

## Supporting Information

### Water-soluble hybrid materials based on $\{\text{Mo}_6\text{X}_8\}^{4+}$ (X = Cl, Br, I) cluster complexes and sodium polystyrene sulfonate

Ekaterina V. Svezhentseva,<sup>ab</sup> Anastasiya O. Solovieva,<sup>c</sup> Yuri A. Vorotnikov,<sup>a</sup> Olga G. Kurskaya,<sup>d</sup> Konstantin A. Brylev,<sup>ab</sup> Alphiya R. Tsygankova,<sup>ab</sup> Mariya V. Edeleva,<sup>e</sup> Svetlana N. Gyrylova,<sup>d</sup> Noboru Kitamura,<sup>f</sup> Olga A. Efremova,<sup>g\*</sup> Michael A. Shestopalov,<sup>abcd\*</sup> Yuri V. Mironov,<sup>ab</sup> Alexander M. Shestopalov<sup>d</sup>

<sup>a</sup>*Nikolaev Institute of Inorganic Chemistry SB RAS, 3 Acad. Lavrentiev Ave., 630090 Novosibirsk, Russian Federation.*

<sup>b</sup>*Novosibirsk State University, 2, Pirogova Str., 630090 Novosibirsk, Russian Federation*

<sup>c</sup>*Scientific Institute of Clinical and Experimental Lymphology, 2 Timakova Str., 630060 Novosibirsk, Russian Federation*

<sup>d</sup>*Research Institute of Experimental and Clinical Medicine, 2 Timakova Str., 630060 Novosibirsk, Russian Federation*

<sup>e</sup>*Vorozhtsov Novosibirsk Institute of Organic Chemistry SB RAS, 9 Acad. Lavrentiev Ave, 630090 Novosibirsk, Russian Federation*

<sup>f</sup>*Department of Chemistry, Faculty of Science, Hokkaido University, 060-0810 Sapporo, Japan*

<sup>g</sup>*Department of Chemistry, University of Hull, Cottingham Road, Hull, HU6 7RX, UK*

\*Corresponding Authors:

Michael A. Shestopalov

Tel. +7-383-330-92-53, Fax +7-383-330-94-89

e-mail: [shtopy@niic.nsc.ru](mailto:shtopy@niic.nsc.ru)

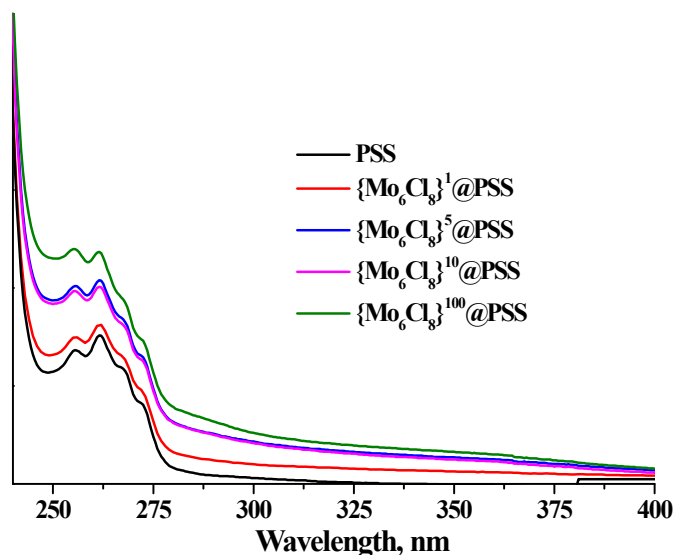
Olga A. Efremova

Tel. +441482465417, Fax +441482466410

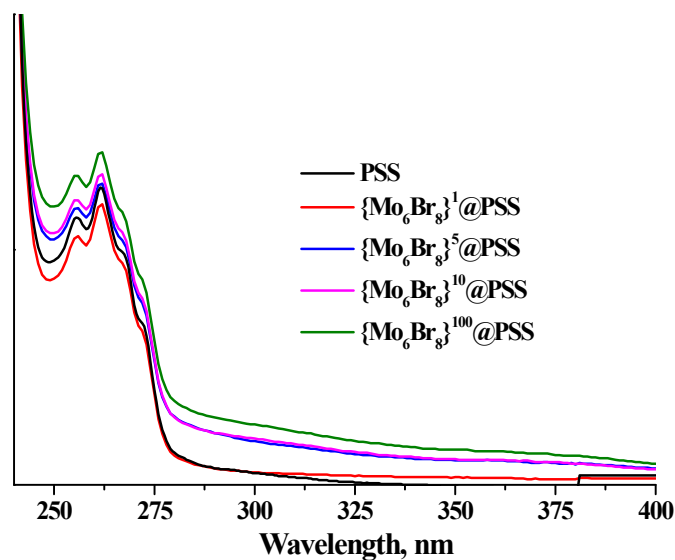
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## Content

