

## Supporting Information

### **Four Polyoxonibate-Based Inorganic-Organic Hybrids Assembly from Bicapped Heteropolyoxonibate with Effective Antitumor Activity**

Ying Zhang,<sup>a</sup> Jian-Qiang Shen,<sup>a</sup> Li-Hua Zheng,<sup>b</sup> Zhi-Ming Zhang,<sup>\*a</sup> Yu-Xin Li<sup>b</sup> and En-Bo Wang<sup>\*a</sup>

*<sup>a</sup>Key laboratory of Polyoxometalate Science of Ministry of Education, Department of Chemistry, Northeast Normal University, 130024, Changchun, Jilin, P. R. China;*

*<sup>b</sup>National Engineering Laboratory for Druggable Gene and Protein Screening, Northeast Normal University, 130024, ChangChun, Jilin, P. R. China;*

*E-mail: zhangzm178@nenu.edu.cn (Z. M. Zhang), wangeb889@nenu.edu.cn (E. B. Wang)*

## Table of Contents

**Figure S1.** The 3D supermolecular structure of **1**.

**Figure S2.** (a) Polyhedron representation of the polyoxoanion  $[\text{SiNb}_{12}\text{V}_2\text{O}_{42}]^{12-}$ ; (b) mixed polyhedral and ball-and-stick representation in **4**.

**Figure S3.** The IR spectra of compounds **1-4**.

**Figure S4.** The UV-Vis spectra of compounds **1-4** in solid state.

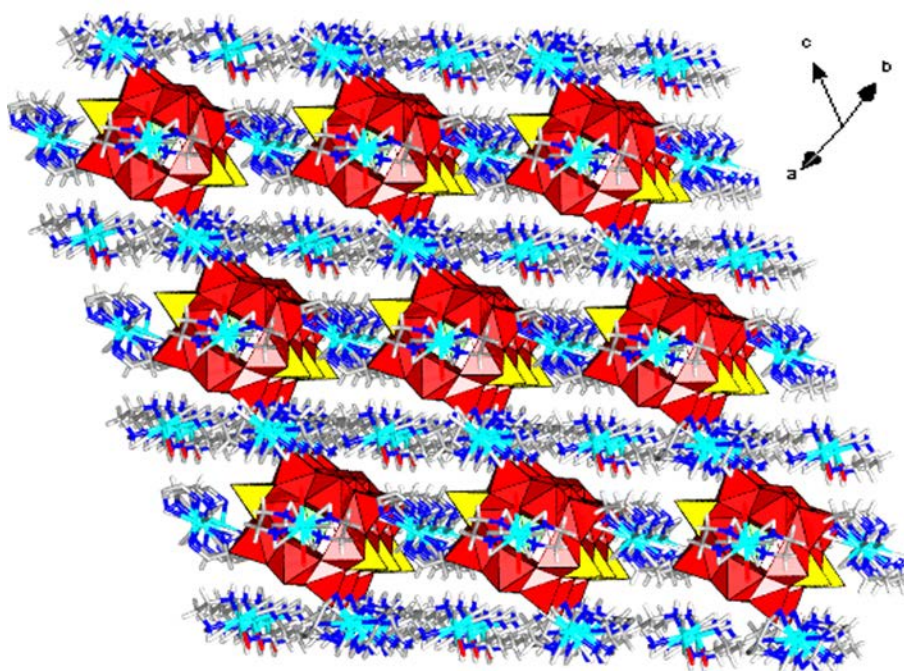
**Figure S5.** The TG curves of compounds **1-4**.

