

## Supporting Information

### **A supramolecular complex based Gd-containing polyoxometalate for MRI/CT imaging and NIR-Triggered Photothermal therapy**

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# Supporting Information

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## Structure Characterization of the peptide

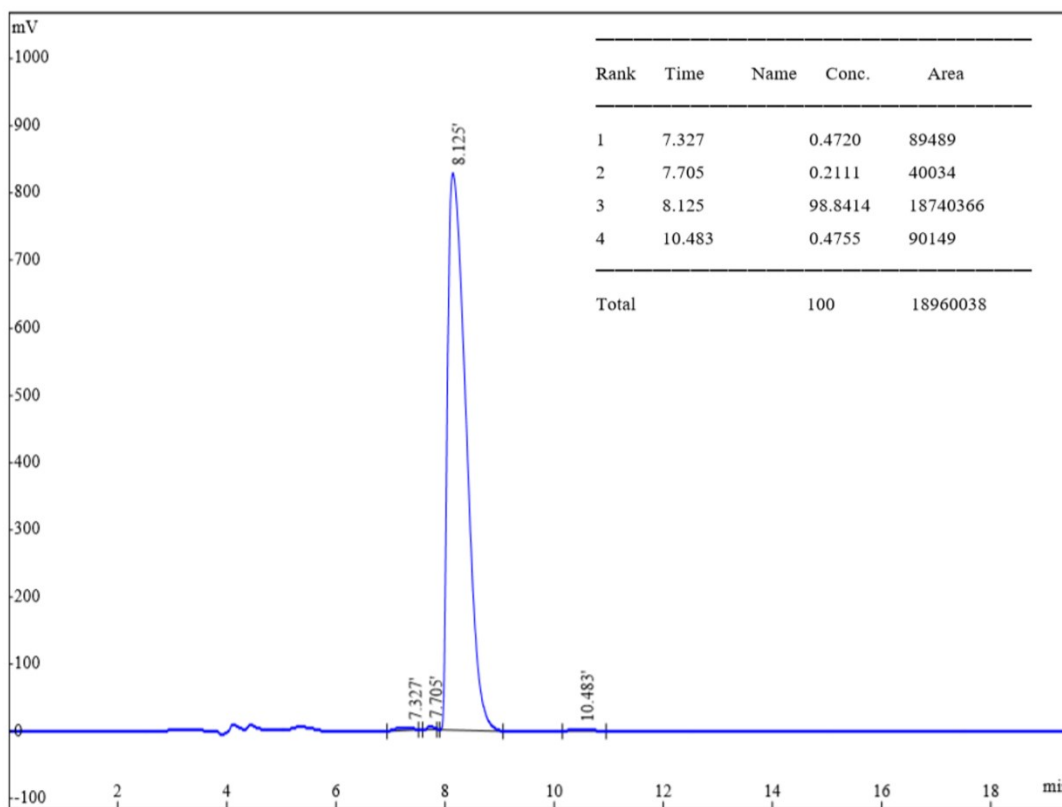


Figure S1. HPLC chromatograms of KDHCCHVTPY.

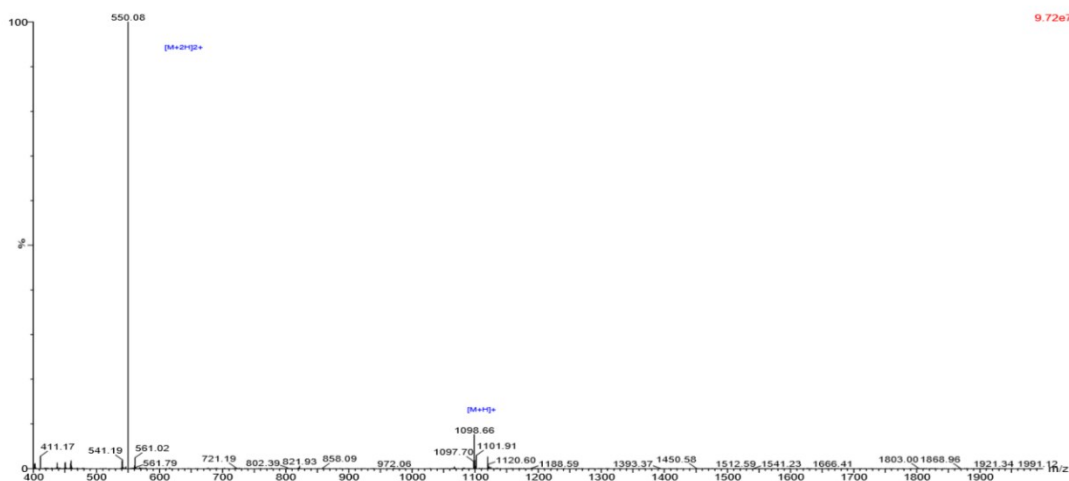
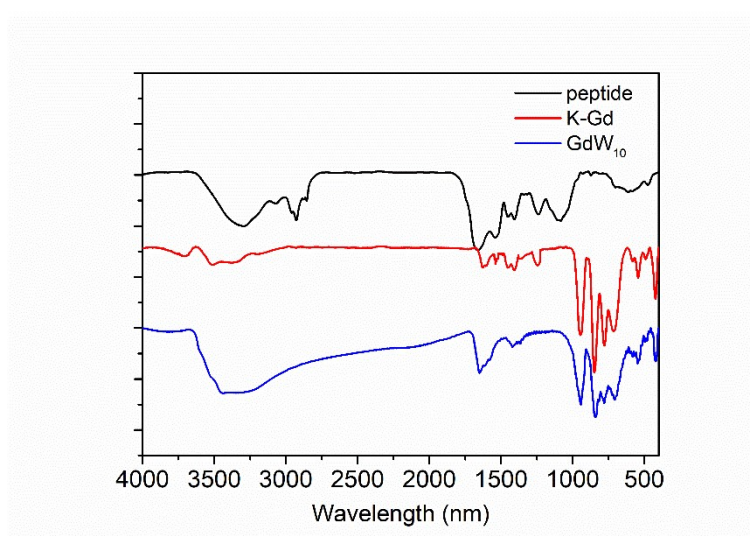