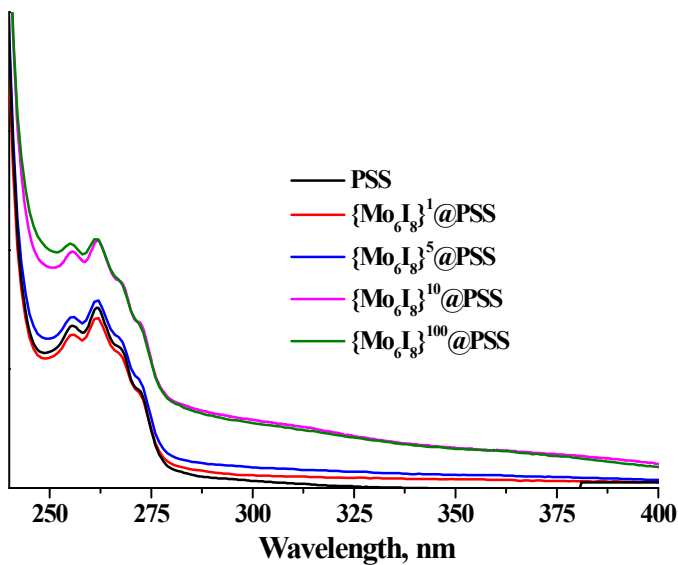
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**Figure S1.** UV-vis spectra of PSS and  $\{\text{Mo}_6\text{Cl}_8\}^n\text{@PSS}$  ( $n = 1, 5, 10, 100$ ) in aqueous solution.



**Figure S2.** UV-vis spectra of PSS and  $\{\text{Mo}_6\text{Br}_8\}^n\text{@PSS}$  ( $n = 1, 5, 10, 100$ ) in aqueous solution.



**Figure S3.** UV-vis spectra of PSS and  $\{\text{Mo}_6\text{I}_8\}^n\text{@PSS}$  ( $n = 1, 5, 10, 100$ ) in aqueous solution.

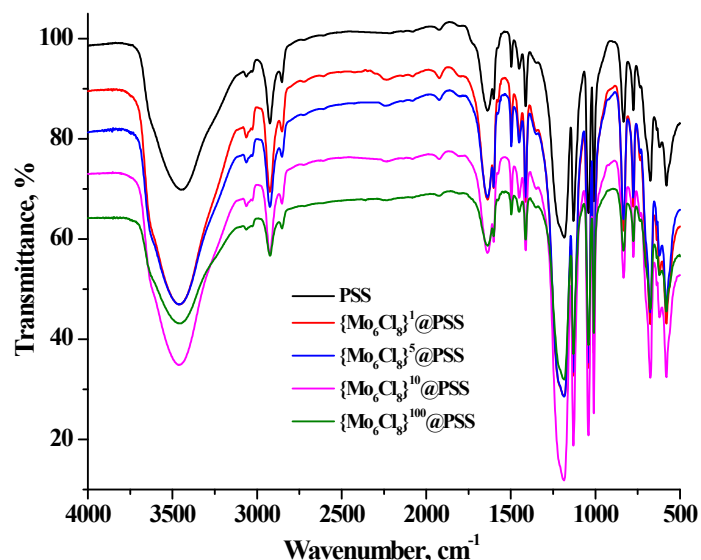


Figure S4. FTIR-spectra of PSS and  $\{\text{Mo}_6\text{Cl}_8\}^n\text{@PSS}$  ( $n = 1, 5, 10, 100$ ).