**Figure S6.** CV for  $\text{K}_7\text{HNb}_6\text{O}_{19}$  in 0.2 M KCl solution.

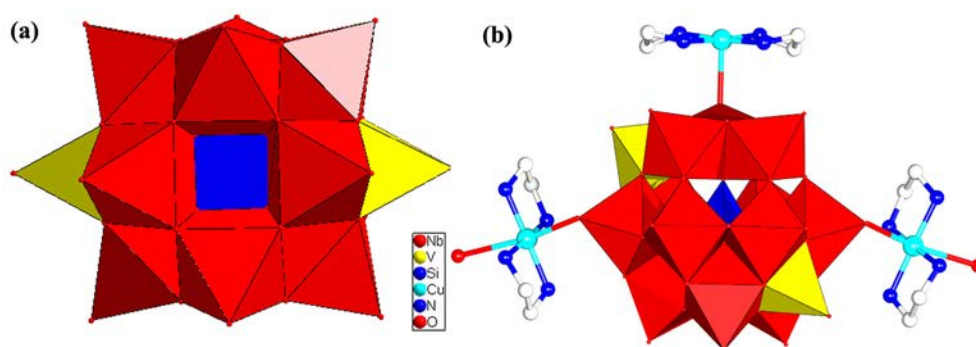
**Figure S7.** The CV and the UV-Vis spectra of **1-4** in 0.2 M KCl solution for five times.

**Figure S8.** Line graph of the inhibition rates of human liver carcinoma HepG2 cells and human gastric cancer SGC7901 cells.

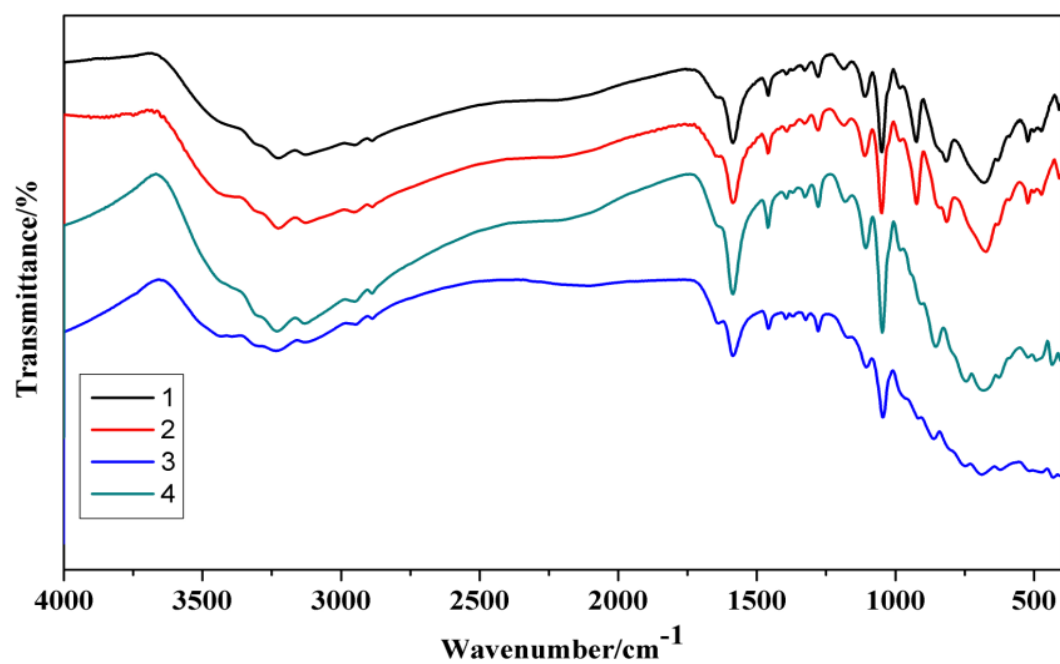
**Table S1.** The IC<sub>50</sub> values of compounds **1-4** against SGC7901 cells and HepG2 cells.