Figure S2. MALDI-TOF mass spectrum of KDHCCHVTPY peptide.



**Figure S3.** FT-IR spectra of pure GdW<sub>10</sub>, peptide KDHCHVTPY, and K-Gd in KBr pellets.

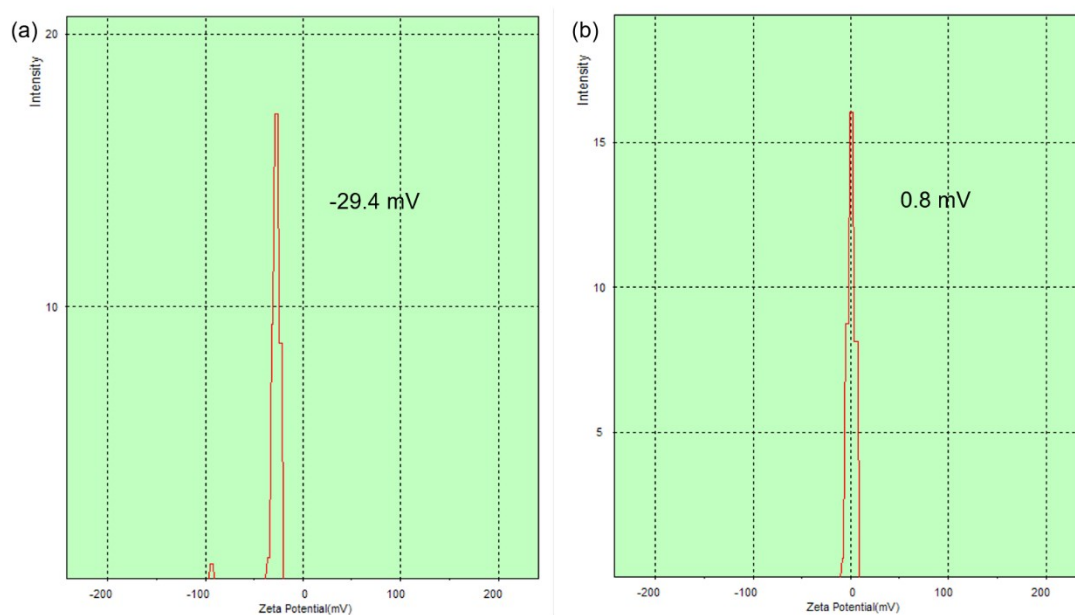
**Table S1.** The assignments of infrared spectra of pure GdW<sub>10</sub>, peptide KDHCHVTPY, and K-Gd in solid state.

peptide /cm <sup>-1</sup>	K-Gd /cm <sup>-1</sup>	Assignment	peptide /cm <sup>-1</sup>	K-Gd /cm <sup>-1</sup>	Assignment
1672	1672	-CO-NH-	1000-1300	1000-1300	C-O, C-OH, C-N
1538	1538	C=C frame str.		946	W=O <sub>d</sub>
1450	1452	CH <sub>2</sub> scissoring		847	W-O <sub>b</sub> -W
1411	1408	CH <sub>2</sub> wagging		782	W-O <sub>c</sub> -W
1335	1333	CH <sub>2</sub> wagging		714	W-O <sub>c</sub> -W
1248	1252	CH <sub>2</sub> twisting	722	722	C-S

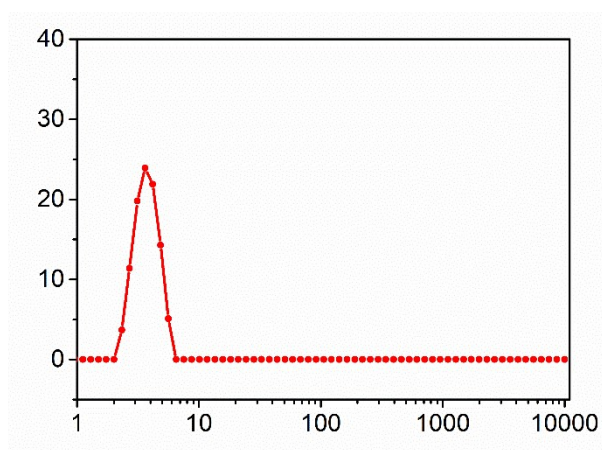
**Table S2.** The summary of elemental analysis for the prepared complex K-Gd.<sup>[a]</sup>