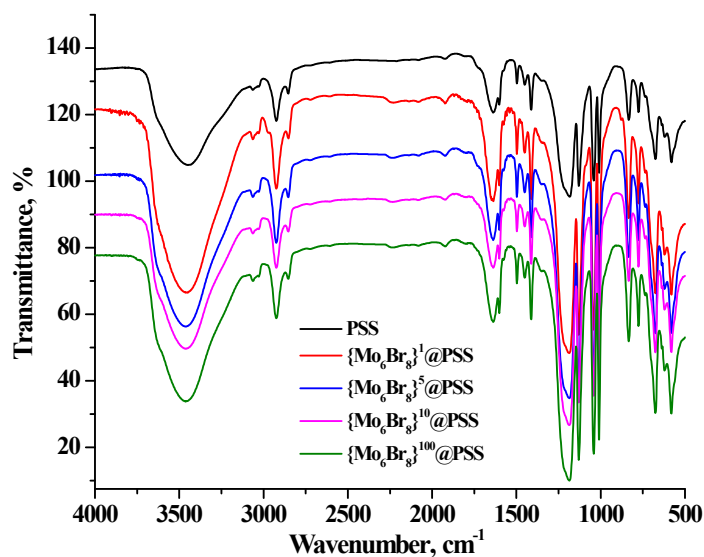


Figure S5. FTIR-spectra of PSS and  $\{\text{Mo}_6\text{Br}_8\}^n\text{@PSS}$  ( $n = 1, 5, 10, 100$ ).

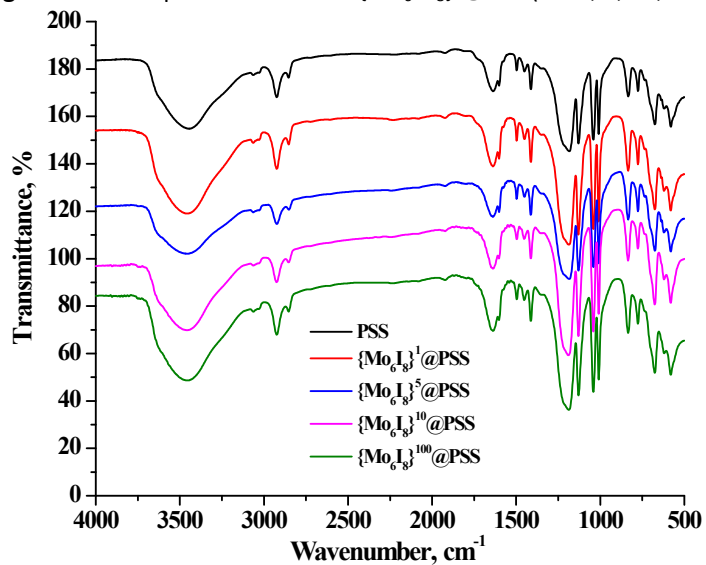
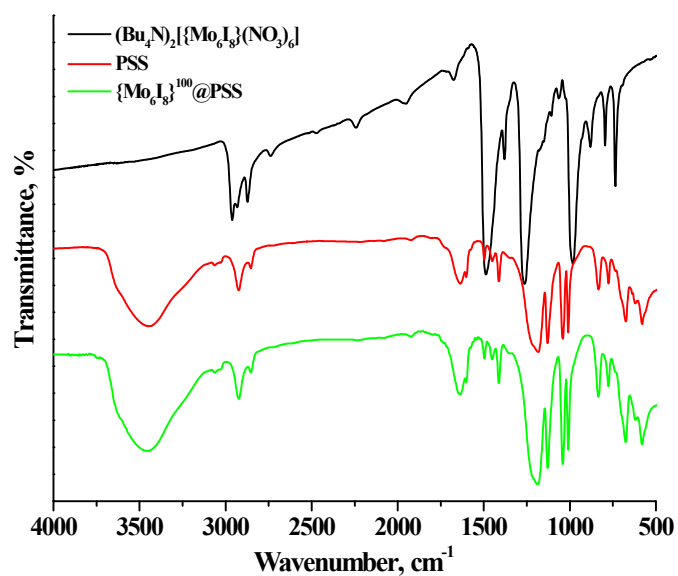
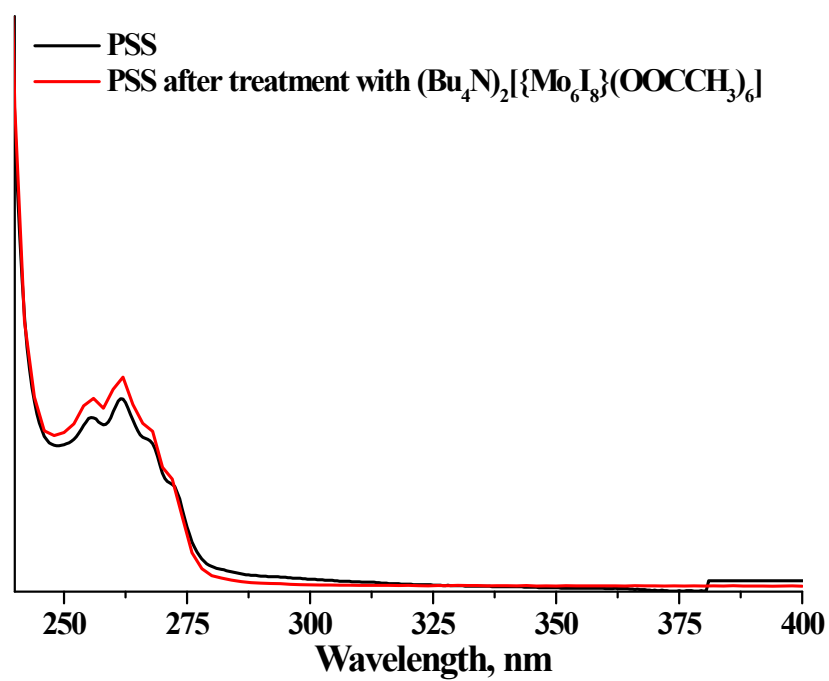