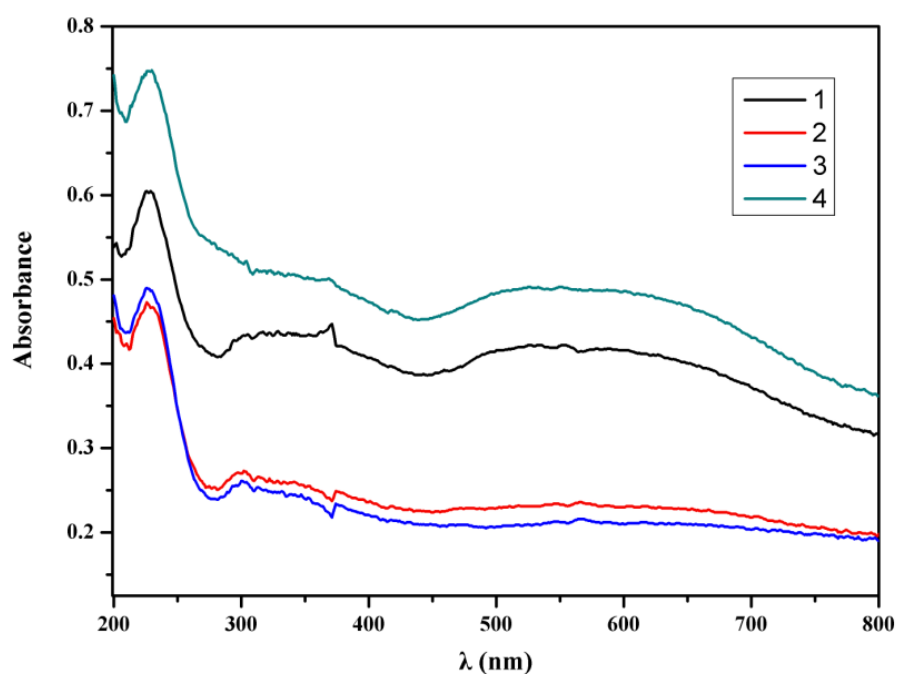
**Figure S1.** The 3D supermolecular structure of **1**.



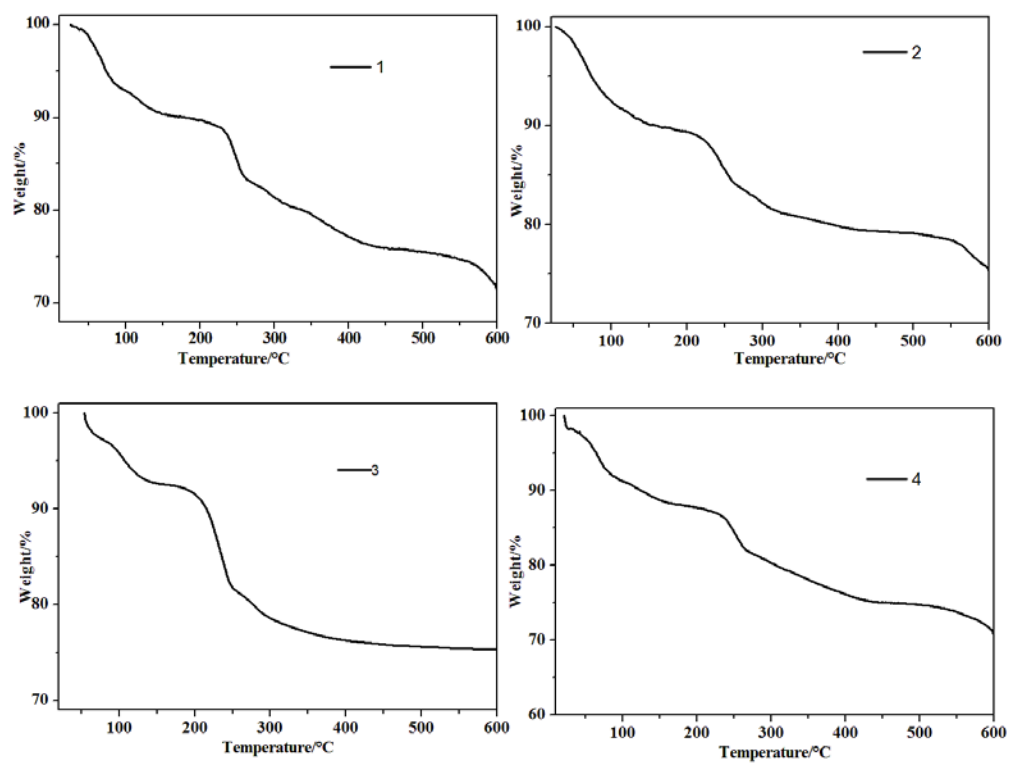
**Figure S2.** (a) Polyhedral representation of the polyoxoanion  $[\text{SiNb}_{12}\text{V}_2\text{O}_{42}]^{12-}$  in **3** and **4**; (b) mixed polyhedral and ball-and-stick representation of tri-supporting polyoxoanion in **4**.