	C	H	N	S	Gd	W
Calcd. (%)	27.49	3.36	9.35	1.53	3.75	43.83
Found (%)	27.12	3.55	9.23	1.33	3.69	43.55

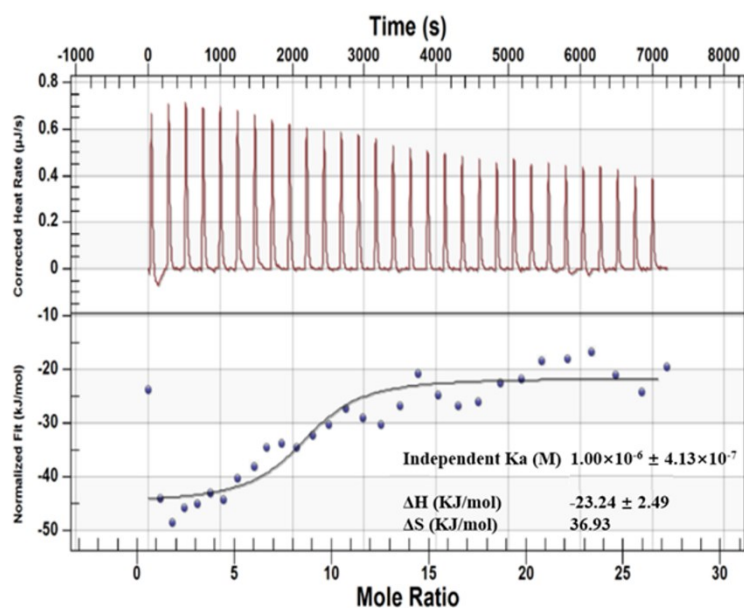
[a] The elemental analytical results of C, H, N and S were obtained from organic elemental analysis, and the elemental analysis of Gd, W was performed on inductive coupled plasma emission spectrometer.



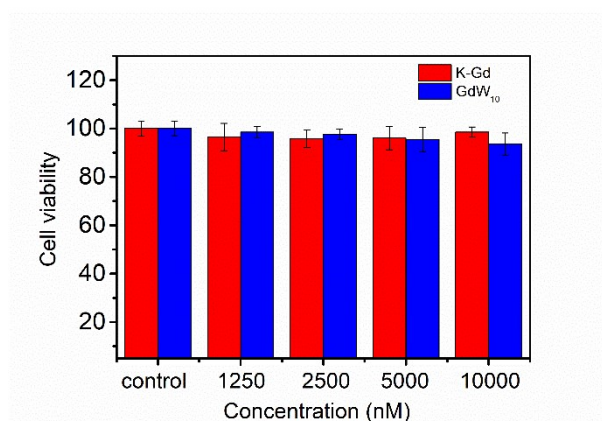
**Figure S4.** Zeta potential of (a) GdW<sub>10</sub> and (b) K-Gd in aqueous solution.



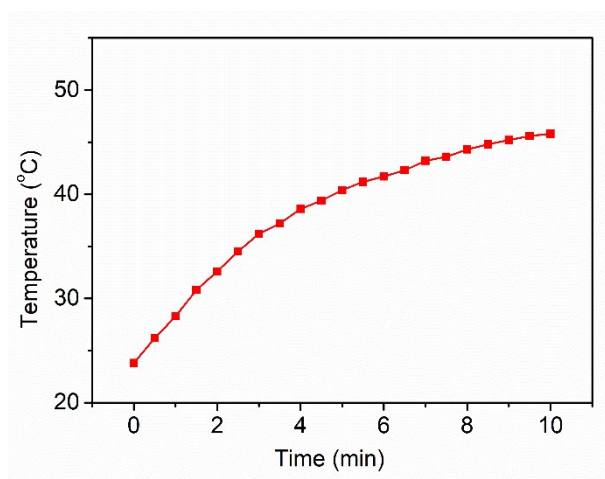
**Figure S5.** DLS curves of K-Gd in dulbecco's modified eagle medium (DMEM) culture medium solution.



**Figure S6.** Isothermal titration calorimetric curves of the thermogram and the isotherm corresponding to  $GdW_{10}$  binding to peptide Lys-Asp-His-Cys-His-Val-Thr-Pro-Tyr.



**Figure S7.** Columnar plots of viability of HepG2 cells after incubation for 24 h in the presence of K-Gd and  $GdW_{10}$  versus the increase in their concentrations.



**Figure S8.** Photothermal heating curves of rK-Gd aqueous solution under 808 nm laser irradiation at a power density of 0.5 W/cm<sup>2</sup> for 10 min.