Figure S6. FTIR-spectra of PSS and  $\{\text{Mo}_6\text{I}_8\}^n\text{@PSS}$  ( $n = 1, 5, 10, 100$ ).



**Figure S7.** FTIR-spectra of PSS, (Bu<sub>4</sub>N)<sub>2</sub>[{Mo<sub>6</sub>I<sub>8</sub>}(NO<sub>3</sub>)<sub>6</sub>] and {Mo<sub>6</sub>I<sub>8</sub>}<sup>100</sup>@PSS.



**Figure S8.** UV-vis spectra of pure PSS and after treatment with (Bu<sub>4</sub>N)<sub>2</sub>[{Mo<sub>6</sub>I<sub>8</sub>}(OOCCH<sub>3</sub>)<sub>6</sub>].

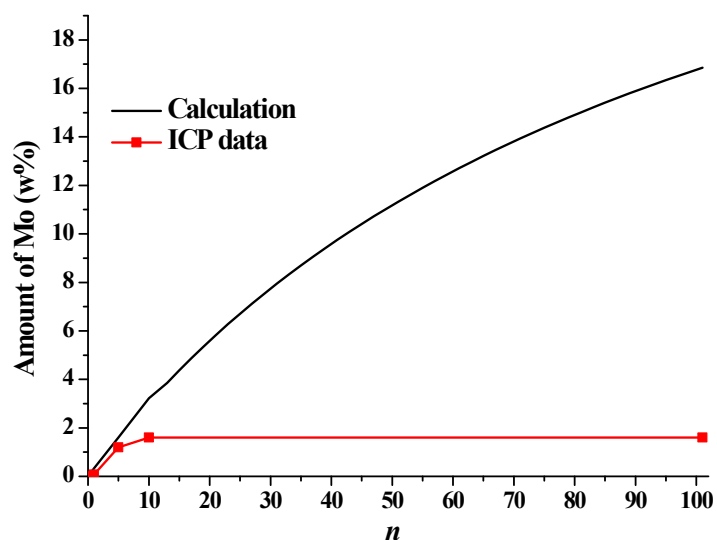


Figure S9. Mo concentration: calculated (black) and based on ICP-AES data (red) for  $\{\text{Mo}_6\text{Cl}_8\}^n\text{@PSS}$  ( $n = 1, 5, 10, 100$ ).