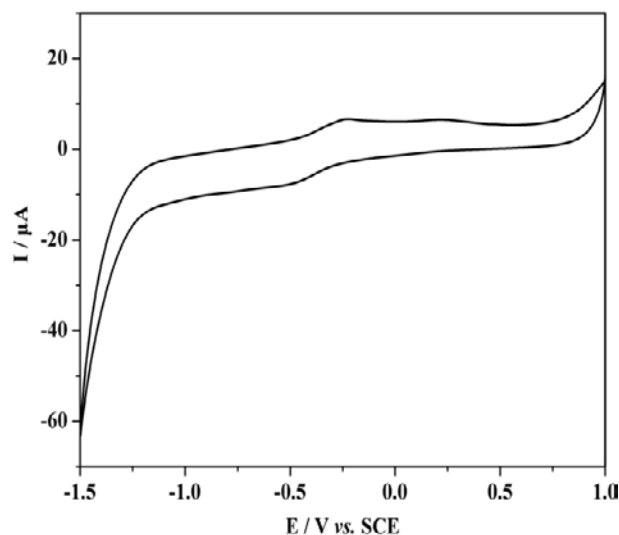
**Figure S3.** The IR spectra of compounds **1-4**.



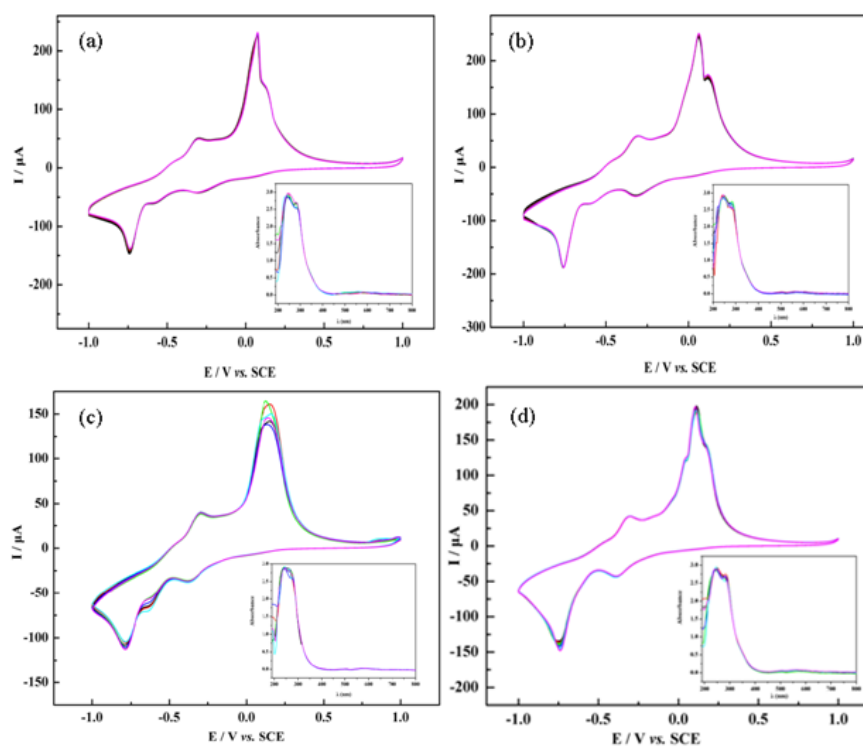
**Figure S4.** The UV-Vis spectra of **1-4** in solid state.



