Supplementary Information file for

# In vitro study of the cytotoxicity of TTF·TCNQ nanoparticles on mammalian cells

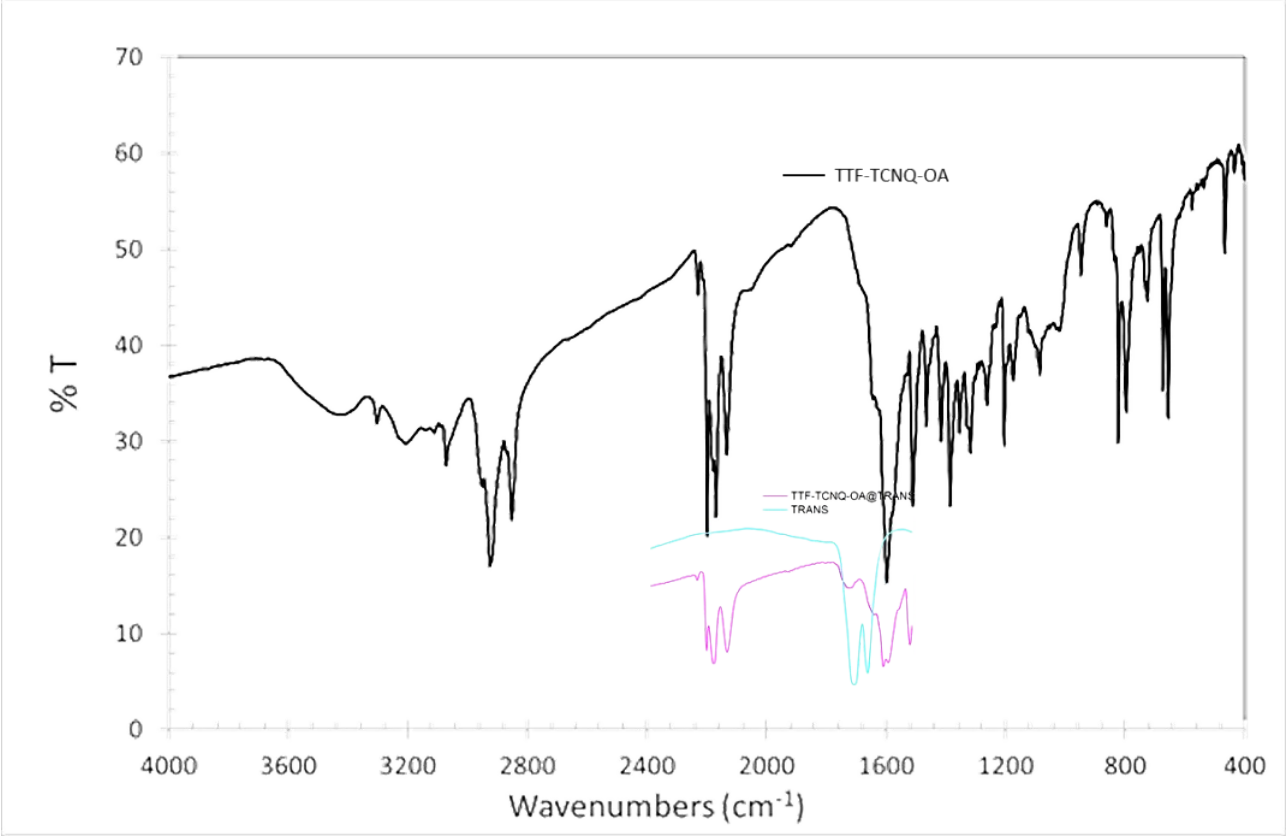
Hongjie Chen, Géraldine Albérola, Dominique de Caro, Christophe Faulmann, Muriel Golzio, Lydie Valade*, and Marie-Pierre Rols*

Content:

S1. IR spectrum of TTF-TCNQ-OA

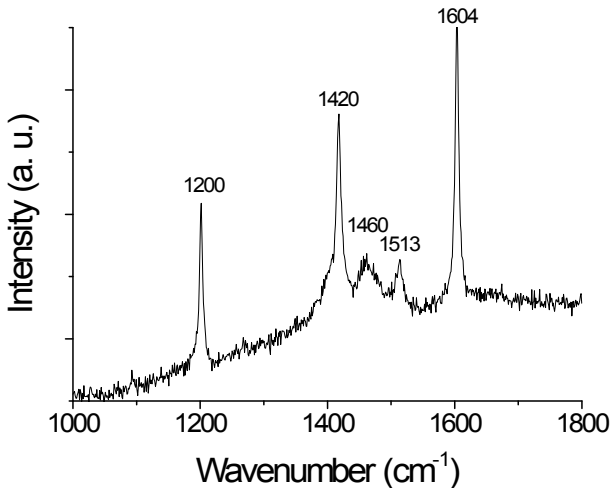
S2. Raman Spectrum of TTF-TCNQ-OA

S3. UV-vis. Spectrum of TTF-TCNQ-OA




## S1. IR spectrum of TTF-TCNQ-OA (in KBr matrix)

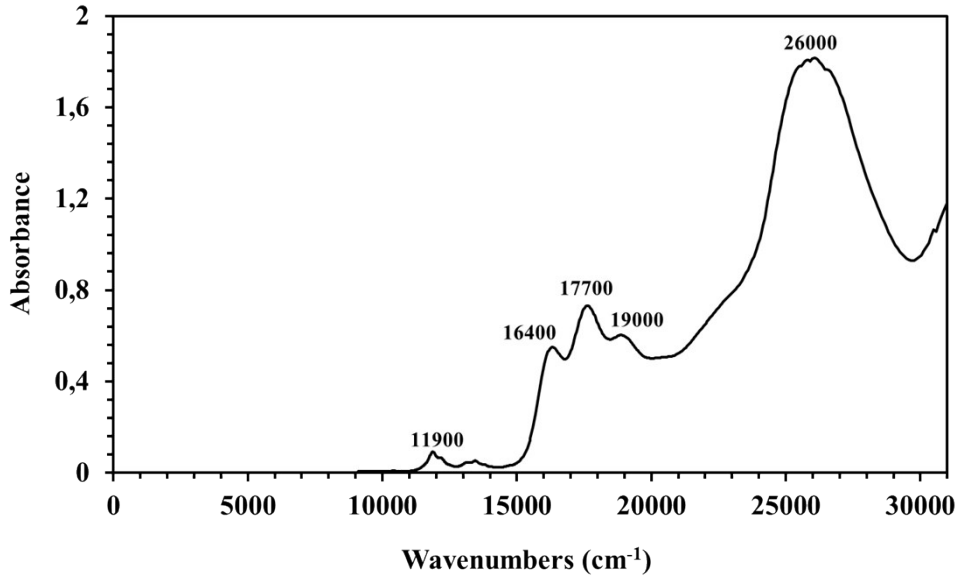
Assignment ($cm^{-1}$): 3072 (CH $sp^2$ stretching); 2926 and 2853 (CH $sp^3$ stretching); 2199, 2169 and 2133 (CN stretching); 1598 and 1512 (C=C stretching); 1086 (S-C-H bending); 797 (CS stretching). Insert (in text Figure 3): CO band area of free *trans*-decenoic acid (1700) and in TTF-TCNQ-OA@TRANS (1710).




| ν ($cm^{-1}$) | Assignment | Symmetry |
|---|---|---|
| 1200 (1202)* | C–C–H bend and C=C ring stretch in TCNQ | $a_g$ ($\nu_5$) |
| 1420 (1423) | C=C stretch in TCNQ | $a_g$ ($\nu_4$) |
| 1460 (1456) | C=C stretch center and C=C ring stretch in TTF | $a_g$ ($\nu_3$) |
| 1513 (1520) | C=C stretch center and C=C ring stretch in TTF | – |
| 1604 (1606) | C=C ring stretch in TCNQ | $a_g$ ($\nu_2$) |

**S2. Raman spectroscopy of TTF-TCNQ-OA**.

Raman modes, assignments, and symmetry. *In parentheses, ν values for TTF-TCNQ single crystal.




**S3. UV-vis. spectrum for TTF-TCNQ-OA in acetonitrile**

Assignment ($cm^{-1}$): 11900 (charge transfer band between TTF and TCNQ); 16400, 17700, 19000 and 26000 (intramolecular transitions for $TCNQ^{\delta-}$)