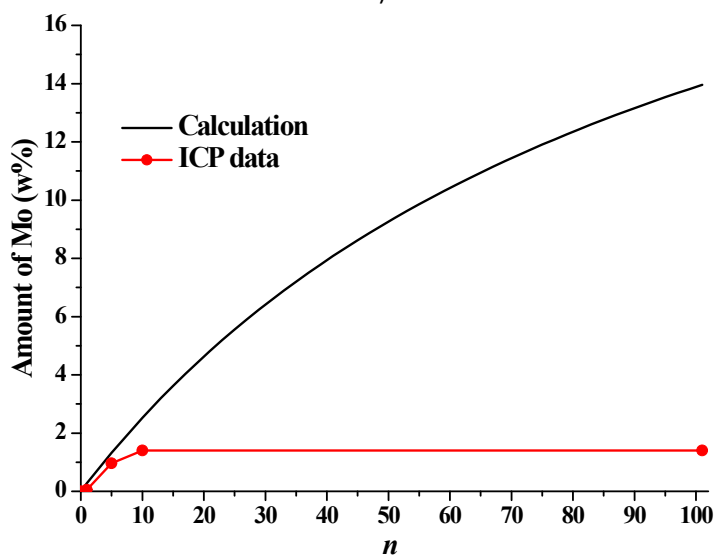


Figure S10. Mo concentration: calculated (black) and based on ICP-AES data (red) for  $\{\text{Mo}_6\text{Br}_8\}^n\text{@PSS}$  ( $n = 1, 5, 10, 100$ ).

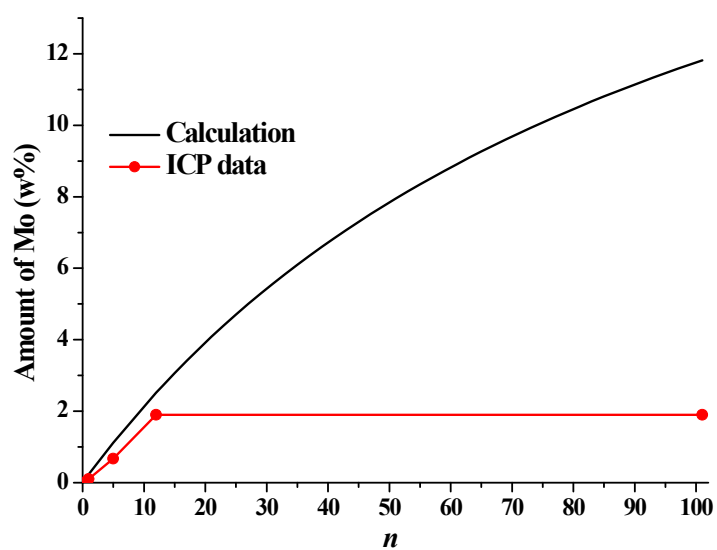
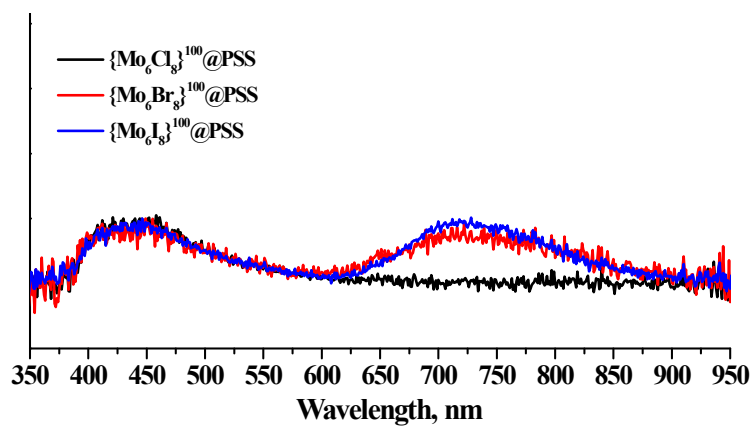
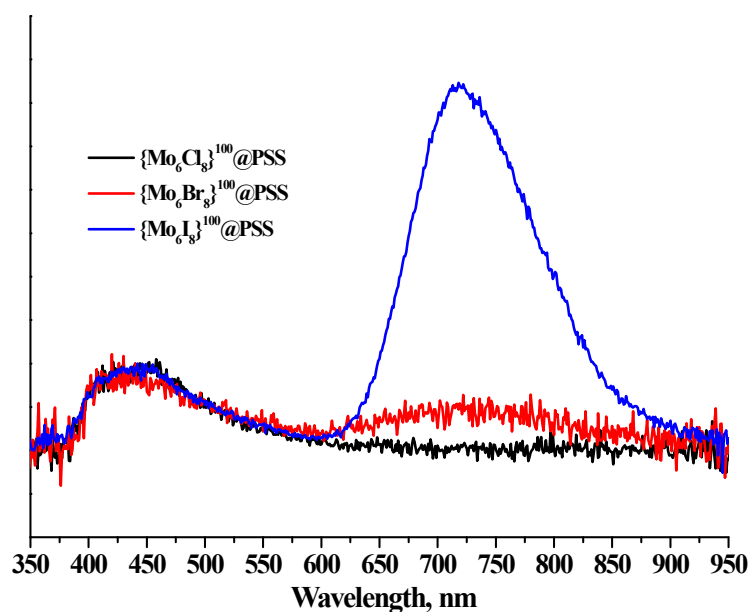


