Supporting Information

{BiW$_8$O$_{30}$} Exerts Antitumor Effect by Triggering Pyroptosis and Upregulating Reactive Oxygen Species

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1. Experimental Procedures

1.1 Measurements and Materials

IR spectra were recorded in the range of 400-4000cm⁻¹ on an Alpha Centaur FT/IR Spectrophotometer with pressed KBr pellets. The X-ray powder diffraction data was collected on a Bruker AXS D8 Advance diffractometer using Cu-Kα radiation (λ=1.5418 Å) in the 2θ range of 5-50° with a step size of 0.02°. Bi, W, Co and Na were analyzed on a PLASMA-SPEC (I) ICP atomic emission spectrometer. TG analyses were performed on a Perkin Elmer TGA7 instrument in flowing O₂ at a heating rate of 10°C/min. The UV-Vis absorption spectra were recorded using a JASCO V550 UV-Visible spectrophotometer (JASCO International Co., LTD., Tokyo, Japan). Glutathione, oxidized glutathione, glutathione reductase, Nicotinamide adenine dinucleotide phosphate (NADPH), glutathione peroxidase (GPX) and o-phthalaldehyde (OPA) were purchased from Sigma-Aldrich (Shanghai, China). Dynamic light scattering (DLS) and ζ-potential measurements were performed at room temperature with a Malvern Zetasizer nano Z (Malvern Instruments Ltd.). All common laboratory chemicals were reagent grade, purchased from commercial sources and used without further purification.

1.2 Synthesis of (BiW₈) and other compounds

Bi(NO₃)₃·5H₂O(1.0 mmol) dissolved in 1 mL of 6M HCl was added to a solution of Na₂WO₄·2H₂O(10.0 mmol) in 40 mL of deionized water and the mixture was heated to 90°C for about 30 min. Then, CoCl₂·6H₂O (2.0 mmol) dissolved in 4 mL water and 4-dimethylaminopyridine (1.0mmol) were added to the clear solution. The pH value of the solution was adjusted to 6.2 at room temperature by the addition of 1M HCl. The mixture was kept 90°C for about 1 h and then cooled to room temperature and filtered. The purple crystal was obtained after 10 days (Yield: 40.3% based on W). Anal. Calcd. For C₃H₃BiO₆W₈: C, 7.78%; H, 1.21%; N, 2.59; Co, 1.82%; Bi, 12.90; W, 51.10; Na, 1.42%. Found: C, 7.54; H, 1.86; N, 2.83; Co, 1.77; Bi, 13.32; W, 50.95; Na, 1.34%. Na₂[Bi₂O₂O₉]·19.5H₂O[1], Na₂[Bi₂O₅]·16H₂O[2] and Na₁₃[Bi₂W₂O₇(H₂O)₄]·34H₂O[3] were synthesized according to some literatures.

1.3 GSH activity of (BiW₈)

The catalytic activity of (BiW₈) was studied using the GR-coupled assay by following the decrease in the concentration of NADPH spectrophotometrically at 340 nm on JASCO V550 UV-Visible spectrophotometer under time drive mode. In a typical assay, the reactants were added in the following order, [BiW₈] (0-3mM), GSH (2 mM), NADPH (0.4 mM), GPX (2.0units), GR (1.7 units), H₂O₂ (240 μM) in 25 mM pH 7.4 phosphate buffer at 25 °C. The fluorescence spectra of [BiW₈](3mM), GSH(2mM), GSSG(2mM) and OPA(10mM) were studied using fluorescence analysis (JASCO FP6500, λex= 334. 4 nm, λem= 424 nm).

1.4 Cell lines and cell culture

The human umbilical vein endothelial cell lines HUVEC, human osteosarcoma cell lines MG63, human rhabdomyosarcoma cell lines RD, human liver cancer cell lines HepG2 and Hep3B, and human breast carcinoma cell lines MCF7 were purchased from the Chinese Academy of Sciences Cell Bank. HUVEC cells, MG63 cells, RD cells, HepG2 cells, Hep3B cells, and MCF7 cells were maintained in high-glucose Dulbecco’s modified Eagle’s medium (DMEM) supplemented with 10% fetal bovine serum and 1% penicillin/streptomycin at 37°C and 5% CO₂ in a humidified incubator. Cells were divided into control group and experimental groups. Control groups were cultured under normal condition. Experimental groups were cultured with complete culture solution containing [BiW₈] in the concentration of IC₅₀ for 24 hours or 48 hours.

1.5 MTT assay

The cells were cultured in a medium containing different concentration of [BiW₈] and three raw materials (50 μmol/L, 100 μmol/L, 200 μmol/L and 400 μmol/L) for 24 hours and 48 hours. The cell proliferation was measured using a MTT dye absorbance assay (Beyotime, China). In brief, the culture medium with [BiW₈] were aspirated after incubations. The MTT reagent (5 mg/ml in PBS, 20 μL/well) and DMEM solution (80 μL/well) were added to each well and further incubated with cells at 37°C for 4 hours. The MTT solution was discarded, and added 150μL DMSO solution to each well for 10 minutes. The optical density (OD) of each well was measured using a microplate reader at 490nm.

1.6 Transmission electron microscopy (TEM) observation

The ultrastructural changes of cells before and after drug application were analyzed by TEM. Cells treated with [BiW₈] for 24h and 48h were collected into a mixture containing paraformaldehyde and 2.5% glutaraldehyde at 4°C for 2h, and then washed with 0.1mol/L phosphoric acid buffer for 3 times for 15 minutes. The solution was fixed with 1% osmium acid solution for 2h, washed with 0.1mol/L phosphoric acid rinse solution for 3 times for 15 minutes, immersed in ethanol dehydration, embedded in a mixture of acetone and embedded solution, and incubated at 37°C overnight. The samples were double stained with 3% uranium acetate and lead citrate and observed by TEM (Hitachi H-7650, Japan).

1.7 Lactate dehydrogenase (LDH) release assay

The cells were cultured in the 96-well plates and incubated with [BiW₈] at 37°C for 24 hours and 48 hours. The activity of LDH were detected by the Lactate dehydrogenase (LDH) release assay kit (Njicbio, Nanjing, China) and measured using a microplate reader at 490 nm.

1.8 Adenosine triphosphate (ATP) assay

Intracellular ATP activities were detected by Cell Titer-Glo Luminescent Cell Viability Assay Kit (Promega, USA). The Cells were added into the 96-well plates and treated with [BiW₈] for 24 hours and 48 hours. Cells after [BiW₈] incubations were treated with 100μL the detection solutions that contained firefly luciferases for 10 minutes and room temperature. The luminescent value of each
well was measured using a microplate reader.

### 1.9 Wound healing assay

For the wound healing assay, MG63 cells were inoculated in 6-well plate until they reached confluence. Create a linear wound with 200 μL pipette tips perpendicular to the bottom of the plate, and wash twice with phosphate buffer saline (PBS). Control cells were cultured under normal condition. Experimental cells were cultured with complete culture solution containing [BiW₈]. The wound healing was observed and photographed by using an inverted microscope at 0h, 24h and 48h.

### 1.10 Transwell matrigel assay

MG63 invasion was assayed by using Boyden chambers consisting of Transwell membrane filter inserts (Corning, USA). We coated the upper chambers with Matrigel (1:5, BD Biosciences, USA). Control cells were cultured under normal condition. Experimental cells were pretreated with [BiW₈] for 24 h. 1 x 10⁵ cells of control and experimental groups were seeded into 24-well Transwell chamber, respectively. Then, complete medium with 10% FBS was added to the lower layer of the chamber. After 24h and 48h of incubation, the chambers were removed, washed with PBS, fixed with formaldehyde, and stained with hematoxylin and eosin. Invading cells in the lower chambers were observed with a microscope. The numbers of invading cells were counted from five fields in a single chamber.

### 1.11 Reactive oxygen species measurement

Use Reactive Oxygen Species Assay Kit (Beyotime, China) to detect the contents of intracellular ROS. MG63 cells were treated with [BiW₈] for 24h, and added 1 mL of DCFH-DA (10 μmol/L). Then, the cells were cultured at 37°C for 20-30min. Fluorescence microscope (Nikon C2, Japan) was used for observation under green fluorescence at 488 nm excitation wavelength and 525 nm emission wavelength. Take photographs and analyze the results.

### 1.12 Intracellular glutathione measurement

The intracellular contents of T-GSH, GSSG and GSH in MG63 cells were detected by TOAL GlutathiOne/Imoxidized GlutathiOne Assay Kit (NJJCBIO, China). MG63 cells were cultured by [BiW₈] for 6h, 12h, 24h, 36h and 48h. The treated cell supernatant and reagents were mixed according to the experimental instructions and added into the 96-well plates. The absorbance value was measured at 405nm using a microplate reader.

### 1.13 Microarray experiment and gene expression analysis Data preparation

RNA isolation form MG63 cells in the control and experimental groups. Control cells were cultured under normal condition. Experimental cells were pretreated with [BiW₈] for 24 h. According to the manufacturer’s instructions, the total RNA of MG63 cells was extracted by using TRizol (Invitrogen, USA). RNA concentration and quality were determined with a NanoDrop Spectrophotometer. Microarray data were converted into recognizable format and annotated with software Genome Studio. The probes detected with p-value lower than 0.01 in at least one sample were accepted as significant and used for further analysis. The raw data were normalized using the quantile algorithm from the package limma of R.

#### 1.13.1 Identification of differentially expressed genes (DEGs).

|Fold change| > 1.5 and adj. P < 0.05 were set as the cut-offs to screen out differentially expressed genes (DEGs).

#### 1.13.2 Heatmaps and volcano plots analysis.

Clustered heatmaps and volcano plots of the control and experimental groups were generated using the package ggplot2 of R.

#### 1.13.3 Enrichment analysis of DEGs.

Functional enrichment analysis of DEGs was performed by DAVID (The Database for Annotation, Visualization and Integrated Discovery) to identify GO categories in by their biological processes (BP), molecular functions (MF), or cellular components (CC). The DAVID database was also used to perform pathway enrichment analysis with reference from KEGG (Kyoto Encyclopedia of Genes and Genomes) pathways. False discovery rate (FDR) < 0.05 was used as the cut-off.

### 1.14 Reverse transcription and qRT-PCR

According to the manufacturer’s instructions, the total RNA of MG63 cells was extracted by using TRizol (Invitrogen, USA). 1μg total RNA was used as a cDNA synthesis template using PrimeScript RT Reagent Kit (Roche, Switzerland). Real-time quantitative PCR was performed on triplicate samples in a reaction mix of SYBR Green (Roche, Switzerland) with CFX96 Touch Real-Time PCR Detection System (Bio-Rad, USA). The levels of total RNA were normalized to GAPDH. The indicated genes was normalized to the endogenous or exogenous reference control by using the 2^(-ΔΔCt) method. Sequences of the primers used for qRT-PCR in this study are listed in Table S1.
Table S1. Sequences of primers used for qRT-PCR

| POMs | Forward (5' → 3') | Reverse (5' → 3') |
|------|------------------|------------------|
| GSDME | GAAGAAGCCAGGAGATGGGAGT | ACGTGCGATTGCTAGAAG |
| TXNIP | CTCGCTGCAAGGCGTGGAG | TGGCTCTCAGAAGAGCCTG |
| NLRP3 | AAAGAATGGAGATGCGAAG | AAGCCTGCTGCTCTCTGT |
| IL-18 | TCACCAGGTCAGTGTGTC | TCCGGAGTGCAAGTGTGTC |
| GSTM1 | TGTCTGGTCTGAGTGGGTC | CGTCCGATCTGCTTGCCTTC |
| GSTT2B | TCACGAGAATCTCCTTCTC | TGGCTCTGCTGCTCTCTG |
| GPX1 | CAGTGGCCTGATGACCTCTG | GAGGGCCGCTGCTGCTG |
| GPX8 | TACCTAGGCTGAGAAGAACGTC | GGCTCGGATCTGCCAAATGTC |
| PARP1 | CGGAGTCTCCTGATAGCTC | TTTCCTCAAACATGGGCGAC |
| NTHL1 | CGCGGAAAGACACAGACGT | CTGATGACAGCTTGAGAC |
| MSH2 | AGGCCATCAAGGAGATGGT | GGAATCCAGAAACCACTCCCA |
| POLD1 | ATCCAGAATTCTGACCTTCCG | RGACAGCGGCTGTAGAG |
| POLE2 | TGAGAGCGCAATCTGCTAC | TCAATGACAGTCGACGTCAT |
| RPA3 | AGTCATATTCTGACAAAGCC | TCTTCAACAGGCGGCTTCCATCA |
| XRCC1 | TCAAGACAGACACTAGGA | TGAAAGAGAGGGCTGCTAGA |
| LIG1 | GAAGAGGCTGATCCTAAGCAG | ACTCTCGGAGAACCTTCATT |
| GAPDH | ACCAGAGAGTGATTGG | ACTACGTAGGATGCUTT |

