

Supplementary information

Tumor-targeted Molybdenum Disulfide@Barium Titanate Core-Shell Nanomedicine for Dual Photothermal and Chemotherapy of Triple-Negative Breast Cancer Cells

Chandran Murugan, Hyoryong Lee, and Sukho Park *

Department of Robotics and Mechatronics Engineering, Daegu Gyeongbuk Institute of Science and
Technology (DGIST), Daegu 42988, Republic of Korea.

***Corresponding author.**

Prof. Sukho Park

Department of Robotics and Mechatronics Engineering,

Multiscale Biomedical Robotics Laboratory,

Daegu Gyeongbuk Institute of Science and Technology, Republic of Korea.

E-mail address: shpark12@dgist.ac.kr (S. Park).

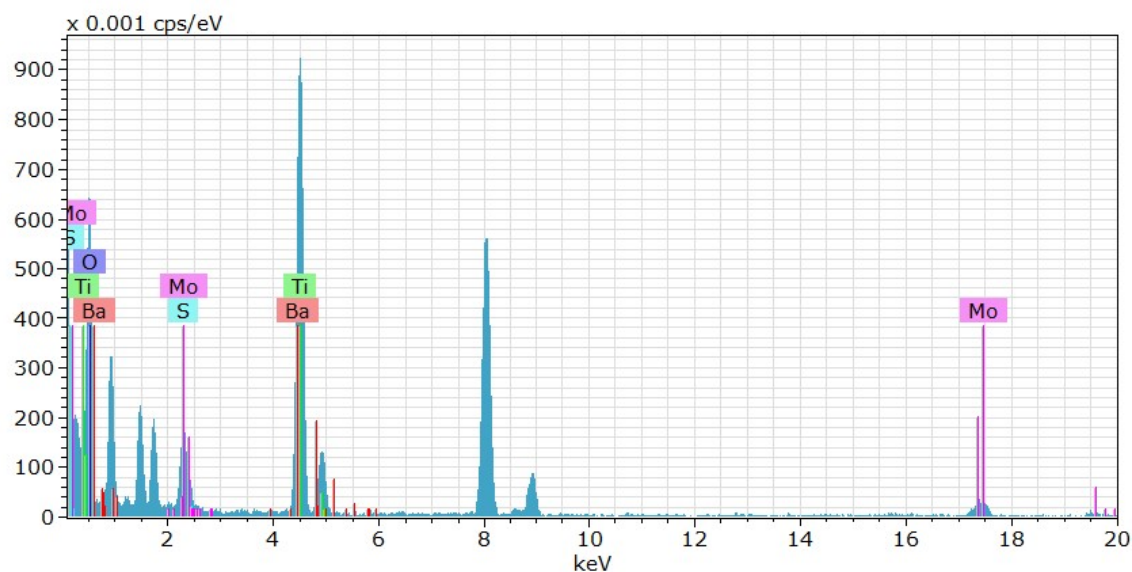


Figure S1. EDAX pattern of MoS₂@BT CSNPs.

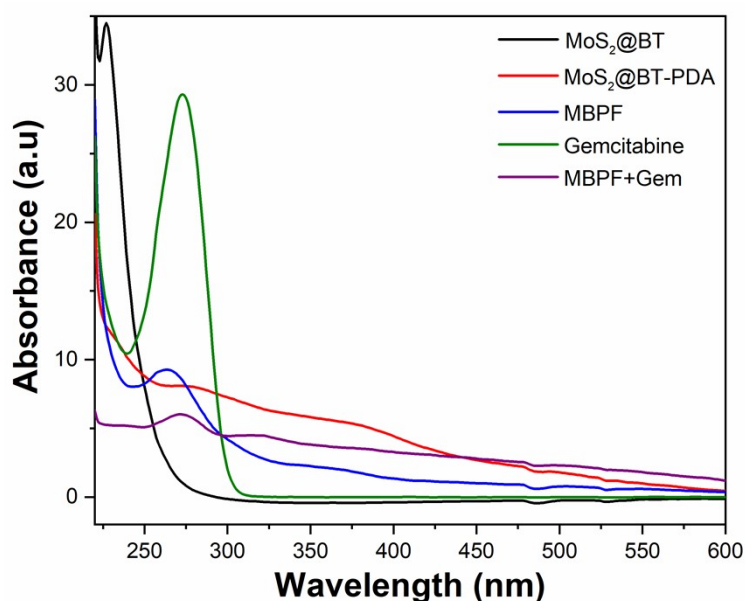


Figure S2. The UV-Visible spectrum of MoS₂@BT, MoS₂@BT-PDA, MBPF, Gemcitabine, and Gem-loaded MBPF (MBPF+Gem) core-shell nanoparticles.

