## Hybrid HPV capsid protein L1 and giant, Mo-containing polyoxometalate improves the stability of virus-like particles and the anti-tumor effect of [Mo<sub>154</sub>]

## (ESI)

Ya-Rong Xue,<sup>a</sup> Yu Wang,<sup>a</sup> Gang Chen,<sup>a</sup> Bo Sun,<sup>\*b</sup> Bao Li,<sup>a</sup> Lixin Wu<sup>a</sup> and Yuqing Wu<sup>\*a</sup>

<sup>a</sup>State Key Laboratory of Supramolecular Structure and Materials, Institute of Theoretical Chemistry, College of Chemistry; <sup>b</sup>National Engineering Laboratory for AIDS Vaccine, School of Life Sciences, Jilin University, Changchun, 130012, China. E-mail: <u>yqwu@jlu.edu.cn</u>.



**Fig. S1** (A) FPLC elution profile of HPV 16 L1 in different NaCl concentrations, and (B) the corresponding SDS-PAGE for the products: panel 6-9 are the elution from 80% NaCl while those at panel 2-5 are from 60% NaCl for comparison.



Fig. S2 UV-vis absorption spectrum and the corresponding intensity of  $[Mo_{154}]$  at different concentrations. No aggregate was shown for  $[Mo_{154}]$  among the test concentration range.



**Fig. S3** DLS histogram of (A)  $[Mo_{154}]$  in buffer A; the mixture of (B) L1-p and  $[Mo_{154}]$ , (C) asprepared VLPs and  $[Mo_{154}]$ , and (D) the extract of F1#b as control after CsCl gradient ultracentrifugation. The final concentration of protein and  $[Mo_{154}]$  is 10  $\mu$ M, respectively.



**Fig. S4** Size distributions of (A)  $[Mo_{154}]@VLPs$ , (C) VLPs@ $[Mo_{154}]$  being stained with 2% phosphotungstate 2 min before measurements; and those of (B)  $[Mo_{154}]@VLPs$ , (D) VLPs@ $[Mo_{154}]$  without negative stain. They are evaluated based on 200 particles obtained from the corresponding TEM images.



**Fig. S5** Energy-dispersive X-ray spectrum (EDS) measured on a representative particle shown in the TEM image for (A)  $[Mo_{154}]@VLPs$ , (C) VLPs@ $[Mo_{154}]$  stained with 2% phosphotungstate 2 min before measurements; (B)  $[Mo_{154}]@VLPs$ , (D) VLPs@ $[Mo_{154}]$  without stain. The Cu shown is a copper net rather than pollutants in the sample.



Fig. S6 UV/Vis absorption spectrum of [Mo154] and [Mo154]@VLPs in assembly buffer solution (4  $\mu$ M), respectively.



Fig. S7 (A) UV-vis absorption spectra of [Mo154] (10  $\mu$ M) under the irradiation of 808 nm for 0, 5, and 10 min, respectively. (B) Photothermal heating curves of 10  $\mu$ M [Mo154] and 10  $\mu$ M [Mo154]@VLPs in the assembly buffer, respectively, and the blank buffer solution under irradiation of 808 nm (1 W cm<sup>-2</sup>).