Table S2. Summarize all the manners of cancer cells death induced by POMs in recent studies.

| POMs | Cell line | Death patterns | Ref. |
|------|-----------|----------------|-----|
| 1 (NH₄)₂H₂[PtMoO₄]₂·nH₂O | S180 | nasopharyngeal cancer KB | Not mentioned [4] |
| 2 K₂H₂[ThAs₆W₆O₄]₁₄ | B16 | Not mentioned | Not mentioned [5] |
| 3 K₃[MoO₄]₂ | H22 | Not mentioned | Not mentioned [5] |
| 4 (NH₄)[MoO₄] | HL-60 | Not mentioned | Not mentioned [5] |
| 5 K₃[MoO₄]₂ | Rectum cancer | Not mentioned | Not mentioned [5] |
| 6 (NH₄)[MoO₄]₂ | Meth A | Not mentioned | Not mentioned [5] |
| 7 [CH₃NH][H₂][MoO₄]·2H₂O·6H₂O | Meth A | Not mentioned | Not mentioned [5] |
| 8 [CH₃NH][H₂][MoO₄]·2H₂O·6H₂O | CO-4 | Not mentioned | Not mentioned [5] |
| 9 [CH₃NH][MoO₄][MoO₄]·2H₂O·6H₂O | CO-4 | Not mentioned | Not mentioned [5] |
| 10 [NH₄][MoO₄]₂ | CO-4 | Not mentioned | Not mentioned [5] |
| 11 Na₂[MoO₄]₂ | CO-4 | Not mentioned | Not mentioned [5] |
| 12 [NH₄][MoO₄]₂ | MX-1 | Not mentioned | Not mentioned [5] |
| 13 α-KH₂[CaH₂O₃Sn]₃SiW₁₁O₃₉ | SSMC-7721 | Not mentioned | Not mentioned [5] |
| 14 β-KH₂[CaH₂O₃Sn]₃SiW₁₁O₃₉ | SSMC-7721 | Not mentioned | Not mentioned [5] |
| 15 α-KH₂[CaH₂O₃Sn]₃SiW₁₁O₃₉ | SSMC-7721 | Not mentioned | Not mentioned [5] |
| 16 β-KH₂[CaH₂O₃Sn]₃SiW₁₁O₃₉ | SSMC-7721 | Not mentioned | Not mentioned [5] |
| 17 α-KH₂[CaH₂O₃Sn]₃SiW₁₁O₃₉ | SSMC-7721 | Not mentioned | Not mentioned [5] |
| 18 β-KH₂[CaH₂O₃Sn]₃SiW₁₁O₃₉ | SSMC-7721 | Not mentioned | Not mentioned [5] |
| 19 α-KH₂[CaH₂O₃Sn]₃SiW₁₁O₃₉ | SSMC-7721 | Not mentioned | Not mentioned [5] |
| 20 β-KH₂[CaH₂O₃Sn]₃SiW₁₁O₃₉ | SSMC-7721 | Not mentioned | Not mentioned [5] |
| 21 α-KH₂[CaH₂O₃Sn]₃SiW₁₁O₃₉ | SSMC-7721 | Not mentioned | Not mentioned [5] |
| 22 β-KH₂[NC₃H₇]₆[SiW₁₁O₃₉] | SSMC-7721 | Not mentioned | Not mentioned [5] |
| 23 K₃[CaH₂O₃Sn]₂PW₁₈O₄₃ | SSMC-7721 | Not mentioned | Not mentioned [5] |
| Entry | Reaction                             | Reference  | Organism  | Cell Line  | Notation   |
|-------|--------------------------------------|------------|-----------|------------|------------|
| 24    | K_d(C(H_O)Sn)PW(O)                  | SSMC-7721  | HeLa      | Not mentioned | [10]       |
| 25    | K_d[(C(H)Sn)PW(O)Os]                | SSMC-7721  | HeLa      | Not mentioned | [10]       |
| 26    | $\alpha$-K_d[(q-C(H)Ti)SiW(O)Os]    | SSMC-7721  | HeLa      | Not mentioned | [10]       |
| 27    | $\beta$-K_d[(q-C(H)Ti)SiW(O)Os]     | SSMC-7721  | HeLa      | Not mentioned | [10]       |
| 28    | $\alpha$-K_d[(q-C(H)Ti)GeW(O)Os]    | SSMC-7721  | HeLa      | Not mentioned | [11]       |
| 29    | K_d[(C(H)O)Sn]PW(O)                  | SSMC-7721  | HeLa      | Not mentioned | [11]       |
| 30    | K_d[(C(H)O)Sn]PW(O)Os               | SSMC-7721  | HeLa      | Not mentioned | [11]       |
| 31    | K_d[(C(H)O)Sn]PW(O)Os               | SSMC-7721  | HeLa      | Not mentioned | [11]       |
| 32    | K_d[(C(H)O)Sn]PW(O)Os               | SSMC-7721  | HeLa      | Not mentioned | [11]       |
| 33    | (HAla)(HeO)PW(O)MoO                  | HeLa      | PC-3m      | Not mentioned | [13]       |
| 34    | $\gamma$-[(C(H)O)(Ni)H][(C(H)O)Sn]HW(O)      | SSMC-7721  | HeLa      | Not mentioned | [14]       |
| 35    | $\gamma$-[(C(H)O)(Ni)H][(C(H)O)Sn]HW(O)      | SSMC-7721  | HeLa      | Not mentioned | [14]       |
| 36    | $\gamma$-[(C(H)O)(Ni)H][(C(H)O)Sn]HW(O)      | SSMC-7721  | HeLa      | Not mentioned | [14]       |
| 37    | $\gamma$-[(TBA)N]C(H)Ti)SiW(O)        | SSMC-7721  | HeLa      | Not mentioned | [14]       |
| 38    | $\gamma$-[(TBA)N]C(H)Ti)SiW(O)        | SSMC-7721  | HeLa      | Not mentioned | [14]       |
| 39    | [(C(H)O)H]_2[(q-C(H)Ti)GeW(O)Os]     | SSMC-7721  | HeLa      | Not mentioned | [15]       |
| 40    | [(C(H)O)H]_2[(q-C(H)Ti)GeW(O)Os]     | SSMC-7721  | HeLa      | Not mentioned | [15]       |
| 41    | [(C(H)O)H]_2[(q-C(H)Ti)GeW(O)Os]     | SSMC-7721  | HeLa      | Not mentioned | [15]       |
| 42    | $\alpha$-K_d[(C(H)O)Sn]SiW(O)        | SSMC-7721  | HeLa      | Not mentioned | [15]       |
| 43    | $\beta$-K_d[(C(H)O)Sn]SiW(O)        | SSMC-7721  | HeLa      | Not mentioned | [15]       |
| 44    | $\alpha$-K_d[(C(H)O)Sn]SiW(O)        | SSMC-7721  | HeLa      | Not mentioned | [16]       |
| 45    | $\beta$-K_d[(C(H)O)Sn]SiW(O)        | SSMC-7721  | HeLa      | Not mentioned | [16]       |
| 46    | $\alpha$-K_d[(C(H)O)Sn]SiW(O)        | SSMC-7721  | HeLa      | Not mentioned | [16]       |
| 47    | $\beta$-K_d[(C(H)O)Sn]SiW(O)        | SSMC-7721  | HeLa      | Not mentioned | [16]       |
| 48    | K_d[(q-C(H)Ti)CoW(O)Os]              | HeLa      | HL-60     | Not mentioned | [17]       |
| 49    | K_d[H_2]CoTiW(O)Os                   | SSMC-7721  | HeLa      | Not mentioned | [17]       |
| 50    | $\alpha$- and $\beta$-Ge(Ti)W(O)     | SSMC-7721  | HeLa      | Not mentioned | [17]       |
| 51    | [(C(H)O)Sn]GeW(O)Os                  | SSMC-7721  | HeLa      | Not mentioned | [17]       |
| 52    | [(C(H)O)Sn]GeW(O)Os                  | SSMC-7721  | HeLa      | Not mentioned | [17]       |
| 53    | [(C(H)O)Sn]GeW(O)Os                  | SSMC-7721  | HeLa      | Not mentioned | [17]       |
| 54    | [SnTiW(O)Os]L-EPE                     | HeLa      | HL-60     | Not mentioned | [18]       |
| 55    | [SnTiW(O)Os]L-EPE                     | HeLa      | HL-60     | Not mentioned | [18]       |
| 56    | K_d[Sn]TiW(O)Os                      | SSMC-7721  | HeLa      | Not mentioned | [18]       |
| 57    | K_d[Sn]TiW(O)Os                      | SSMC-7721  | HeLa      | Not mentioned | [18]       |
| 58    | [(CoTiW(O)Os]SEP                     | HeLa      | HL-60     | Not mentioned | [19]       |
| 59    | K_d[CoTiW(O)Os]                      | HeLa      | HL-60     | Not mentioned | [19]       |
| 60    | K_d[CoTiW(O)Os]                      | HeLa      | HL-60     | Not mentioned | [19]       |
| 61    | K_d[(q-C(H)Ti)P(Si)Os]               | SSMC-7721  | HeLa      | Not mentioned | [20]       |
| 62    | (TBA)N[(q-C(H)Zr)P(Si)Os]            | SSMC-7721  | HeLa      | Not mentioned | [20]       |
| 63    | K_d[(q-C(H)O)Sn]P(Si)W(O)           | SSMC-7721  | HeLa      | Not mentioned | [20]       |
| No. | Chemical Formula | Cells | Growth Inhibition | Source |
|-----|------------------|-------|-------------------|--------|
| 64  | K4[(CH3O)2Sn]PF6 | HeLa  | Not mentioned     | [20]   |
| 65  | (C2H2N3)H[BF4]   | SMMC-7721 | HeLa           | Not mentioned  | [20] |
| 66  | 5-FU (C4H4F3O2) | SMMC-7721 | Not mentioned |        | [21] |
| 67  | K4[BW10O42]     | SMMC-7721 | Not mentioned |        | [21] |
| 68  | [CoTiW10O38]LEP | SMMC-7721 | Not mentioned |        | [22] |
| 69  | K4[Co2TiW10O4]  | SMMC-7721 | Not mentioned |        | [22] |
| 70  | [n5-C5H4Ti]C6W11O39-LEP | SMMC-7721 | Not mentioned |        | [23] |
| 71  | K4[Si2TiW10O4]  | SMMC-7721 | Not mentioned |        | [23] |
| 72  | [SiTiW10O4]LEP  | SMMC-7721 | Not mentioned |        | [24] |
| 73  | K4[SiTiW10O4]  | SMMC-7721 | Not mentioned |        | [24] |
| 74  | [NH4Pr][MoO4]   | AsPC-1 | apoptosis        | [25]   |
| 75  | [NH4Pr][MoO4]   | KB     | Not mentioned    | [26]   |
| 76  | [NH4Ho][CoMoO4] | KB     | Not mentioned    | [26]   |
| 77  | [NH4Ho][PMoO4]  | KB     | Not mentioned    | [26]   |
| 78  | [NH3Ho][NMnO4]  | KB     | Not mentioned    | [26]   |
| 79  | [NH3Ho][RhMoO4] | KB     | Not mentioned    | [26]   |
| 80  | Na2[PMoO4]      | KB     | Not mentioned    | [26]   |
| 81  | Na2[SiMoO4]     | KB     | Not mentioned    | [26]   |
| 82  | Na2[GeMoO4]     | KB     | Not mentioned    | [26]   |
| 83  | Na2[AsMoO4]     | KB     | Not mentioned    | [26]   |
| 84  | Na2[PMoO4]      | KB     | Not mentioned    | [26]   |
| 85  | Na2[SiMoO4]     | KB     | Not mentioned    | [26]   |
| 86  | Na2[AsMoO4]     | KB     | Not mentioned    | [26]   |
| 87  | Na2[PMoO4]      | KB     | Not mentioned    | [26]   |
| 88  | Na2[AsMoO4]     | KB     | Not mentioned    | [26]   |
| 89  | Na2[PMoO4]      | KB     | Not mentioned    | [26]   |
| 90  | Na2[PW2O7]      | KB     | Not mentioned    | [26]   |
| 91  | Na2[PMoO4]      | KB     | Not mentioned    | [26]   |