The UV-Vis spectra of MoS₂@BT, MoS₂@BT-PDA, MBPF, gemcitabine, and Gem-loaded MBPF core-shell nanoparticles are shown in Figure S3. The UV-vis absorption spectrum of pure MoS₂@BT indicates that it can absorb light from 200 to 800 nm, which is consistent with the findings of other studies [1-3]. The characteristic absorption peak of PDA is visible after its coating on the MoS₂@BT, and it was noted at 350 nm due to the formation of quinone, which is consistent with the proposed mechanism of polymerization [4]. Pure folic acid displays two UV-Vis absorbance peaks at 280 nm and 360 nm for the n-π* and π-π* transitions, respectively. These two distinct peaks in the MBPF demonstrate that folic acid is effectively attached to the MBPF [5]. Gemcitabine exhibits a

prominent peak at about 270 nm, and the presence of Gem in the MBPF CSNPs was confirmed by a slight shift in the peak in the Gem-loaded MBPF [6].

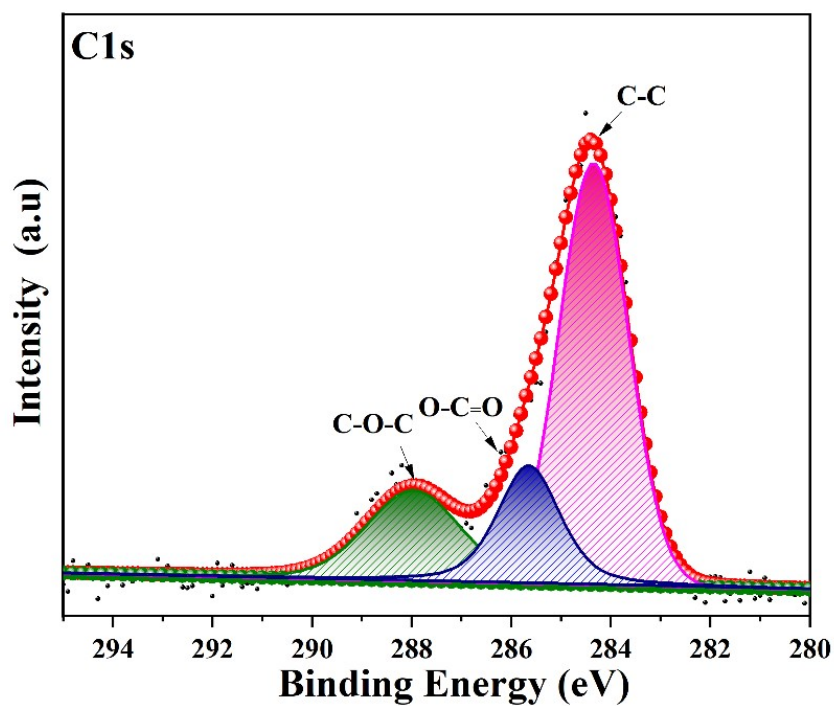


Figure S3. XPS spectrum of carbon atom in the MoS₂@BT CSNPs.

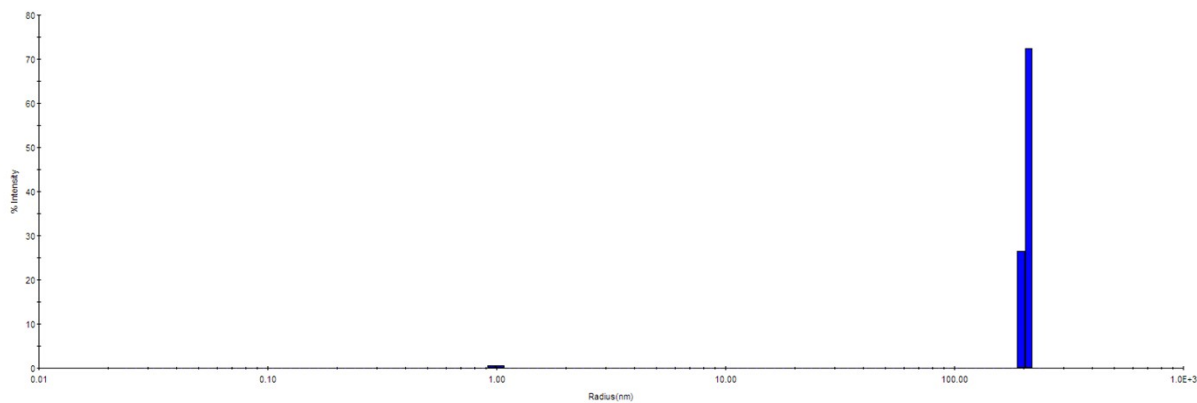


Figure S4. Dynamic light scattering (DLS) measurement showed the size distribution of MBPF CSNPs.

