

## Supporting Information

### Hybrid system {W<sub>6</sub>I<sub>8</sub>}-cluster/dsDNA as an agent for targeted X-ray induced photodynamic therapy of cancer stem cells

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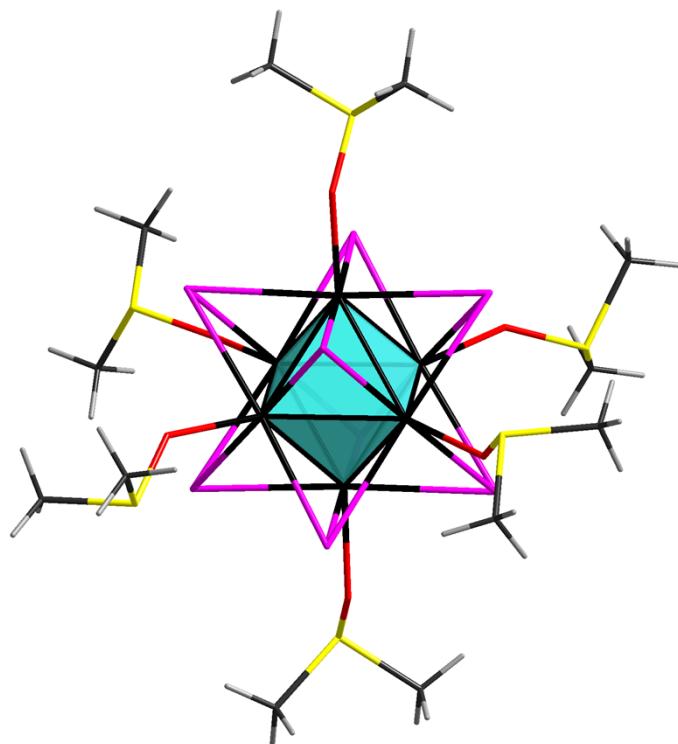
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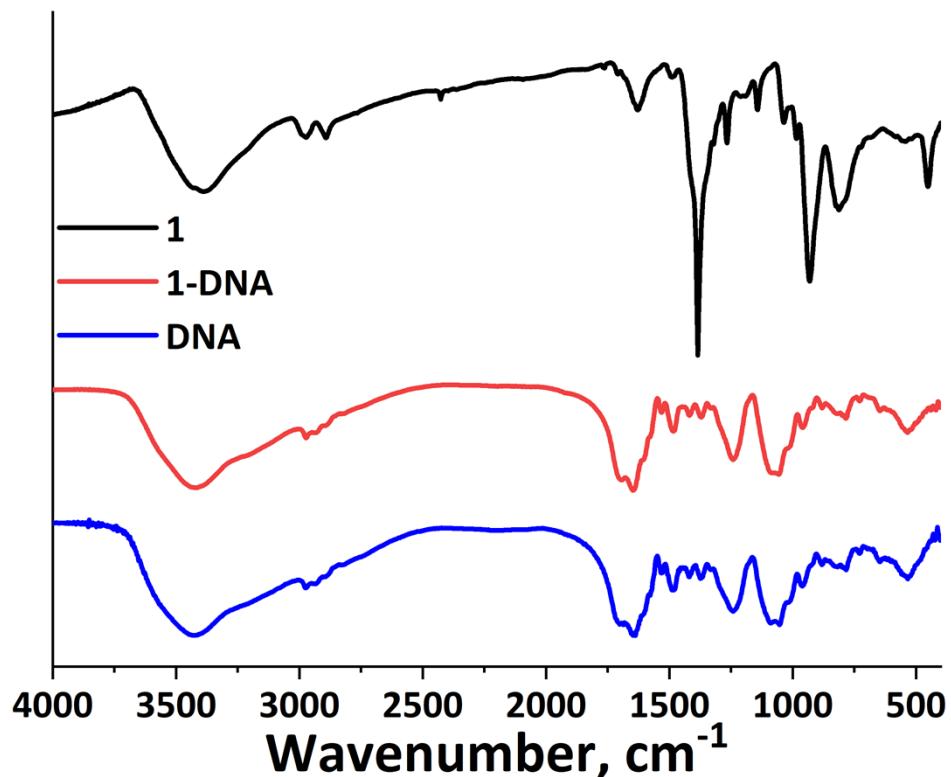
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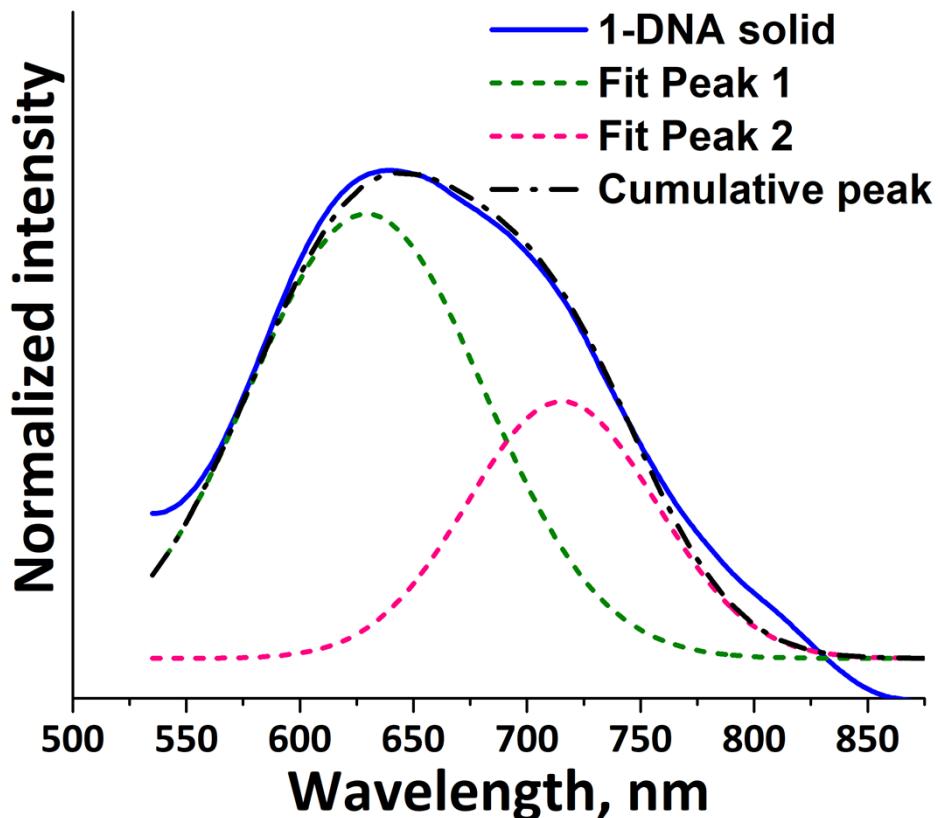
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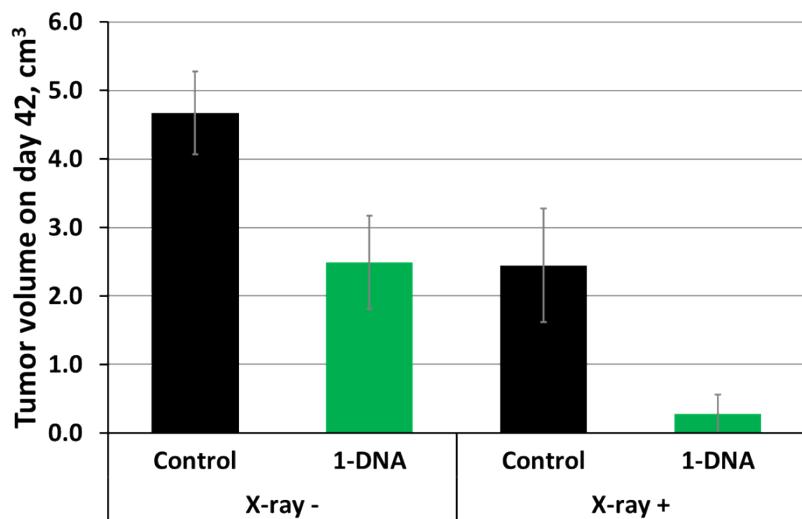
**Figure S1.** Structure of the cation  $[\{Mo_6I_8\}(DMSO)_6]^{4+}$  which is isostructural to  $[\{W_6I_8\}(DMSO)_6]^{4+}$ .<sup>1</sup>



**Figure S2.** FTIR spectra of **1**, DNA and **1**-DNA.



**Figure S3.** Deconvolution of the emission spectra of 1-DNA in solid state.  $\lambda_{\text{max}}$  (peak 1) = 629 nm,  $\lambda_{\text{max}}$  (peak 2) = 715 nm.



**Figure S4.** Tumor volume on day 42 after injection with non-irradiated (X-ray -) and irradiated with X-rays (X-ray +) control Krebs-2 cells (black) and cells incubated with 1-DNA (green).

## References

1. E. V. Svezhentseva, Y. A. Vorotnikov, A. O. Solovieva, T. N. Pozmogova, I. V. Eltsov, A. A. Ivanov, D. V. Evtushok, S. M. Miroshnichenko, V. V. Yanshole, C. J. Eling, A. M. Adawi, J. S. G. Bouillard, N. V. Kuratieva, M. S. Fufaeva, L. V. Shestopalova, Y. V. Mironov, O. A. Efremova and M. A. Shestopalov, *Chem-Eur J*, 2018, **24**, 17915-17920. <https://doi.org/10.1002/chem.201804663>