| 92  | K3[LiV3O8]      | KB     | Not mentioned    | [26]   |
| 93  | Pr3[LiV3O8]     | KB     | Not mentioned    | [26]   |
| 94  | K3[Mo3O8]       | KB     | Not mentioned    | [26]   |
| 95  | K3[PMo4]        | KB     | Not mentioned    | [26]   |
| 96  | (Horn)[H2O]2[PMo5O14] | HeLa | PC-3m | Not mentioned | [27] |
| 97  | (Horn)[SiMo4O12] | HeLa  | PC-3m           | Not mentioned  | [27] |
| 98  | (Horn)[GeMo4O12] | HeLa  | PC-3m           | Not mentioned  | [27] |
| 99  | Na2[Ca(H2O)2(HLw2O42)] | SHEP-SF | KCN  | Not mentioned | [28] |
| 100 | (H2m)2[WO4(OH)]2[Zn(H2O)2]Na2[H2O]2[BiW2O5(O)] | SHEP-SF | KCN  | Not mentioned | [28] |
| 101 | NaNi[NH3][Mo6(H2O)3(SbW6O30)] | SHEP-SF | KCN  | Not mentioned | [28] |
| 102 | NaNi[NH3][Mo6(H2O)3(SbW6O30)] | SHEP-SF | KCN  | Not mentioned | [28] |
| 103 | NaNi[NH3][Mo6(H2O)3(SbW6O30)] | SHEP-SF | KCN  | Not mentioned | [28] |
| 104 | LPVO [(NH4)(HCl)2(HCl)(NH4)[V2O7]] | SHEP-SF | KCN  | Not mentioned | [28] |
| 105 | [NH4Pr][MoO4]   | M-45   | apoptosis        | [30]   |
| 106 | [NH4Pr][MoO4]   | M-45   | apoptosis        | [30]   |
| 107 | Na2[MoO4][μ-H2O] | MCF-7  | Hep-G2          | [31]   |
|      |                 |        | HeLa            | [31]   |
|      |                 |        | Hep-2           | [31]   |
|      |                 |        | SW-620          | [31]   |
|      |                 |        | WI-38           | [31]   |
| 108 | Na₂MoO₄(glyglyO)₂·15H₂O | MCF-7 | Hep-G2 | HeLa | Hep-2 | SW-620 | WI-38 | Not mentioned | [31] | [31] | [31] | [31] | [31] | [31] | [31] |
| 109 | Na₂MoO₄(glyglyO)₂·12H₂O | MCF-7 | Hep-G2 | HeLa | Hep-2 | SW-620 | WI-38 | Not mentioned | [31] | [31] | [31] | [31] | [31] | [31] | [31] |
| 110 | [Hmorph]₄[Mo₆O₁₅(OH)₃(metO₃)·4H₂O | MCF-7 | Hep-G2 | HeLa | Hep-2 | SW-620 | WI-38 | Not mentioned | [31] | [31] | [31] | [31] | [31] | [31] |
| 111 | [Hmorph]₄[Mo₆O₁₅(OH)₃(metO₃)·4CH₃OH | MCF-7 | Hep-G2 | HeLa | Hep-2 | SW-620 | WI-38 | Not mentioned | [31] | [31] | [31] | [31] | [31] | [31] |
| 112 | [Hmorph]₄[MoO₃(OH)₃(alhO₃) | MCF-7 | Hep-G2 | HeLa | Hep-2 | SW-620 | WI-38 | Not mentioned | [31] | [31] | [31] | [31] | [31] | [31] |
| 113 | (C₆H₅)₃N(CH₃O)(H₂)₃(OSiW₅(OH)) | PC-3m | Not mentioned | [32] |
| 114 | (C₆H₅)₃O₂(H₂)₂P₂Z₃M₀₆O₄₂ | PC-3m | Not mentioned | [32] |
| 115 | K₃Na₃SiW₁₂O₄₃ | S180 | leucocytoma | Not mentioned | [33] |
| 116 | (C₆H₅)₃N(CH₃O)(H₂)₃(OSiW₅(OH)) | S180 | leucocytoma | Not mentioned | [33] |
| 117 | (C₆H₅)₃N(CH₃O)(H₂)₂P₂Z₃M₀₆O₄₂ | S180 | leucocytoma | Not mentioned | [33] |
| 118 | (C₆H₅)₃N(CH₃O)(H₂)₃(OSiW₅(OH)) | S180 | leucocytoma | Not mentioned | [33] |
| 119 | (C₆H₅)₃N(CH₃O)(H₂)₂P₂Z₃M₀₆O₄₂ | S180 | leucocytoma | Not mentioned | [33] |
| 120 | (C₆H₅)₃N(CH₃O)(H₂)₂P₂Z₃M₀₆O₄₂ | S180 | leucocytoma | Not mentioned | [33] |
| 121 | (C₆H₅)₃N(CH₃O)(H₂)₂P₂Z₃M₀₆O₄₂ | S180 | leucocytoma | Not mentioned | [33] |
| 122 | (C₆H₅)₃N(CH₃O)(H₂)₂P₂Z₃M₀₆O₄₂ | HL-60 | K-562 | Not mentioned | [34] |
| 123 | [TBA]₃[MoO₃(OH)₆]-[NC₆H₅-CH₄-N₃]- | K-562 | Not mentioned | [35] |
| 124 | [TBA]₃[MoO₃(OH)₆]-[NC₆H₅-CH₄-N₃]- | K-562 | Not mentioned | [35] |
| 125 | [TBA]₃[MoO₃(OH)₆]-[NC₆H₅-CH₄-N₃]- | K-562 | Not mentioned | [35] |
| 126 | [St₅Th₄W₆O₃₂]·2H₂O | H₂O | H₂O | Not mentioned | [36] |
| 127 | K₃[H₂(N₃)₃W₄O₁₃] | H₂O | H₂O | Not mentioned | [36] |
| 128 | α-K₃[H₂(N₃)₃W₄O₁₃] | H₂O | H₂O | Not mentioned | [36] |
| 129 | [(CH₃)₃NH]₃[CH₃(OH)₃(N₃)₃][Mo(VI)₃O₃] | AsPC-1 | AsPC-1 | MKN-45 | [37] | [37] | [37] |
| 130 | [P₂Mo₆O₃₂]²⁺ | Protein kinase CK2 | Not mentioned | [38,51] |
| 131 | K₃[P₂Mo₆O₃₂]-14H₂O | breast cancer MCF-7 | Not mentioned | [39] |
| 132 | [Ni(C₅H₅N)₃][MoO₃(OH)₆]-7H₂O | breast cancer MCF-7 | Not mentioned | [40] |
| 133 | Na₂[V₃O₈] | SMCC-7721 | SK-OV-3 | Not mentioned | [41] |
| 134 | Na₂C₁₀H₁₈O₁₀ | Hep-A-22 | SMCC-7721 | Not mentioned | [41] |
| 135 | (C₆H₅)₃N(CH₃O)(H₂)₃(OSiW₅(OH)) | H₂O | H₂O | Not mentioned | [42,43] |
| 136 | [H₂O][C₆H₅N(CH₃O)(H₂)₃(OSiW₅(OH)) | H₂O | H₂O | Not mentioned | [43] |
| 137 | Na₂[H₂W₁₂O₄₀] | B16-F10 | MCA-38 | Not mentioned | [44] |
| 138 | K₃[H₃N(CH₃O)(phen)] | K-562 | K-562 | Not mentioned | [45] |
| 139 | K₂[Na₃(C₆H₅O)(phen)] | K-562 | K-562 | Not mentioned | [45] |
| 140 | K₂[Na₃(C₆H₅O)(phen)] | K-562 | K-562 | Not mentioned | [45] |
| 141 | K₂[Na₃(C₆H₅O)(phen)] | K-562 | K-562 | Not mentioned | [45] |
| Entry | Formula | Topics | Cell Lines |
|-------|---------|--------|------------|
| 142   | (NH₃)[MoO₃] | NCI-H460, MCF-7, SF-268 | Not mentioned |
| 143   | Li₄[MoV₂O₇(H₂O)₆]PC(C₂H₅NH₃)₃ | NCI-H460, MCF-7, SF-268 | Not mentioned |
| 144   | Li₄[MoV₂O₇(H₂O)₆]PC(C₂H₅NH₃)₃ | NCI-H460, MCF-7, SF-268 | Not mentioned |
| 145   | Li₄[MoV₂O₇(H₂O)₆]PC(C₂H₅NH₃)₃ | NCI-H460, MCF-7, SF-268 | Not mentioned |
| 146   | Na₄H₂[Mo₄V₄O₁₆(C₅H₇NO)₃]PC(C₂H₅NH₃)₃ | NCI-H460, MCF-7, SF-268 | Not mentioned |
| 147   | H₂[men]₃[V₁₂O₄] | A-549, P388, L-02 | Not mentioned |
| 148   | H₂[en]₃[V₁₂O₄] | A-549, P388, L-02 | Not mentioned |
| 149   | Na₄K₃[Sn(C₃H₇OH)₃][Sn(C₃H₇OH)₃]PC(C₂H₅NH₃)₃ | cervical cancer HeLa | Not mentioned |
| 150   | K₃[MoF₆] | HeLa | Not mentioned |
| 151   | [En]₂[SiW₁₈O₆₄]·CMC | HeLa | Not mentioned |
| 152   | [En]₂[SiW₁₈O₆₄]·CMC | HeLa | Not mentioned |
| 153   | [En]₂[SiW₁₈O₆₄]·CMC | HeLa | Not mentioned |
| 154   | H₂[SiW₁₈O₆₄] | HeLa | Not mentioned |
| 155   | PPA | HeLa | Not mentioned |
| 156   | [Cu₂P₂O₇][H₂O] | HeLa | Not mentioned |
| 157   | [Cu₂P₂O₇][H₂O] | HeLa | Not mentioned |
| 158   | Na₂[C₅C₆H₄N₃] | KB, MCF-7, PC-3, A-549 | Apoptosis |
| 159   | Na₂[C₅C₆H₄N₃] | KB, MCF-7, PC-3, A-549 | Apoptosis |
| 160   | [Cr(C₃H₇OH)₂]₄[Mo₄O₄] | Hep-G2, MCF-7, SK-OV-3 | Not mentioned |
| 161   | [Sn(C₃H₇OH)₂]₄[Mo₄O₄] | Hep-G2, MCF-7, SK-OV-3 | Not mentioned |
| 162   | [Sn(C₃H₇OH)₂]₄[Mo₄O₄] | Hep-G2, MCF-7, SK-OV-3 | Not mentioned |
| 163   | K₂[PC(W₁₂O₄₃)] | Hep-G2, MCF-7, SK-OV-3 | Apoptosis |
| 164   | [Cr(C₃H₇OH)₂][PW₁₂O₄₃] | PC-3, HeLa, Hep-G2 | Not mentioned |
| 165   | [HPPA]₃[CdPW₄] | PC-3, HeLa, Hep-G2 | Not mentioned |
| 166   | [HPPA]₃[CdPW₄] | PC-3, HeLa, Hep-G2 | Not mentioned |
| 167   | H₂[PC(W₁₂O₄₃)] | PC-3, HeLa, Hep-G2 | Not mentioned |
| 168   | K₂[Cr(C₃H₇OH)₂][PW₁₂O₄₃] | HeLa | Not mentioned |
| 169   | [Cr(C₃H₇OH)₂][PW₁₂O₄₃]·CMC | HeLa | Not mentioned |
| 170   | K₂[Cr(C₃H₇OH)₂][PW₁₂O₄₃] | HeLa | Not mentioned |
| 171   | [MoO₃]₃[η¹-p-carboxylatole] | H22, BGC-823 | Not mentioned |
| 172   | [NH₃]₃[Mo₄O₄] | H22, BGC-823 | Not mentioned |
| 173   | [NH₃]₃[Mo₄O₄] | H22, BGC-823 | Not mentioned |
| 174   | K₃H₁[(η-Bu-NH₂)₃]GeW₆O₃₆ | H22, H22, SW-620, MGC-803, A-549, MM-231, Hep-G2 | Not mentioned |
| L-62 | NCI-H460 | MCF-7 | SF-268 |
|---|---|---|---|
| 175 | Rh₂₀[NH₄]₂[(MoO₄)O(O)PC(CH₂NH₃)OPO₄]₂ | Not mentioned | [59] |
| 176 | (NH₄)₂[(MoO₄)O(O)PC(CH₂NH₃)OPO₄]₂ | Not mentioned | [60] |
| 177 | Rh₂₀[NH₄]₂[(MoO₄)O(O)PC(CH₂H₅)OPO₄]₂ | Not mentioned | [60] |
| 178 | Na₂[Rh₂O₃(OH)₃(O)PC(CH₂H₅)OPO₄]₂ | Not mentioned | [60] |
| 179 | Na₂[V₂O₅(H₂O)]₂[(MoO₄)O(O)PC(CH₂H₅)OPO₄]₂ | Not mentioned | [60] |
| 180 | (NH₄)₂[Rh₂O₃(OH)₃(O)PC(CH₂H₅)OPO₄]₂ | Not mentioned | [60] |
| 181 | (NH₄)₂[K₉[(V₂O₅(H₂O)]₂[(MoO₄)O(O)PC(CH₂H₅)OPO₄]₂ | Not mentioned | [60] |
| 182 | Na₂[V₄O₅] | Not mentioned | [60] |
| 183 | [Cu₂(Enro)₂(H₂O)]₂[Mo₃(OH)₆]Mo₃O₆ | SGC-7901 | Not mentioned | [61] |
| 184 | [Cu₂(PPA)₂][Mo₃(OH)₆]Mo₃O₆ | SGC-7901 | Not mentioned | [61] |
| 185 | [Cu₂(Norf)(H₂O)]₂[Mo₃(OH)₆]Mo₃O₆ | SGC-7901 | Not mentioned | [61] |
| 186 | [Cu₂(Enro)(H₂O)]₂[Mo₃(OH)₆]Mo₃O₆ | SGC-7901 | Not mentioned | [61] |
| 187 | Na₂[H₂W₁₀O₴] | H₂-157 | HEC | HEC | HEC | [62] |
| 188 | Na₂[H₂W₁₀O₴] | H₂-157 | HEC | HEC | [62] |
| 189 | [Cu₂(Norf)(H₂O)]₂[Mo₃(OH)₆]Mo₃O₆ | Not mentioned | [61] |
| 190 | Na₂[H₂W₁₀O₴] | H₂-157 | HEC | HEC | [62] |
| 191 | Na₂[H₂W₁₀O₄] | H₂-157 | HEC | HEC | [62] |
| 192 | (C₂H₄F₂N₅O₂H₂)[PW₁₂O₄] | HeLa | HEP-G2 | HEK-293 | [63] |
| 193 | K₉[(C₂H₄F₂N₅O₂H₂)[PW₁₂O₄] | HeLa | HEP-G2 | HEK-293 | [63] |
| 194 | [Cu₂(Norf)(H₂O)]₂[Mo₃(OH)₆]Mo₃O₆ | Not mentioned | [61] |
| 195 | [Cu₂(Norf)(H₂O)]₂[Mo₃(OH)₆]Mo₃O₆ | Not mentioned | [61] |
| 196 | [Cu₂(Norf)(H₂O)]₂[Mo₃(OH)₆]Mo₃O₆ | Not mentioned | [61] |
| 197 | 5-FU (C₂H₄F₂N₅O₂) | HeLa | HEP-G2 | HEK-293 | [63] |
| 198 | [Cu₂(Norf)(H₂O)]₂[Mo₃(OH)₆]Mo₃O₆ | Not mentioned | [61] |