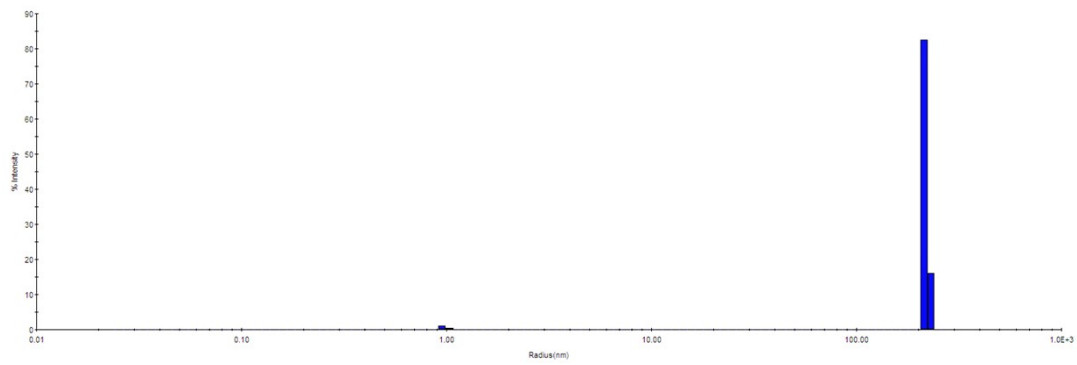


Figure S5. The stability of MBPF CSNPs was determined after 1 week of incubation with PBS (pH 7.4).

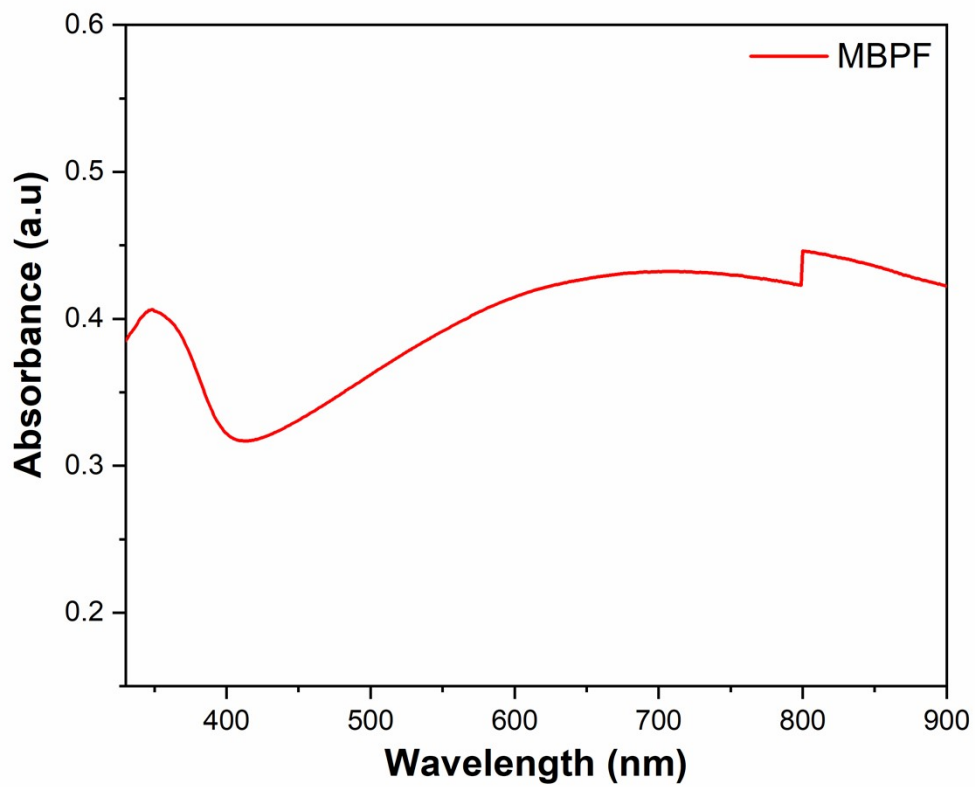


Figure S6. UV-Visible NIR spectrum of MBPF showed a strong band at NIR region.

