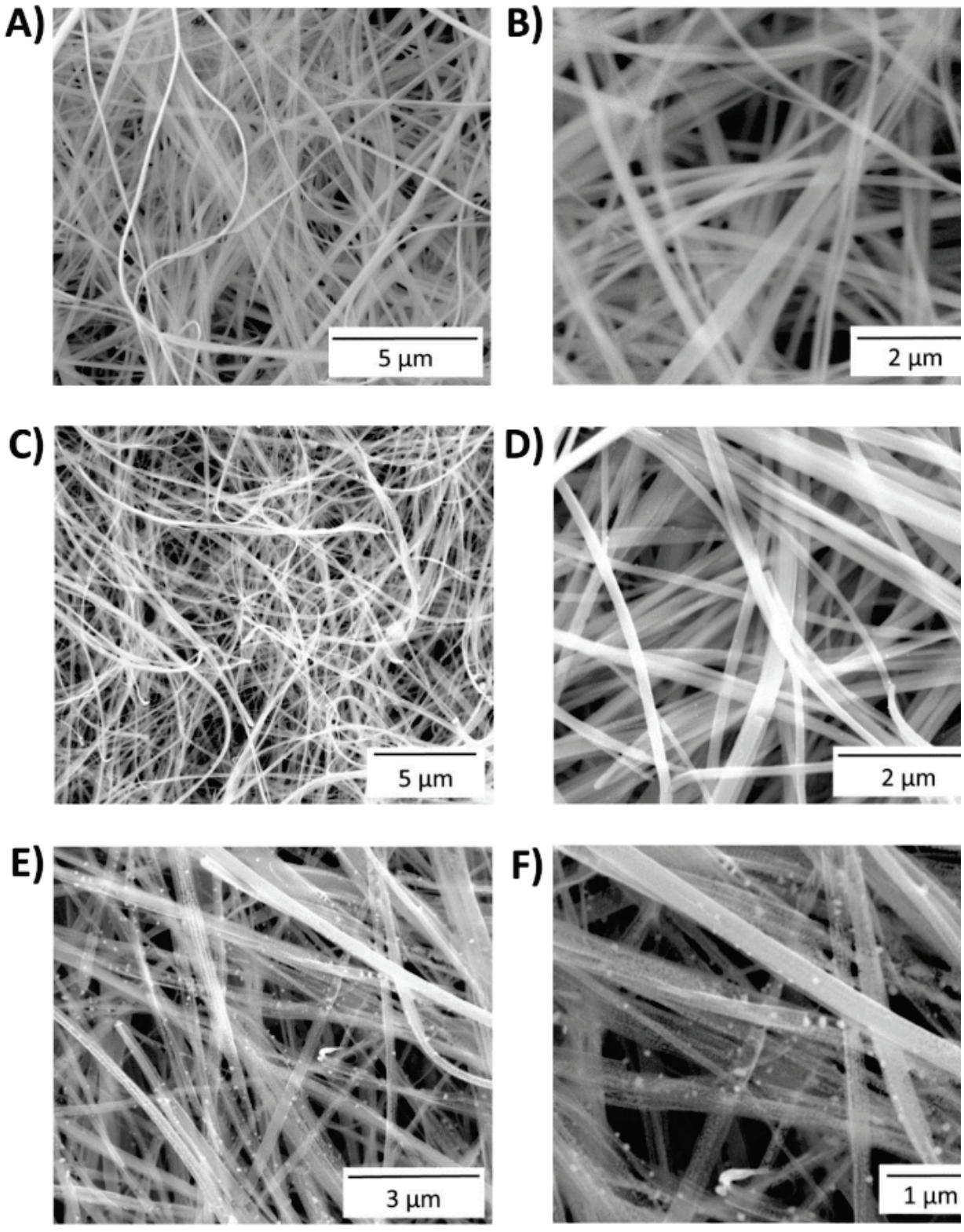


Figure S13. Remaining organic content after the calcinations at different temperatures and times of the $[Au(SPh)]_n$ fibers.