| 199 | Na₂[K₉[β-SiC₅W₁₀O₄][OH]₂(H₂O)]₂ | SMMC-7721 | SK-OV-3 | Not mentioned | [64] |
| 200 | (TBA)₃[p+−(C₃H₇)₄]PW₁₀O₄ | HL-60 | B16 | Not mentioned | [65] |
| 201 | K₀[(C₂H₄F₂N₅O₂H₂)[Sm(PW₁₀)]₂ | HeLa | HEP-G2 | HEK-293 | Apoptosis | [66] |
| 202 | K₀[(C₂H₄F₂N₅O₂H₂)[Er(PW₁₀)]₂ | HeLa | HEP-G2 | HEK-293 | Apoptosis | [66] |
| 203 | K₀[(C₂H₄F₂N₅O₂H₂)[Pr(SiW₁₀O₄)] | HeLa | HEP-G2 | HEK-293 | Not mentioned | [67] |
| 204 | K₀[(C₂H₄F₂N₅O₂H₂)[Sm(SiW₁₀O₄)] | HeLa | HEP-G2 | HEK-293 | Not mentioned | [67] |
| 205 | (Mn₂OsO₆)[(OClO)₃(C₂H₆)] | MCF-7 | MDA-MB-231 | MCF-10A | Not mentioned | [68] |
| 206 | (Mn₂OsO₆)[(OClO)₃(C₂H₆)] | MCF-7 | MDA-MB-231 | MCF-10A | Not mentioned | [68] |
| 207 | (Mn₂OsO₆)[(OClO)₃(C₂H₆)] | MCF-7 | MDA-MB-231 | MCF-10A | Not mentioned | [68] |
| 208 | (Mn₂OsO₆)[(OClO)₃(C₂H₆)] | MCF-7 | MDA-MB-231 | MCF-10A | Not mentioned | [68] |
|   | MCF-10A | MCF-7 | MDA-MB-231 | Not mentioned |   |
|---|---------|-------|-------------|---------------|---|
| 209 | [MnMoO₄(OCH₃CNHCH₃(OH)₃)]⁺ | MCF-7 | MDA-MB-231 | MCF-10A | Not mentioned |
| 210 | [MnMoO₄(OCH₃CNHCH₃(OH)₃)]⁺ | MCF-7 | Not mentioned | MCF-10A | Not mentioned |
| 211 | [{Cu(En)}(OH)₂][SiW₄O₁₄]| SGC-7901 | Not mentioned | SMMC-7721 | Not mentioned |
| 212 | [{Cu(Norf)₃}][SiW₄O₁₄] | SGC-7901 | Not mentioned | SMMC-7721 | Not mentioned |
| 213 | H₂[Na(En)]{SiW₄O₁₄} | SGC-7901 | Not mentioned | SMMC-7721 | Not mentioned |
| 214 | K₁₀[(n-pentafluorophenyl)C₁₀H₄] | MCF-7 | Not mentioned | HEK-293 | Not mentioned |
| 215 | K₁₀[(n-pentafluorophenyl)C₁₀H₄] | MCF-7 | Not mentioned | HEK-293 | Not mentioned |
| 216 | K₀[(n-pentafluorophenyl)C₁₀H₄] | MCF-7 | Not mentioned | HEK-293 | Not mentioned |
| 217 | (Him)₃[{W(OH)}₃(Mn(H₂O)₃][Na(H₂O)₃](BiW₁₂O₄₀)] | SGC-7901 | Apoptosis | Not mentioned | |
| 218 | (CoTi₇W₄O₃₀)@TMC | Hel-a | Not mentioned |   | |
| 219 | Kₓ[CoTi₇W₄O₃₀] | Hel-a | Not mentioned |   | |
| 220 | (P₂W₁₆(Nb₂O₉)₉)@TMC | Hel-a | Not mentioned |   | |
| 221 | Kₓ[P₂W₁₆(Nb₂O₉)₉] | Hel-a | Not mentioned |   | |
| 222 | α-[Na₅(AsW₆O₁₉)] | K-562 | Not mentioned |   | |
| 223 | Naₓ[Ca₄H₄O₁₂(α-AsW₆O₁₉)] | K-562 | Not mentioned | Hep-G2 | Not mentioned |
| 224 | Naₙ[(Ca₄H₄O₁₂)(α-AsW₆O₁₉)] | K-562 | Apoptosis | Hep-G2 | Not mentioned |
| 225 | [{Cu[PPA]₃}][H₂PMo₆O₁₆] | SGC-7901 | Not mentioned |   | |
| 226 | [{Cu[PPA]₃}][H₂PMo₆O₁₆] | SGC-7901 | Not mentioned |   | |
| 227 | H₂[PMo₆O₁₆] | SGC-7901 | Not mentioned |   | |
| 228 | Naₙ[PMo₆O₁₆] | SGC-7901 | Not mentioned |   | |
| 229 | Kₓ[(CH₃N′CH₂COO)₃]₁[(VO₃)₂] | MCF-7 | Not mentioned | A-549 | Not mentioned |
| 230 | [{[(CH₃)₂N′CH₂COOH]·[(VO₃)₂]}],[(CH₃)₂N′CH₂COO]⁺ | MCF-7 | A-549 | MCF-10A | Not mentioned |
| 231 | [{Cu(H₂O)₃}[Mo₃Os₆(µ₆-O)] | MCF-7 | A-549 | Not mentioned | |
| 232 | [{Zn(H₂O)₃}[Mo₃Os₆(µ₆-O)] | MCF-7 | Not mentioned | Hep-G2 | Not mentioned |
| 233 | [{Co(H₂O)₃}[Mo₃Os₆(µ₆-O)] | MCF-7 | Not mentioned | Hep-G2 | Not mentioned |
| 234 | [{Cr(H₂O)₃[lys]₀}[Mo₃Os₆] | MCF-7 | Not mentioned | Hep-G2 | Not mentioned |
| 235 | [{Zn(H₂O)₃}[Mo₃Os₆[lys]₁] | MCF-7 | Not mentioned | Hep-G2 | Not mentioned |
| 236 | [{Cr(H₂O)₃}[Mo₃Os₆[lys]₁] | MCF-7 | Not mentioned | Hep-G2 | Not mentioned |
| 237 | Naₓ[Mo₃Os₆[lys]₁] | MCF-7 | Not mentioned | Hep-G2 | Not mentioned |
| 238 | Naₓ[Mo₃Os₆[lys]₁] | MCF-7 | Not mentioned | Hep-G2 | Not mentioned |
| 239 | AnNP₇Tyr@ H₂PW₁₆O₃₀ | A-549 | Not mentioned |   | |
| 240 | AnNP₇Tyr@ H₂PW₁₆O₃₀ | A-549 | Not mentioned |   | |
| 241 | [{Bi₃L₆NO₃}₂(CH₃CH₃O)₃] (HL = 2-acetylpyridine N(4)-phenylthiosemicarbazone) | Hept0₂ | Apoptosis |   | |
| 242 | (TBA)₃[Mo₃Os₆(O₅)(NC₃H₄-C₆H₅)] | K-562 | Not mentioned |   | |
| 243 | (TBA)₃[Mo₃Os₆(O₅)(NC₃H₄-C₆H₅)] | MCF-7 | Not mentioned |   | |
| 244 | (TBA)₃[Mo₃Os₆] | K-562 | Not mentioned | MCF-7 | Not mentioned |
| 245 | [TeW₁₂O₴₀]⁻ | HeLa | Not mentioned | Vero | Not mentioned |
| 246 | Naₓ[TeW₁₂O₴₀] | HeLa | Not mentioned | Vero | Not mentioned |
| 247 | [Na₉PW₁₆SO₄₁₆]⁻ | HeLa | Not mentioned | Vero | Not mentioned |
| 248 | [Ni₉(Na₉PW₁₆SO₄₁₆)]⁻ | HeLa | Not mentioned | Vero | Not mentioned |
| 249 | [VₓO₁₆]⁻ | HeLa | Not mentioned | Vero | Not mentioned |
| 250 | Naₓ[VₓO₁₆] | HeLa | Not mentioned | Vero | Not mentioned |
| 251 | Naₓ[TeW₁₂O₴₀] | HeLa | Not mentioned | Vero | Not mentioned |
| 252 | M₁₂[Na₉PW₁₆SO₄₁₆] | HeLa | Not mentioned | Vero | Not mentioned |
| 253 | Naₓ[VₓO₁₆] | HeLa | Not mentioned | Vero | Not mentioned |
| 254 | [Co₃H₃O₃Ni₃(W₄O₁₄)]·SEP | MCF-7 | Not mentioned | HEK-293 | Not mentioned |
| No. | Formula | Cell Lines | Apoptosis | Ref. |
|-----|---------|------------|-----------|------|
| 255 | K₃[CoCl₃(OH)₂SiW₁₆O₅₆] | MCF-7 | Not mentioned | [82] |
| 256 | [Co(H₂O)₆]Cl₂EP | MCF-7 | Not mentioned | [82] |
| 257 | K₂[Co(H₂O)₆]2EP | MCF-7 | Not mentioned | [82] |
| 258 | (Him)₂[(W(OH)₃)₃Co₂H₄O₇]Na₂H₄O₇·10H₂O | HT-29 | Apoptosis | [83] |
| 259 | (chlorin)₂[SiMo₇O₃4] | A-549 | Not mentioned | [84] |
| 260 | Na₂[SiMo₇O₃₄] | MCF-7 | Not mentioned | [85] |
| 261 | Na₂[MoO₄] | SK-OV-3 | Not mentioned | [85] |
| 262 | Na₂[(Na₂Si₃O₇)(Co₃O₇)](Mo₆O₂₃(NO₃)₀)·23H₂O | Hep-G2 | Not mentioned | [85] |
| 263 | Zn₃PM₆₃O₃₈·23H₂O | SGC-7901 | Not mentioned | [86] |
| 264 | K₃[Na₂(Cu₂H₃O₇)₈(P₈O₇)] | MG-63 | Apoptosis | [87] |
| 265 | (NH₄)_₄[(MoV)₃MoV₆₃O₆₄(H₂O)₉]·(MoVO₄CH₃COO)₉ | Hep-G2 | Apoptosis | [88] |
| 266 | (NH₄)_₄[(MoV)₃MoV₆₃O₆₄(H₂O)₉]·(MoVO₄CH₃COO)₉ | Hep-G2 | Apoptosis | [88] |
| 267 | (CH₃NH₃)₃[(CH₃NH₃)₃[(MoV)₃MoV₆₃O₆₄(H₂O)₉]·(MoVO₄CH₃COO)₉ | Hep-G2 | Apoptosis | [88] |
| 268 | K₃[Na₂MoO₄] | SGC-7901 | Not mentioned | [89] |
| 269 | SK-OV-3 | SGC-7901 | Not mentioned | [89] |
| 270 | [H₂en][Na₂[(Zn(en)₂H(en)][(Zn(en)₂(H₂O)][(P₈O₇)] | SGC-7901 | Not mentioned | [89] |
| 271 | K₃[Na₂MoO₄] | SGC-7901 | Not mentioned | [89] |
| 272 | (Cu(en)₃)₃[GeNH₃]₃[V₄O₉]·20H₂O | SC-1680 | Gastric cancer | [90] |
| 273 | Na₂[MoO₃(C₆H₅NCH₂CH₃)(CH₃N(OPO₄))] | MCF-7 | Not mentioned | [91] |
| 274 | Na₂[MoO₃(C₆H₅NCH₂CH₃)(CH₃N(OPO₄))] | MCF-7 | Not mentioned | [91] |
| 275 | Na₂[MoO₃(C₆H₅NCH₂CH₃)(CH₃N(OPO₄))] | MCF-7 | Not mentioned | [91] |
| 276 | Na₂[MoO₃(C₆H₅NCH₂CH₃)(CH₃N(OPO₄))] | MCF-7 | Not mentioned | [91] |
| 277 | Na₂[MoO₃(C₆H₅NCH₂CH₃)(CH₃N(OPO₄))] | MCF-7 | Not mentioned | [91] |
| 278 | Na₂[MoO₃(C₆H₅NCH₂CH₃)(CH₃N(OPO₄))] | MCF-7 | Not mentioned | [91] |
| 279 | Na₂[MoO₃(C₆H₅NCH₂CH₃)(CH₃N(OPO₄))] | MCF-7 | Not mentioned | [91] |
| 280 | Na₂[MoO₃(C₆H₅NCH₂CH₃)(CH₃N(OPO₄))] | MCF-7 | Not mentioned | [91] |
| 281 | Na₂[MoO₃(C₆H₅NCH₂CH₃)(CH₃N(OPO₄))] | MCF-7 | Not mentioned | [91] |
| 282 | Na₂[MoO₃(C₆H₅NCH₂CH₃)(CH₃N(OPO₄))] | MCF-7 | Not mentioned | [91] |
| 283 | Na₂[MoO₃(C₆H₅NCH₂CH₃)(CH₃N(OPO₄))] | MCF-7 | Not mentioned | [91] |
| 284 | Na₂[MoO₃(C₆H₅NCH₂CH₃)(CH₃N(OPO₄))] | MCF-7 | Not mentioned | [91] |
| 285 | Na₂[MoO₃(C₆H₅NCH₂CH₃)(CH₃N(OPO₄))] | MCF-7 | Not mentioned | [91] |
| 286 | β-Na₂[As₂W₁₈O₆₃] | HeLa | Not mentioned | [91] |
| 287 | Na₂[MoO₃(C₆H₅NCH₂CH₃)(CH₃N(OPO₄))] | HeLa | Not mentioned | [91] |
| 288 | Na₂[MoO₃(C₆H₅NCH₂CH₃)(CH₃N(OPO₄))] | HeLa | Not mentioned | [91] |
| 289 | Na₂[MoO₃(C₆H₅NCH₂CH₃)(CH₃N(OPO₄))] | HeLa | Not mentioned | [91] |
| 290 | Na₂[MoO₃(C₆H₅NCH₂CH₃)(CH₃N(OPO₄))] | HeLa | Not mentioned | [91] |
| 291 | Na₂[MoO₃(C₆H₅NCH₂CH₃)(CH₃N(OPO₄))] | HeLa | Not mentioned | [91] |
| 292 | [P₂W₁₈O₆₃] | HeLa | Apoptosis | [96] |
| 293 | Na₂[MoO₃(C₆H₅NCH₂CH₃)(CH₃N(OPO₄))] | HeLa | Apoptosis | [96] |
| No. | Formula/Type | Cell Line(s) | Effect | Reference |
|-----|--------------|--------------|--------|-----------|
| 294 | [TtPW6O19]-CT | HeLa, Vero | apoptosis | [96] |
| 295 | K₄H₂[TtPW6O19] | HeLa, Vero | apoptosis | [96] |
| 296 | [CoTiW11O38]-CT | HeLa, Vero | apoptosis | [96] |
| 297 | K₂H₂[CoTiW₁₁O₃₈] | HeLa, Vero | apoptosis | [96] |
| 298 | SiW₁₁O₃₉-FePt NP | Rat Primary Cortical Astrocytes | Not mentioned | [97] |
| 299 | SiW₁₁O₃₉-FePt NP | Rat Primary Cortical Astrocytes | Not mentioned | [97] |
| 300 | Pt⁴⁺-P516-DSPF-PEG2000 | HT-29, HUVEC | apoptosis | [98] |
| 301 | [PW₁₁O₃₉SiCH₃NH₃][Pt(NH₃)₂Cl₂]²⁺ | HT-29, HUVEC | apoptosis | [98] |
| 302 | Na₂[Pt₁₁O₃₉] | HT-29, HUVEC | apoptosis | [98] |
| 303 | K₁₀(C₄H₉F₉N₃O₂)₂Er[PW₁₁O₃₉] | HeLa, Hep-G2, HEK-293 | Not mentioned | [99] |