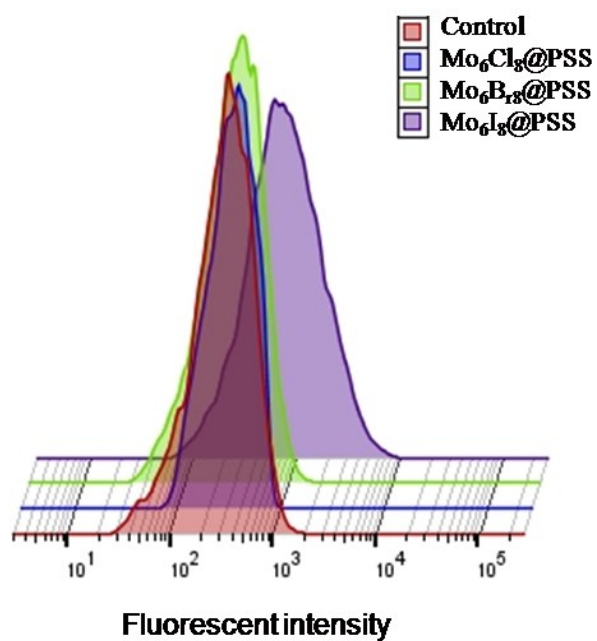
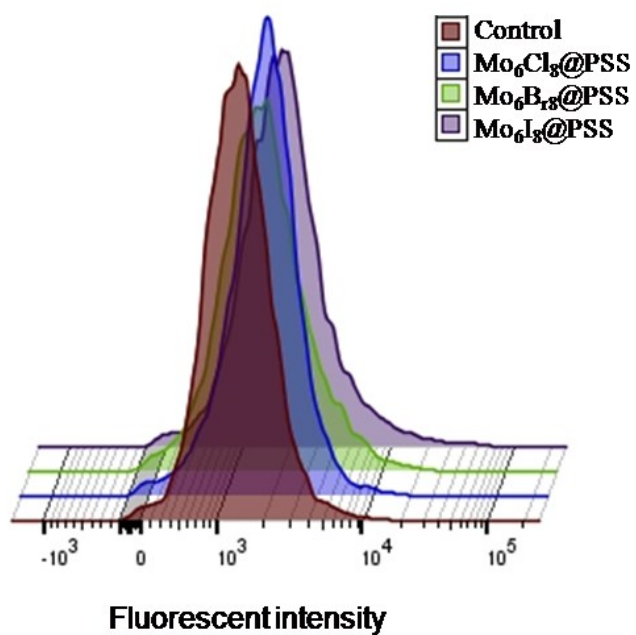
Figure S11. Mo concentration: calculated (black) and based on ICP-AES data (red) for  $\{\text{Mo}_6\text{I}_8\}^n\text{@PSS}$  ( $n = 1, 5, 10, 100$ ).



**Figure S12.** Emission spectra of  $\{\text{Mo}_6\text{X}_8\}^{100}\text{@PSS}$  normalized on maximum of PSS emission in aerated aqueous solution.



**Figure S13.** Emission spectra of  $\{\text{Mo}_6\text{X}_8\}^{100}\text{@PSS}$  normalized on maximum of PSS emission in deaerated aqueous solution.



**Figure S14.** Cellular uptake of  $\{\text{Mo}_6\text{X}_8\}^{100}@\text{PSS}$  determined by FACS. Representative flow cytometry histogram plot of HeLa (left) and Hep-2 (right) cells incubated for 24 hours with  $\{\text{Mo}_6\text{X}_8\}^{100}@\text{PSS}$ . Excitation wavelength – 488 nm; emission filter – 695 nm.