A)
5 µm
B)
2 µm
C)
5 µm
D)
2 µm
E)
3 µm
F)
1 µm

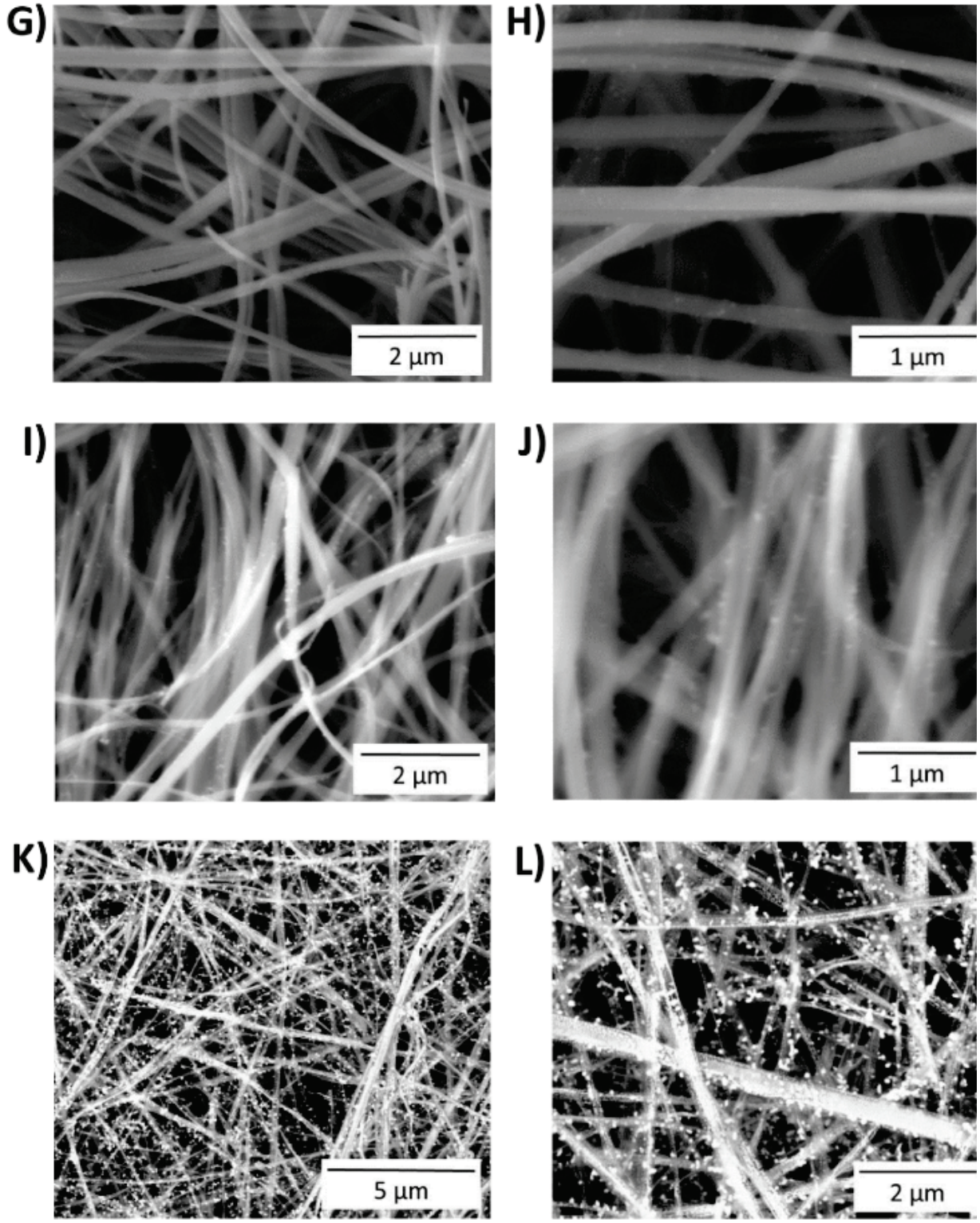


Figure S14. SEM images of the fibers calcined at the (A and B) 180 °C – 1 h, (C and D) 180 °C – 4 h, (E and F) 180 °C – 12 h, (G and H) 200 °C – 1 h, (I and J) 200 °C – 4 h and (K and L) 200 °C – 12 h.