| 304 | K₁₀[Er₂[PW₁₁O₃₉]] | HeLa, Hep-G2, HEK-293 | Not mentioned | [99] |
| 305 | K₁₀(C₄H₉F₉N₃O₂)₂Gd[PW₁₁O₃₉] | HeLa, Hep-G2, HEK-293 | Not mentioned | [99] |
| 306 | K₁₀[Gd₂[PW₁₁O₃₉]] | HeLa, Hep-G2, HEK-293 | Not mentioned | [99] |
| 307 | K₁₀(C₄H₉F₉N₃O₂)₂Dy[PW₁₁O₃₉] | HeLa, Hep-G2, HEK-293 | Not mentioned | [99] |
| 308 | K₁₀[Dy₂[PW₁₁O₃₉]] | HeLa, Hep-G2, HEK-293 | Not mentioned | [99] |
| 309 | (NH₃)₁₂[Co₉Sb₉O₁₅] | A2780, A2780cisR, OVGAR-3, SKOV-3, CT-26, HT-29, A-549, MCF-7, HEK-293 | apoptosis | [100] |
| 310 | (NH₃)₁₂[Co₉Sb₉O₁₅] | A2780, A2780cisR, OVGAR-3, SKOV-3, CT-26, HT-29, A-549, MCF-7, HEK-293 | apoptosis | [100] |
| 311 | (NH₃)₁₂[Na₉Sb₉W₃O₃₉] | A2780, A2780cisR, OVGAR-3, SKOV-3, CT-26, HT-29, A-549, MCF-7, HEK-293 | apoptosis | [100] |
| 312 | [Co₂(H₂O)SiMo₆O₁₅]-SEP | MCF-7, HEK-293, NHF | Not mentioned | [101] |
| 313 | K₄[Co₂(H₂O)SiMo₆O₁₅] | MCF-7, HEK-293, NHF | Not mentioned | [101] |
| 314 | [Co₂(H₂O)SiMo₆O₁₅]-LEP | MCF-7, HEK-293, NHF | Not mentioned | [101] |
| 315 | K₄[SiCo₂(H₂O)Mo₆O₁₅] | MCF-7, HEK-293, NHF | Not mentioned | [101] |
| 316 | (NH₃)₁₂[Fe₂(AsMo₆O₂₆)(H₂O)₂] | Hep-G2, Vero | Not mentioned | [102] |
| 317 | (NH₃)₁₂[Fe₂(AsMo₆O₂₆)] | Hep-G2, Vero | Not mentioned | [102] |
| 318 | K₄(AsMo₆O₂₆)(H₂O)₂ | A-549 | apoptosis and necrosis | [103] |
| 319 | K₄(Na₉Mo₆O₁₅) | A-549 | Not mentioned | [103] |
| 320 | AuNP@POM | B16, Vero | apoptosis/necrosis | [104] |
| 321 | (NH₃)₁₂[Na₉(As₂Mo₆O₂₆)] | B16, Vero | apoptosis/necrosis | [104] |
| 322 | Na₂[CoPMO₆O₁₅] | B16 | Not mentioned | [105] |
| Reaction | [H][βliz][HMoF₄O₃] | SHSY5 | SKOV-3 | HeLa | HepG2 | EVC-304 | Not mentioned | [110] |
|----------|---------------------|-------|-------|------|-------|---------|---------------|------|
| 335 | [Na₂P₂MoO₆] | SHSY5 | SKOV-3 | HeLa | HepG2 | EVC-304 | Not mentioned | [110] |
| 336 | [K₂[GeMo₄O₁₃]] | HCT-116 | SMMC-7721 | HL-7702 | HEP-G2 | HEP-2 | HEP-2 | Not mentioned | [111] |
| 337 | [Na₂P₂MoO₆] | HCT-116 | SMMC-7721 | HL-7702 | HEP-G2 | HEP-2 | HEP-2 | Not mentioned | [111] |
| 338 | [K₂[GeMo₄O₁₃]] | HCT-116 | SMMC-7721 | HL-7702 | HEP-G2 | HEP-2 | HEP-2 | Not mentioned | [111] |
| 339 | [Na₂P₂MoO₆] | HCT-116 | SMMC-7721 | HL-7702 | HEP-G2 | HEP-2 | HEP-2 | Not mentioned | [111] |
| 340 | [K₂[GeMo₄O₁₃]] | HCT-116 | SMMC-7721 | HL-7702 | HEP-G2 | HEP-2 | HEP-2 | Not mentioned | [111] |
| 341 | [K₂[GeMo₄O₁₃]] | HCT-116 | SMMC-7721 | HL-7702 | HEP-G2 | HEP-2 | HEP-2 | Not mentioned | [111] |
| 342 | [H][βliz][HMoF₄O₃] | SHSY5 | SKOV-3 | HeLa | HepG2 | EVC-304 | Not mentioned | [110] |
| 343 | [K₂[GeMo₄O₁₃]] | HCT-116 | SMMC-7721 | HL-7702 | HEP-G2 | HEP-2 | HEP-2 | Not mentioned | [111] |
| 344 | [Na₂P₂MoO₆] | HCT-116 | SMMC-7721 | HL-7702 | HEP-G2 | HEP-2 | HEP-2 | Not mentioned | [111] |
| 345 | [K₂[GeMo₄O₁₃]] | HCT-116 | SMMC-7721 | HL-7702 | HEP-G2 | HEP-2 | HEP-2 | Not mentioned | [111] |
| 346 | [Na₂P₂MoO₆] | HCT-116 | SMMC-7721 | HL-7702 | HEP-G2 | HEP-2 | HEP-2 | Not mentioned | [111] |
| 347 | [K₂[GeMo₄O₁₃]] | HCT-116 | SMMC-7721 | HL-7702 | HEP-G2 | HEP-2 | HEP-2 | Not mentioned | [111] |
| 348 | [Na₂P₂MoO₆] | HCT-116 | SMMC-7721 | HL-7702 | HEP-G2 | HEP-2 | HEP-2 | Not mentioned | [111] |
| 349 | [K₂[GeMo₄O₁₃]] | HCT-116 | SMMC-7721 | HL-7702 | HEP-G2 | HEP-2 | HEP-2 | Not mentioned | [111] |
| 350 | [Na₂P₂MoO₆] | HCT-116 | SMMC-7721 | HL-7702 | HEP-G2 | HEP-2 | HEP-2 | Not mentioned | [111] |
| 351 | [K₂[GeMo₄O₁₃]] | HCT-116 | SMMC-7721 | HL-7702 | HEP-G2 | HEP-2 | HEP-2 | Not mentioned | [111] |
| 352 | [Na₂P₂MoO₆] | HCT-116 | SMMC-7721 | HL-7702 | HEP-G2 | HEP-2 | HEP-2 | Not mentioned | [111] |
| 353 | [K₂[GeMo₄O₁₃]] | HCT-116 | SMMC-7721 | HL-7702 | HEP-G2 | HEP-2 | HEP-2 | Not mentioned | [111] |
| 354 | [Na₂P₂MoO₆] | HCT-116 | SMMC-7721 | HL-7702 | HEP-G2 | HEP-2 | HEP-2 | Not mentioned | [111] |
| 355 | [K₂[GeMo₄O₁₃]] | HCT-116 | SMMC-7721 | HL-7702 | HEP-G2 | HEP-2 | HEP-2 | Not mentioned | [111] |
| 356 | [Na₂P₂MoO₆] | HCT-116 | SMMC-7721 | HL-7702 | HEP-G2 | HEP-2 | HEP-2 | Not mentioned | [111] |
| 357 | [K₂[GeMo₄O₁₃]] | HCT-116 | SMMC-7721 | HL-7702 | HEP-G2 | HEP-2 | HEP-2 | Not mentioned | [111] |
| 358 | [Na₂P₂MoO₆] | HCT-116 | SMMC-7721 | HL-7702 | HEP-G2 | HEP-2 | HEP-2 | Not mentioned | [111] |
| 359 | [K₂[GeMo₄O₁₃]] | HCT-116 | SMMC-7721 | HL-7702 | HEP-G2 | HEP-2 | HEP-2 | Not mentioned | [111] |
| 360 | [Na₂P₂MoO₆] | HCT-116 | SMMC-7721 | HL-7702 | HEP-G2 | HEP-2 | HEP-2 | Not mentioned | [111] |
| 361 | [K₂[GeMo₄O₁₃]] | HCT-116 | SMMC-7721 | HL-7702 | HEP-G2 | HEP-2 | HEP-2 | Not mentioned | [111] |
| 362 | [Na₂P₂MoO₆] | HCT-116 | SMMC-7721 | HL-7702 | HEP-G2 | HEP-2 | HEP-2 | Not mentioned | [111] |
| 363 | [K₂[GeMo₄O₁₃]] | HCT-116 | SMMC-7721 | HL-7702 | HEP-G2 | HEP-2 | HEP-2 | Not mentioned | [111] |
| 364 | [Na₂P₂MoO₆] | HCT-116 | SMMC-7721 | HL-7702 | HEP-G2 | HEP-2 | HEP-2 | Not mentioned | [111] |
| 365 | [K₂[GeMo₄O₁₃]] | HCT-116 | SMMC-7721 | HL-7702 | HEP-G2 | HEP-2 | HEP-2 | Not mentioned | [111] |
| 366 | [Na₂P₂MoO₆] | HCT-116 | SMMC-7721 | HL-7702 | HEP-G2 | HEP-2 | HEP-2 | Not mentioned | [111] |
| 367 | [K₂[GeMo₄O₁₃]] | HCT-116 | SMMC-7721 | HL-7702 | HEP-G2 | HEP-2 | HEP-2 | Not mentioned | [111] |
| 368 | [Na₂P₂MoO₆] | HCT-116 | SMMC-7721 | HL-7702 | HEP-G2 | HEP-2 | HEP-2 | Not mentioned | [111] |
| 369 | [K₂[GeMo₄O₁₃]] | HCT-116 | SMMC-7721 | HL-7702 | HEP-G2 | HEP-2 | HEP-2 | Not mentioned | [111] |
| 370 | [Na₂P₂MoO₆] | HCT-116 | SMMC-7721 | HL-7702 | HEP-G2 | HEP-2 | HEP-2 | Not mentioned | [111] |
| 371 | [K₂[GeMo₄O₁₃]] | HCT-116 | SMMC-7721 | HL-7702 | HEP-G2 | HEP-2 | HEP-2 | Not mentioned | [111] |
| Compound | Cells (Effects) |
|----------|----------------|
| [AsMoO$_4$(O$_2$CCH$_2$NH$_3$)$_2$]@SiO$_2$ | U937 | apoptosis and necrosis | [119] |
| Na$_2$Gd(WO$_4$)$_2$·CT | BEL-7402 | Not mentioned | [120] |
| Na$_2$Gd(WO$_4$)$_2$·CT + X-rays | BEL-7402 | Not mentioned | [120] |
| Na$_2$Gd(WO$_4$)$_2$·CT + siRNA | BEL-7402 | Not mentioned | [120] |
| Na$_2$Gd(WO$_4$)$_2$·CT + siRNA + X-rays | BEL-7402 | Not mentioned | [120] |
| [Ag(diz)$_2$][Ag(diz)$_2$·(AsMo$_4$O$_2$)]·H$_2$O | gastric cancer | SGC-7901 | Not mentioned | [121] |
| K$_2$(LiF:N$_2$O)$_2$·2SH$_2$O (FNdPW) | A549 | apoptosis | [122] |
| [PdWO$_4$]·CMC-PMMA | MCF-7, HeLa, Vero | Not mentioned | [123] |
| K$_2$(P$_2$Mo$_5$O$_{18}$) | breast cancer 4T1 | Not mentioned | [124] |
| [Na$_2$Ni$_2$O$_4$·H$_2$O$_2$](imid)$_2$(Sh$_2$W$_2$O$_3$)$_2$ | HeptG2, SMMC-7721, A549, H1299, AGS, BGC-823, HEK293T | in the S-phase and inducing cell apoptosis | [127] |
| [Na$_2$Co$_2$O$_4$·H$_2$O$_2$](imid)$_2$(Sh$_2$W$_2$O$_3$)$_2$ | AGS, BGC-823, HEK293T | in the S-phase and inducing cell apoptosis | [127] |
| [Sh$_2$W$_2$O$_7$] | AGS, BGC-823, HEK293T | in the S-phase and inducing cell apoptosis | [127] |
| [SB$_2$W$_3$] | AGS, BGC-823, HEK293T | in the S-phase and inducing cell apoptosis | [127] |
| Imi = imidazole | AGS, BGC-823, HEK293T | in the S-phase and inducing cell apoptosis | [127] |
| Cisplatin | AGS, BGC-823, HEK293T | in the S-phase and inducing cell apoptosis | [127] |
| [Ag(p-H$_2$pyttz)$_2$][H$_2$SiMo$_5$O$_9$]+4H$_2$O | MDA-MB-231, CHO, MIA-PaCa-2, J82, HCT-8, HEK-293 | mitochondrial apoptotic pathway | [128] |
| [Cu(m-pyttz)$_2$(H$_2$O)$_2$][H$_2$SiMo$_5$O$_9$] | MDA-MB-231, CHO, MIA-PaCa-2, J82, HCT-8, HEK-293 | mitochondrial apoptotic pathway | [128] |
| 5-FU | MDA-MB-231, CHO, MIA-PaCa-2, J82, HCT-8, HEK-293 | mitochondrial apoptotic pathway | [128] |
| H$_2$SiMo$_5$O$_9$ | MDA-MB-231, CHO, MIA-PaCa-2, J82, HCT-8, HEK-293 | mitochondrial apoptotic pathway | [128] |
| [Na$_2$H$_2$O$_2$]$_2$[(Na$_2$H$_5$O)$_2$][Mn$_3$(bppy)$_3$](Sh$_2$W$_2$O$_3$)$_2$]·8H$_2$O (Mn$\equiv$Sh$\equiv$W- bppy) (bppy = 1,3-bis(4-pyridyl) propane) | SGC-7901, HT-29, HeptG2, Hela, U2OS, Saos2, HMC | apoptosis | [129] |
| VMOP-31 | SMCC-7721 | apoptosis | [130] |
| Sh$_2$W$_3$ | NSCLC | apoptosis | [131] |
| NLP(Ph$_2$H$_2$N$_2$[NaP$_2$WO$_8$]$_{10}$) | HeptG2 cells, normal cells | Not mentioned | [132] |
| PMA/adenine·[AuCl$_4$]$_2$ | MDA-MB-231, PC-3, HaCaT | Not mentioned | [133] |
| PMA/thymine·Ag$^+$ | MDA-MB-231, PC-3, HaCaT | Not mentioned | [133] |
| PMA/adenine·Ag$^+$ | MDA-MB-231, PC-3 | Not mentioned | [133] |
2. Results and Discussion