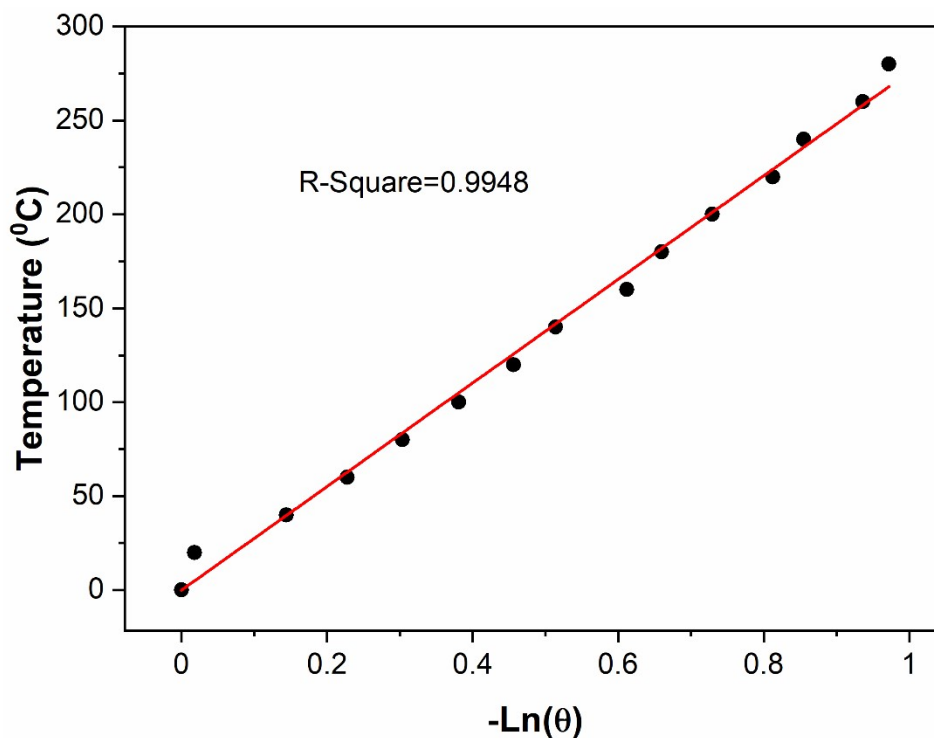


Figure S7. Linear fitting curve of T and $-\ln(\theta)$ at cooling phase.

References

1. Li, J., Liu, X., Pan, L., Qin, W., Chen, T. and Sun, Z., 2014. MoS₂-reduced graphene oxide composites synthesized via a microwave-assisted method for visible-light photocatalytic degradation of methylene blue. *RSC Adv* 4:9647–9651.
2. Laursen, A.B., Pedersen, T., Malacrida, P., Seger, B., Hansen, O., Vesborg, P.C. and Chorkendorff, I., 2013. MoS₂—an integrated protective and active layer on n+ p-Si for solar H₂ evolution. *Physical Chemistry Chemical Physics*, 15(46), pp.20000-20004.
3. Rastogi, M., Kushwaha, H.S. and Vaish, R., 2016. Highly efficient visible light-mediated azo dye degradation through barium titanate decorated reduced graphene oxide sheets. *Electronic Materials Letters*, 12(2), pp.281-289.
4. Mazario, E., Sánchez-Marcos, J., Menéndez, N., Herrasti, P., García-Hernández, M. and Muñoz-Bonilla, A., 2014. One-pot electrochemical synthesis of polydopamine coated magnetite nanoparticles. *RSC Advances*, 4(89), pp.48353-48361.
5. Chowdhuri, A.R., Laha, D., Pal, S., Karmakar, P. and Sahu, S.K., 2016. One-pot synthesis of folic acid encapsulated upconversion nanoscale metal organic frameworks for targeting, imaging and pH responsive drug release. *Dalton Transactions*, 45(45), pp.18120-18132.
6. Mishra, S., Narendran, S.T., Babu, B., Mukherjee, K. and Meyyanathan, S.N., 2019. Validated Analytical Method for the Estimation of Gemcitabine from its Pharmaceutical Formulation by RP-HPLC. *Research Journal of Pharmacy and Technology*, 12(11), pp.5407-5412.