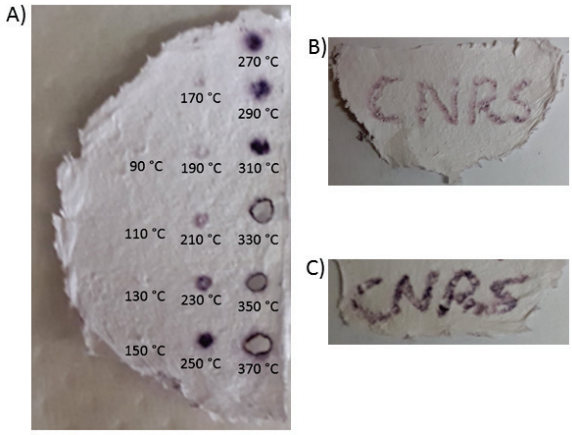


Figure S15. Photographs of marks left on the fibrous film after the contact with a soldering iron at A) different temperatures, B) 230 °C and C) 270 °C.

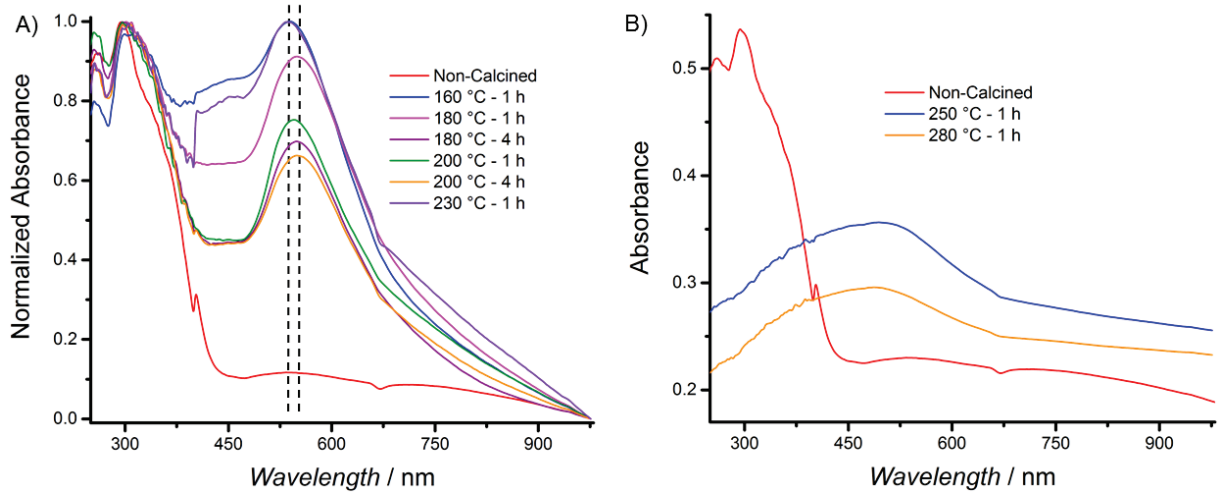


Figure S16. A) and B) UV-Vis spectra of the $[Au(SPh)]_n$ fibers heated at different temperatures and times.

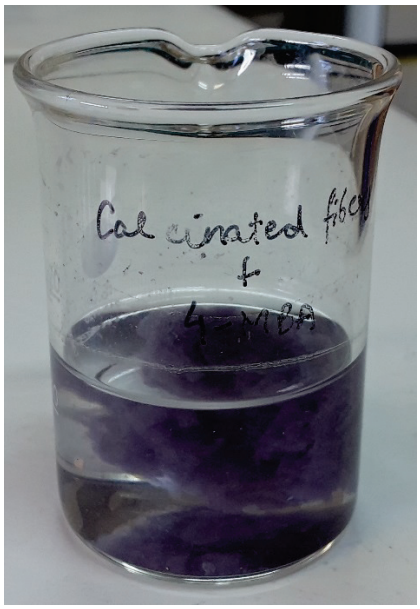


Figure S17. Photograph of the calcined fibers along with 4-MBA (1.25 x 10^{-3} M) after studying the SERS effect. No leaching of the AuNPs can be seen clearly.