2.1 The structural diagrams of \{BiW₈\}

Table S3. Crystal data and structure refinement for \{BiW₈\}

| Compound | \(\text{[BiW}_8\text{]}\) |
|----------|------------------|
| Formula  | \(\text{Co}_3\text{H}_{38}\text{Bi}_2\text{Co}_2\text{N}_6\text{Na}_2\text{O}_{44}\text{W}_9\) |
| Mr       | 3241.01 |
| Crystal. size, mm³ | 0.19 x 0.15 x 0.18 |
| Crystal system | triclinic |
| Space group | \(\text{P} \cdot 1\) |
| a, Å | 12.8345(3) |
| b, Å | 13.0070(3) |
| c, Å | 19.4287(5) |
| \(\beta\), deg | 98.795(2) |
| \(V\) (Å³) | 2997.03(13) |
| \(Z\) | 2 |
| \(D_{calcld, \text{Kg} \text{m}^{-3}}\) | 3.592 |
| \(\mu\)(MoKα), mm⁻¹ | 23.425 |
| \(F\)(000), e | 2864.0 |
| \(\theta\) range, deg° | 3.24 - 26.34 |
| Reflections collected / unique / Rint | 37943 / 23.425 / 0.0539 |
| Data/restraints/parameters | 13546 / 938 / 764 |
| \(R1\) / \(wR2\) \((I \geq 2\sigma(I))\) | 0.0449 / 0.1116 |
| \(GoF (F^2)\) | 1.036 |
| \(\Delta \rho_{\text{f}}\) (max/min), e Å⁻³ | 5.399 / -4.567 |