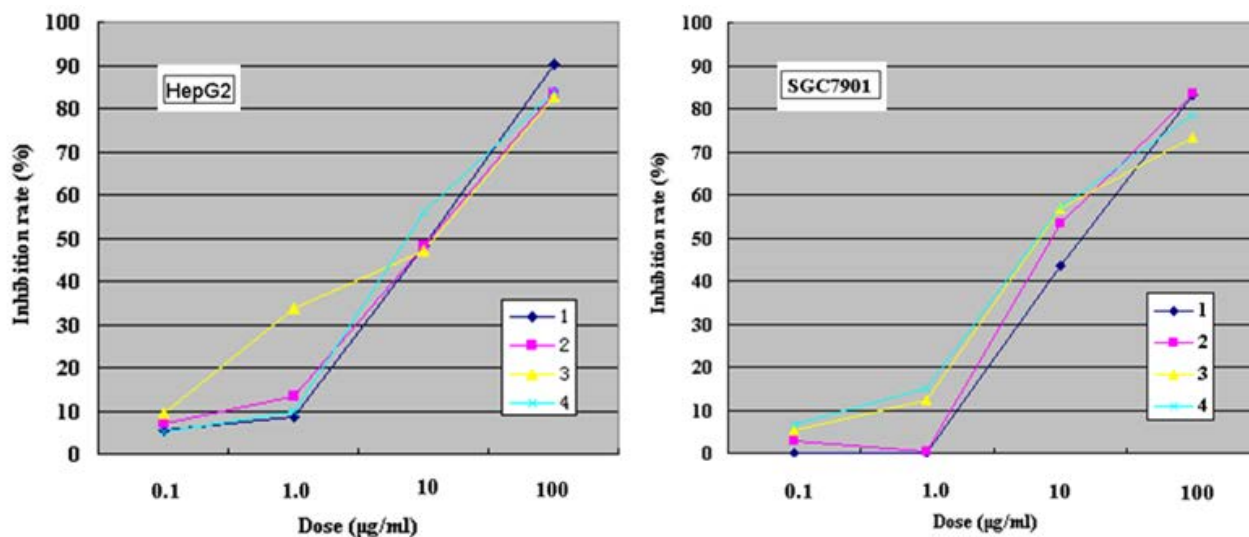
**Figure S5.** The TG curves of compounds **1-4**.



**Figure S6.** CV for  $\text{K}_7\text{HNB}_6\text{O}_{19}$  ( $1.0 \times 10^{-4}$  M) in 0.2 M KCl solution at the scan rate of  $100 \text{ mV s}^{-1}$ ; a GC electrode was used as a working electrode, a platinum wire served as the counter electrode and a  $\text{Hg}/\text{Hg}_2\text{Cl}_2$  electrode as the reference electrode.



**Figure S7.** The CV curves at  $100 \text{ mV s}^{-1}$  and the UV-Vis spectra of **1-4** in 0.2 M KCl solution were detected in every 24 hours and totally detected for five times. A GC electrode was used as a working electrode, a platinum wire served as the counter electrode and a  $\text{Hg}/\text{Hg}_2\text{Cl}_2$  electrode as the reference electrode.



**Figure S8.** Line graph of the inhibition rates of human liver carcinoma HepG2 cells and human gastric cancer SGC7901 cells.

Compound	IC50 values SGC7901 cells (µg/mL)	IC50 values HepG2 cells (µg/mL)
<b>1</b>	17.65 ± 2.53	10.06 ± 3.45
<b>2</b>	13.13 ± 0.64	11.93 ± 0.79
<b>3</b>	12.77 ± 3.19	12.01 ± 2.73
<b>4</b>	9.53 ± 2.68	9.93 ± 1.83

**Table S1.** The IC50 values of compounds **1-4** against SGC7901 cells and HepG2 cells.