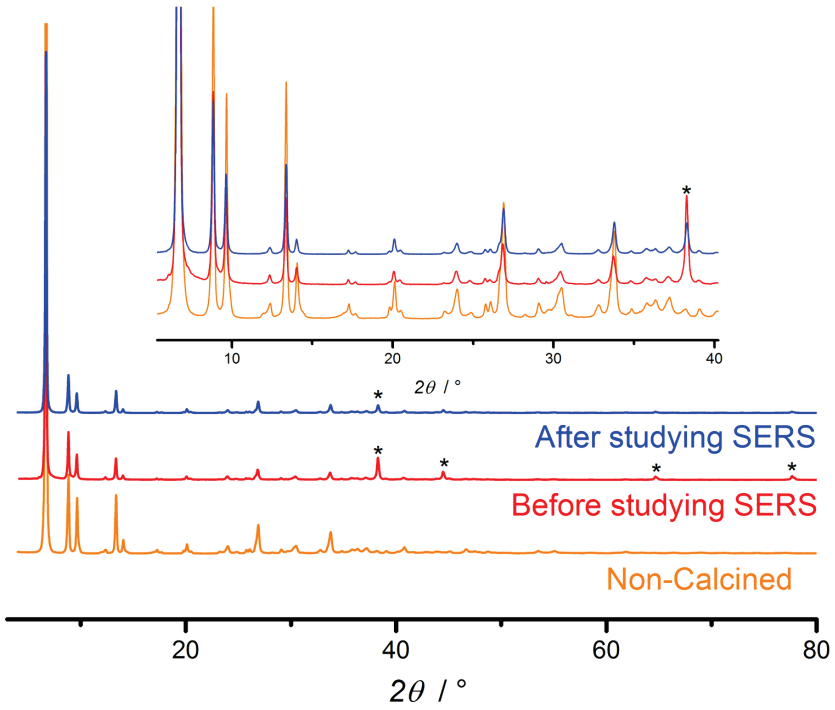


Figure S18. Comparison of the PXRD of the $[Au(SPh)]_n$ fibers, the composite material obtained at 230°C-1h before and after the SERS effect study. The asterisks denote the FCC gold of the AuNPs.

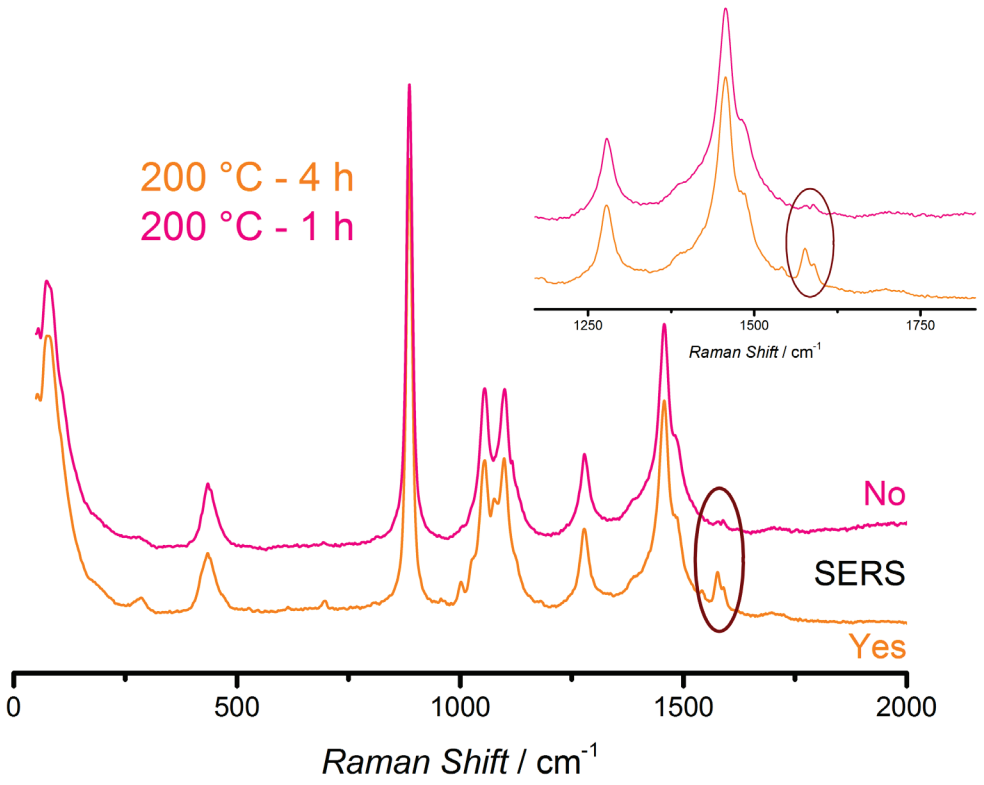


Figure S19. Comparison of the Raman spectra of the composite materials obtained after calcination of the fibers at 200 °C for 1 h and 4 h. The samples are mixed with 4-MBA (1.25 x 10^{-3} M) to show the SERS effect.