| Bond | Dist. | Bond | Dist. | Bond | Dist. |
|------|-------|------|-------|------|-------|
| \(\text{Bi(1)-O(36)}\) | 2.143(9) | \(\text{Bi(1)-O(38)}\) | 2.150(9) | \(\text{Bi(1)-O(40)}\) | 2.132(9) |
| Angle | (°) | Angle | (°) | Angle | (°) |
|-------|-----|-------|-----|-------|-----|
| Bi(2)-O(3) | 1.762(10) | Bi(2)-O(9) | 1.756(9) | Bi(2)-O(26) | 2.116(9) |
| Bi(2)-O(30) | 2.145(9) | Bi(2)-O(32) | 1.964(9) | Bi(2)-O(34) | 1.971(9) |
| W(1)-O(5) | 1.866(9) | W(1)-O(11) | 1.899(9) | W(1)-O(12) | 1.994(10) |
| W(1)-O(16) | 1.724(10) | W(1)-O(36) | 2.244(9) | W(1)-O(41) | 1.973(9) |
| W(2)-O(2) | 1.857(10) | W(2)-O(2) | 1.711(9) | W(2)-O(5) | 2.016(8) |
| W(2)-O(29) | 1.892(9) | W(2)-O(35) | 1.927(10) | W(3)-O(38) | 2.318(9) |
| W(3)-O(15) | 1.732(9) | W(3)-O(28) | 1.954(9) | W(3)-O(31) | 1.932(9) |
| W(3)-O(34) | 1.906(10) | W(3)-O(40) | 2.234(9) | W(3)-O(42) | 1.919(10) |
| W(4)-O(10) | 1.907(10) | W(4)-O(28) | 1.887(9) | W(4)-O(33) | 1.964(9) |
| W(4)-O(35) | 1.925(9) | W(4)-O(38) | 2.301(9) | W(4)-O(44) | 1.730(10) |
| W(5)-O(8) | 1.736(10) | W(5)-O(11) | 1.919(9) | W(5)-O(33) | 1.919(8) |
| W(5)-O(40) | 2.276(9) | W(5)-O(42) | 1.942(9) | W(5)-O(43) | 1.885(9) |
| W(6)-O(1) | 2.083(9) | W(6)-O(4) | 1.752(10) | W(6)-O(10) | 2.030(10) |
| W(6)-O(26) | 1.813(9) | W(6)-O(30) | 1.805(9) | W(6)-O(38) | 2.193(8) |
| W(7)-O(14) | 1.717(10) | W(7)-O(29) | 1.966(9) | W(7)-O(32) | 1.905(9) |
| W(7)-O(36) | 2.264(9) | W(7)-O(39) | 1.908(9) | W(7)-O(41) | 1.887(10) |
| W(8)-O(6) | 1.960(10) | W(8)-O(12) | 1.931(10) | W(8)-O(13) | 1.706(10) |
| W(8)-O(36) | 2.253(9) | W(8)-O(37) | 1.872(9) | W(8)-O(39) | 2.002(9) |
| W(9)-O(7) | 1.728(9) | W(9)-O(27) | 1.793(9) | W(9)-O(31) | 1.967(9) |
| W(9)-O(37) | 1.966(9) | W(9)-O(40) | 2.244(8) | W(9)-O(43) | 2.031(10) |
| Co(1)-O(4) | 2.087(10) | Co(1)-O(6) | 2.094(9) | Co(1)-O(17) | 2.124(11) |
| Co(1)-O(18) | 2.072(11) | Co(1)-O(19) | 2.121(13) | Co(1)-O(27) | 2.072(10) |
| Na(1)-O(1) | 2.463(11) | Na(1)-O(17) | 2.462(13) | Na(1)-O(20) | 2.328(13) |
| Na(1)-O(20) | 2.446(11) | Na(1)-O(21) | 2.352(16) | Na(1)-O(22) | 2.496(13) |
| Na(2)-O(3) | 2.826(13) | Na(2)-O(6) | 2.852(15) | Na(2)-O(19) | 2.905(16) |
| Bond                        | Angle (°) | Bond                        | Angle (°) |
|-----------------------------|-----------|-----------------------------|-----------|
| O(20)-Na(1)-O(21)          | 172.5(5)  | O(20)-Na(1)-O(22)          | 165.1(4)  |
| O(3)-Na(2)-O(6)            | 115.3(4)  | O(3)-Na(2)-O(19)           | 143.2(5)  |
| O(6)-Na(2)-O(19)           | 65.3(4)   | O(6)-Na(2)-O(19)           | 65.3(4)   |

Symmetry transformations used to generate equivalent atoms: 
#1: -x, -y, -z; #2: -x+1/2, -y+1/2, -z

Figure S1. The view of the basic units in \( \{\text{BiW}_8\} \) with 50% thermal ellipsoid

Figure S2. The 1-D chain of \( \{\text{BiW}_8\} \).
Figure S3. (a) The 2D structure for \{BiW₈\} (b) Simplified diagram of 2D structure for \{BiW₈\} (Some O atoms are omitted).

Figure S4. (a) The 3D structure for \{BiW₈\} (b) Simplified diagram of 3D structure for \{BiW₈\} (Some O atoms are omitted)

Figure S5. Simplified diagram of 3D structure for \{BiW₈\} with other direction (Some O atoms are omitted).
Table S5. The hydrogen bonding and supramolecular interaction of \{BiW\}_8

| Donor | H   | Acceptor | D-H   | H...A | D...A   | D-H...A |
|-------|-----|----------|-------|-------|---------|---------|
| N3    | H1N | O35      | 0.86  | 2.29  | 2.9908(1)| 138     |
| N3    | H1N | O33      | 0.86  | 2.26  | 2.9692(1)| 140     |
| N2    | H2N | O3      | 0.86  | 2.03  | 2.8170(1)| 152     |
| N2    | H2N | O15      | 0.86  | 2.56  | 3.0049(1)| 113     |
| C3    | H3B | O2       | 0.96  | 2.57  | 3.5150(1)| 168     |
| C4    | H4A | O15      | 0.93  | 2.46  | 3.1689(1)| 133     |
| C10   | H10C| O2       | 0.96  | 2.51  | 3.4395(1)| 162     |
| C21   | H21C| O11      | 0.96  | 2.52  | 3.4407(1)| 161     |

2.2 The characterization diagrams of \{BiW\}_8

- Figure S6. IR spectra of compound \{BiW\}_8
- Figure S7. TG curve of \{BiW\}_8 compound
- Figure S8. XRD for compound \{BiW\}_8
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**Figure S9.** The stability of the \(\text{BiW}_8\) compound in PBS buffer was obtained via UV spectroscopy after 0, 24, and 48 h of incubation (pH=7.4) at 37°C.

**Figure S10.** The DLS test of compound 5 mM \(\text{BiW}_8\) in PBS buffer (pH=7.4) after 0 h incubation (pH=7.4) at 37°C.

**Figure S11.** The DLS test of compound 5 mM \(\text{BiW}_8\) in PBS buffer (pH=7.4) after 24 h incubation (pH=7.4) at 37°C.
Figure S12. The DLS test of compound 5 mM {BiW₈} in PBS buffer (pH=7.4) after 48 h incubation (pH=7.4) at 37°C.

2.3 Calculation of IC₅₀

To determine the effect of {BiW₈} on cell proliferation, the cell viabilities of one normal cell line (human umbilical vein endothelial cell line [HUVEC]) and five carcinoma cell lines (human osteosarcoma cell line, MG63; human rhabdomyosarcoma cell line, RD; human liver cancer cell lines, HepG2 and Hep3B; and human breast carcinoma cell line, MCF7) were measured via MTT assays. As shown in Figure S13, {BiW₈} caused nonlinear inhibition of cell growth.

Figure S13. MTT assay was performed to evaluate the cell viability after treated with the increased concentration (0, 50, 100, 200, and 400 μM) of {BiW₈} for 24 and 48 h. (a) HUVEC; (b) MG63; (c) RD; (d) Hep3B; (e) HepG2; (f) MCF7. Data are presented as the Mean ± SD. Statistical significances were determined by Student’s t-test. *p < 0.05.

As shown in the Figure S14, linear regression equation were applied to calculate the IC₅₀. When set the X is the logarithmic concentration of {BiW₈}, Y is the probit of cell inhibitory rate, and A and B are constants, we obtained the linear regression equation of Y=A×X+B. The log₁₀(IC₅₀) was obtained by setting the value of Y to 5. And the equation and IC₅₀ were list in Table S6.
Figure S14. MTT assay was performed to evaluate the cell viability after treated with the increased concentration (0, 50, 100, 200, and 400 μM) of \(\text{BiW}_8\) for 24 and 48 h. Linear regression equation were applied to calculate the IC\(_{50}\). The straight line was fitted to the log dose-inhibitory rate probit curve by regression analysis. And the equation and IC\(_{50}\) were list in Table S6.

| Human cell lines | Time/h | Regression equation | \(\log_{10}(\text{IC}_{50})\) | \text{IC}_{50} / μM | \(R^2\) | 95% confidence interval / μM |
|------------------|--------|---------------------|--------------------------|---------------------|------|----------------------------|
| HUVEC            | 24     | \(Y = 1.3594X + 0.9868\) | 2.9522                   | 895.8               | 0.9943 | 864.2-927.3                |
|                  | 48     | \(Y = 1.4823X + 1.1733\) | 2.5816                   | 381.6               | 0.9512 | 352.4-403.9                |
| MG63             | 24     | \(Y = 2.0044X + 0.7809\) | 2.1048                   | 127.3               | 0.9948 | 117.7-145.1                |
|                  | 48     | \(Y = 2.1270X + 1.1700\) | 1.8007                   | 63.2                | 0.9813 | 57.01-73.67                |
| RD               | 24     | \(Y = 1.4417X + 1.3425\) | 2.5369                   | 344.3               | 0.9911 | 335.1-371.6                |
|                  | 48     | \(Y = 1.4230X + 1.8470\) | 2.2156                   | 164.3               | 0.9936 | 150.3-187.1                |
| Hep3B            | 24     | \(Y = 1.4698X + 1.0932\) | 2.6580                   | 455.0               | 0.9886 | 445.8-462.7                |
|                  | 48     | \(Y = 1.6575X + 1.1269\) | 2.3367                   | 217.1               | 0.9960 | 198.5-231.2                |
The growth inhibition in MG63 cells treated with {BiW₈} and three raw materials (Na₂WO₄·2H₂O, CoCl₂·6H₂O, and dmap) for 24 and 48 h was measured. As shown in Figure S15, {BiW₈} and three raw materials caused nonlinear inhibition of cell growth.

As shown in the Figure S16, linear regression equation were applied to calculate the IC₅₀. When set the X is the logarithmic concentration of drug, Y is the probit of cell inhibitory rate, and A and B are constants, we obtained the linear regression equation of Y=A×X+B. The log₁₀ (IC₅₀) was obtained by setting the value of Y to 5. And the equation and IC₅₀ were list in Table S7.

![Figure S15. MTB assay analysis {BiW₈} and three raw materials treatment (0, 50, 100, 200, and 400 μM) against MG63 cells for (a) 24 and (b) 48 h. Data are presented as the mean ± SD. Statistical significances were calculated by Student’s t-test or two-way ANOVA, *** p < 0.001, **** p < 0.0001.](image)

![Figure S16. MTB assay analysis {BiW₈} and three raw materials treatment (0, 50, 100, 200, and 400 μM) against MG63 cells for 24 and 48 h. Linear regression equation were applied to calculate the IC₅₀. And the straight line was fitted to the log dose-inhibitory rate probit curve by regression analysis. (a) MG63 cells were treated with {BiW₈} for 24 h; (b) MG63 cells were treated with {BiW₈} for 48 h; (c) MG63 cells were treated with Na₂WO₄·2H₂O for 24 h; (d) MG63 cells were treated with Na₂WO₄·2H₂O for 48 h; (e) MG63 cells were treated with CoCl₂·6H₂O for 24 h; (f) MG63 cells were treated with CoCl₂·6H₂O for 48 h; (g) MG63 cells were treated with dmap for 24 h; (h) MG63 cells were treated with dmap for 48 h. Data are presented as the Mean ± SD. Statistical significances were determined by Student’s t-test. *p < 0.05.](image)
Table S7. The IC<sub>50</sub> values of drugs to MG63 cells

| Drugs                | Time/h | Regression equation | log<sub>10</sub>(IC<sub>50</sub>) | IC<sub>50</sub> / μM | R<sup>2</sup> | 95% confidence interval / μM |
|----------------------|--------|---------------------|-------------------------------|----------------------|--------------|-------------------------------|
| (BiW<sub>8</sub>)    | 24     | Y = 2.0044X + 0.7809 | 2.1048                        | 127.3                | 0.9948       | 117.7 - 145.1                 |
|                      | 48     | Y = 2.127X + 1.17   | 1.8007                        | 63.2                 | 0.9813       | 57.01 - 73.67                 |
| Na<sub>2</sub>WO<sub>4</sub>·2H<sub>2</sub>O | 24     | Y = 0.7034X + 2.7867 | 3.0013                        | 1003.0               | 0.9748       | 730.3 - 1377                  |
|                      | 48     | Y = 1.0435X + 2.4168 | 2.4755                        | 298.9                | 0.999        | 266.3 - 356.9                 |
| CoCl·6H<sub>2</sub>O  | 24     | Y = 0.5473X + 2.7756 | 4.0643                        | 11596.2              | 0.9498       | 5754 - 37813                  |
|                      | 48     | Y = 0.655X + 3.1583  | 2.8118                        | 648.3                | 0.9603       | 411.9 - 992.4                 |
| dmap                 | 24     | Y = 1.357X + 1.5958  | 2.5629                        | 365.5                | 0.9895       | 328.7 - 406.4                 |
|                      | 48     | Y = 1.3755X + 2.1609 | 2.0641                        | 115.9                | 0.9578       | 110.3 - 166.1                 |

Linear regression equation were applied to calculate the IC<sub>50</sub>. According to the linear regression equation of Y = A×X + B, X is the logarithmic concentration of drugs, Y is the probit of cell inhibitory rate, and A and B are constants. log<sub>10</sub>(IC<sub>50</sub>) values were obtained by setting the value of Y to 5.

For further comparison, the growth inhibition in MG63 cells treated with (BiW<sub>8</sub>) and three other POM drugs (Na<sub>9</sub>[SbW<sub>9</sub>O<sub>33</sub>]·19.5H<sub>2</sub>O, Na<sub>6</sub>H<sub>4</sub>[Bi<sub>2</sub>W<sub>10</sub>Co<sub>2</sub>O<sub>30</sub>(H<sub>2</sub>O)<sub>6</sub>·34H<sub>2</sub>O, and Na<sub>9</sub>[BiW<sub>9</sub>O<sub>33</sub>]·16H<sub>2</sub>O) for 24 and 48 h was measured (Figure S16-17). At 24 h post-incubation, the IC<sub>50</sub> values of (BiW<sub>8</sub>), Na<sub>9</sub>[SbW<sub>9</sub>O<sub>33</sub>]·19.5H<sub>2</sub>O, Na<sub>9</sub>[BiW<sub>9</sub>O<sub>33</sub>]·16H<sub>2</sub>O were 127.3, 912.7, 389.5, and 696.3 μM, respectively (Table S8). At 48 h post-incubation, their IC<sub>50</sub> values were 63.2, 398.8, 194.2, and 304.9 μM, respectively.

**Figure S17.** MTT assay analysis (BiW<sub>8</sub>) and three POM drugs (0, 50, 100, 200, and 400 μM) against MG63 cells for (a) 24 and (b) 48 h. Data are presented as the mean ± SD. Statistical significances were calculated by Student’s t-test or two-way ANOVA, *p < 0.05 **p < 0.01 ***p < 0.001 ****p < 0.0001.
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Figure S18. MTT assay analysis (BiW₈) and three other POM drugs (0, 50, 100, 200, and 400 μM) against MG63 cells for 24 and 48 h. Linear regression equation were applied to calculate the IC₅₀. The straight line was fitted to the log dose-inhibitory rate probit curve by regression analysis. And the equation and IC₅₀ were listed in Table S8.

(a) MG63 cells were treated with BiW₈ for 24 h; (b) MG63 cells were treated with BiW₈ for 48 h; (c) MG63 cells were treated with Na₉[SbW₉O₃₃]·19.5H₂O for 24 h; (d) MG63 cells were treated with Na₉[SbW₉O₃₃]·19.5H₂O for 48 h; (e) MG63 cells were treated with Na₁₀[Bi₂W₂₀Co₂O₇₀(H₂O)₆]·41H₂O for 24 h; (f) MG63 cells were treated with Na₁₀[Bi₂W₂₀Co₂O₇₀(H₂O)₆]·41H₂O for 48 h; (g) MG63 cells were treated with Na₉[BiW₉O₃₃]·16H₂O for 24 h; (h) MG63 cells were treated with Na₉[BiW₉O₃₃]·16H₂O for 48 h. Data are presented as the Mean ± SD. Statistical significances were determined by Student's t-test. *p < 0.05.

Table S8. The IC₅₀ values of drugs to MG63 cells

| Drugs                  | Time/h | Regression equation       | Log₁₀ (IC₅₀) | IC₅₀/μM | R²       | 95% confidence interval / μM |
|------------------------|--------|---------------------------|-------------|--------|----------|-----------------------------|
| BiW₈                   | 24     | Y = 2.0044X+0.7809        | 2.1048      | 127.3  | 0.9948   | 117.7-145.1                |
| BiW₈                   | 48     | Y = 2.1270X+1.1700        | 1.8007      | 63.2   | 0.9813   | 57.0-73.7                  |
| Na₉[SbW₉O₃₃]·19.5H₂O  | 24     | Y = 0.7639X+2.7386        | 2.9603      | 912.7  | 0.9856   | 764.6-1439.3               |
| Na₁₀[Bi₂W₂₀Co₂O₇₀(H₂O)₆]·41H₂O | 24  | Y = 0.6226X+3.3808        | 2.6008      | 398.8  | 0.9957   | 379.9-430.7                |
| Na₉[Bi₂W₂₀Co₂O₇₀(H₂O)₆]·41H₂O | 48  | Y = 1.1498X+2.0214        | 2.5905      | 389.5  | 0.9817   | 383.2-412.6                |
| Na₁₀[BiW₉O₃₃]·16H₂O   | 24     | Y = 1.5239X+1.5131        | 2.2882      | 194.2  | 0.9997   | 185.7-236.7                |
| Na₁₀[BiW₉O₃₃]·16H₂O   | 48     | Y = 0.7312X+3.1836        | 2.4842      | 304.9  | 0.9707   | 281.5-351.5                |

Linear regression equation were applied to calculate the IC₅₀. According to the linear regression equation of Y=A×X+B, X is the logarithmic concentration of drugs, Y is the probit of cell inhibitory rate, and A and B are constants. log₁₀ (IC₅₀) values were obtained by setting the value of Y to 5.

2.4 Effects of (BiW₈) on invasion and migration

In the wound healing assay (Figure S19), the gap of the control group largely closed, and the wound was stationary at the centroid position (45.95% and 86.4% confluence at 24 and 48 h post-scratch, respectively), while the experimental group (10.36% and 26.77% confluence at 24 and 48 h post-scratch, respectively) failed to fill large portions of the scratch. This indicates that (BiW₈) reduced the migration ability of the MG63 cells.
Figure S19. Before and after treated with 127.3 μM {BiWs} for 24 and 48h, MG63 cells migration were analysed by the wound healing assay. (a) Representative phase-contrast microscopic images of the wound healing assay (magnification 40×, scale bars=200μm). (b) Quantification of the wound-healing assay. Data are presented as the mean ± SD of three independent experiments. Statistical significances were calculated by two-way ANOVA, **p < 0.01, ***p < 0.001.

In the Transwell Matrigel assay (Figure S20), the numbers of invading cells of the control group increased by more than four and seven times those of the experimental group after 24 and 48 h, respectively. This indicates that {BiWs} repressed the invasion ability of the MG63 cells.

Figure S20. Before and after treated with 127.3 μM {BiWs} for 24 and 48h, MG63 cells invasion were analysed by the Transwell Matrigel assay. (a) Representative phase-contrast microscopic images of the Transwell Matrigel assay (magnification 40×, scale bars=100μm). (b) Quantification of the Transwell Matrigel assay. Data are presented as the mean ± SD of three independent experiments. Statistical significances were calculated by two-way ANOVA, **p < 0.01, ***p < 0.001.

2.5 Effects of {BiWs} on GSH

Figure S21. (a) The absorbance changes of NADPH in different concentrations of {BiWs} (b) The relationship between the concentration of {BiWs} and the inhibition rate.
2.6 Effects of (BiW8) on transcriptome

We performed RNA sequencing in three biological replicates to compare global gene expression profiles. We first compared the gene expression profiles of MG63 cells incubated with 127.3 μM (BiW8) for 24 h as the experimental group and normal MG63 cells as the control group.

When the cutoff was set to a false discovery rate (FDR)<0.05, a total of 20 Gene Ontology (GO) terms of biological process (BP), 14 GO terms of cellular component (CC), and 9 GO terms of molecular function (MF) were identified (Figure S25a–c). These data indicate that (BiW8) altered the expression profiles of DEGs mostly located in the cell nuclei or cytoplasm with functions related to DNA repair, replication, transcription, energy, and enzymes. We performed further enrichment analysis using the Kyoto Encyclopedia of Genes and Genomes (KEGG). When the cutoff was set to the top 3000 upregulated and downregulated DEGs, a total of 24 Kyoto Encyclopedia of Genes and Genomes (KEGG) pathways enriched by 1739 DEGs (Figure S25d, 8) were obtained. Most of the 24 pathways could be summarized and classified into four functional categories: DNA repair/replication, glutathione metabolism, ECM-cell/cell-cell interactions, and signaling pathways in cancer.
Figure S25. GO term and KEGG pathway analysis for 3000 up- and downregulated DEGs (experimental group vs. control group). Top pathways with FDR< 0.05, -log FDR> 1.301 are shown: (a) biological process, (b) cellular component, (c) molecular function, and (d) KEGG pathway.

When the cutoff was to the top 3000 downregulated DEGs, 14 KEGG pathways were identified (Figure S26). These 14 KEGG pathways could be sorted with the abovementioned identical functional categories.

Figure S26. KEGG pathway analysis for 3000 downregulated DEGs (experimental vs. control group). Top pathways with FDR< 0.05, -log FDR> 1.301.
### Table S9. DEGs in RNA-sequencing

| Gene Name | FoldChange | Log2FoldChange | adj.p | Up/Down |
|-----------|------------|----------------|-------|---------|
| APEX1     | 0.555536811| -0.848045585   | 5.14×10⁻²² | down   |
| APEX2     | 0.441600567| -1.17918607    | 4.27×10⁻²⁵ | down   |
| EXO1      | 0.403608027| -1.308973227   | 5.87×10⁻³⁵ | down   |
| FEN1      | 0.291740538| -1.777242231   | 3.89×10⁻¹¹⁵ | down |
| LIG1      | 0.088204608| -3.503902158   | 1.89×10⁻¹⁶ | down   |
| MSH2      | 0.225319167| -2.149958053   | 1.01×10⁻¹² | down   |
| MSH3      | 0.511280157| -0.967814061   | 5.55×10⁻¹⁵ | down   |
| MUTYH     | 0.382067271| -1.388101419   | 6.10×10⁻⁹  | down   |
| NEIL2     | 0.526180922| -0.926391555   | 1.46×10⁻⁴  | down   |
| NTHL1     | 0.211546498| -2.240953292   | 1.04×10⁻³³ | down   |
| OGG1      | 0.476266855| -1.07015855    | 1.62×10⁻⁶  | down   |
| PARP1     | 0.206554402| -2.275406289   | 4.11×10⁻⁸  | down   |
| PCNA      | 0.146240994| -2.773580315   | 1.74×10⁻²⁰ | down   |
| POLD1     | 0.261441988| -1.935437731   | 1.52×10⁻⁸  | down   |
| POLD3     | 0.293376679| -1.769173902   | 1.50×10⁻⁷  | down   |
| POLE      | 0.402673611| -1.312317164   | 3.43×10⁻⁸  | down   |
| POLE2     | 0.244754198| -2.030594492   | 4.92×10⁻⁰  | down   |
| RPA1      | 0.315782593| -1.662969447   | 1.58×10⁻¹² | down   |
| RPA3      | 0.285862457| -1.806606935   | 7.60×10⁻³⁸ | down   |
| UNG       | 0.245566517| -2.025814233   | 5.82×10⁻¹⁴ | down   |
| XRCC1     | 0.302848364| -1.723332476   | 3.74×10⁻⁵² | down   |
| GSTA1     | 0.054767445| -4.190537612   | 9.47×10⁻²² | down   |
| GSTA2     | 0.122829987| -3.025265284   | 2.86×10⁻⁸  | down   |
| GSTA4     | 0.585531707| -0.7721808     | 2.43×10⁻³  | down   |
| GSTK1     | 0.496422134| -1.010360654   | 1.27×10⁻¹⁴ | down   |
| GSTM1     | 0.498118936| -1.00543784    | 1.03×10⁻³⁸ | down   |
| GSTM2     | 0.407736822| -1.294289851   | 1.43×10⁻¹⁰ | down   |
| GSTM4     | 0.633515432| -0.658543332   | 2.48×10⁻¹⁰ | down   |
| GSTT2B    | 0.395136605| -1.339576592   | 3.97×10⁻¹⁰ | down   |
| GPX1      | 0.567733751| -0.816713584   | 2.42×10⁻²² | down   |
| GPX2      | 0.161122328| -2.633771661   | 3.60×10⁻²  | down   |
| GPX7      | 0.81076994| -0.302635495   | 6.51×10⁻⁴  | down   |
| GPX8      | 0.635329722| -0.654225822   | 6.06×10⁻²  | down   |
| CASP3     | 1.950516553| 0.963856242    | 1.25168×10⁻²⁷ | up |
| CASP4     | 2.37326709| 1.24693526    | 6.57×10⁻²⁷ | up |
| CASP5     | 4.92755801| 5.489528743   | 8.14×10⁻⁴  | up |
| GSDMB     | 1.437232816| 0.523293782    | 3.24×10⁻²  | up |
| GSDME     | 2.029902366| 1.021410338   | 2.11×10⁻⁸  | up |
| IL16      | 3.590645223| 1.844243113    | 1.30×10⁻⁶³ | up |
| NLRP3     | 6.241318275| 2.641850784   | 6.01×10⁻⁸  | up |
| NLRC4     | 2.151562653| 1.105384852   | 3.46×10⁻⁶  | up |
| NLRP10    | 4.55175399| 2.186422462   | 2.21×10⁻⁵  | up |
| TXNIP     | 10.08182719| 3.333685226   | 1.76×10⁻⁴  | up |

**Experimental vs. control group, FoldChange>1.5 or <0.67, |Log2FoldChange|>0.58, adj.p<0.05.**

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