

Supporting Information:

Inhibitory Effects of New Cobalt-Based Polyoxometalates on Growth of Human Cancer Cells**

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Table S1 Crystal data and refinement parameters for Compound BWCN.

Compound	BWCN
Empirical formula	H ₈₈ Na ₄ Bi ₂ Co ₂ W ₂₀ O ₁₀₇ C ₆ N ₄
Formula weight	6152.74
Temperature, K	273
Crystal system	triclinic
Space group	P -1
a, Å	12.4832(5)
b, Å	13.6886(5)
c, Å	16.9954(6)
α , deg	69.4680(10)
β , deg	83.0670(10)
γ , deg	64.6840(10)
Volume, Å ³	2457.00(16)
Z	1
D _{calcd} (g cm ⁻³)	4.158
μ (Mo K α), mm ⁻¹	27.339
F(000)	2672
Reflections collected/unique (R _{int})	17826 / 11657
GOF on F ²	1.035
Final R indices [I > 2 σ (I)]	R1 = 0.0533, wR2 = 0.1430
R (all data)	R1 = 0.0640, wR2 = 0.1512

(* R₁ = $\sum||F_o| - |F_c|| / \sum|F_o|$, wR₂ = $[\sum(w(F_o^2 - F_c^2)^2) / \sum(wF_o^2)^2]^{1/2}$).

Table S2: Selected bond lengths (Å) and angles (deg) for Compound BWCN.

bond and bond angles	bond lengths (Å) and angles (deg)	bond and bond angles	bond lengths (Å) and angles (deg)	bond and bond angles	bond lengths (Å) and angles (deg)
W1-O25	1.797(12)	W1-O37	1.741(12)	W1-O38	2.077(11)
W1-O40	2.201(11)	W1-O44	2.075(11)	W1-O18	1.803(12)
W2-O20	1.720(13)	W2-O27	1.915(12)	W2-O28	1.899(11)
W2-O34	1.892(12)	W2-O43	1.937(11)	W2-O45	2.285(10)
W3-O31	1.698(12)	W3-O34	1.967(12)	W3-O36	1.952(11)
W3-O38	1.859(11)	W3-O40	2.303(11)	W3-O41	1.864(10)
W4-O12	1.707(12)	W4-O30	1.898(12)	W4-O32	1.873(12)
W4-O41	1.978(10)	W4-O43	1.956(11)	W4-O45	2.247(10)
W5-O26	1.910(12)	W5-O33	1.722(11)	W5-O36	1.909(11)
W5-O40	2.307(11)	W5-O42	1.937(11)	W5-O44	1.870(11)
W6-O23	1.704(13)	W6-O22	1.914(12)	W6-O27	1.909(12)
W6-O35	1.939(12)	W6-O39	2.297(11)	W6-O42	1.914(12)
W7-O16	1.727(12)	W7-O17	1.782(12)	W7-O19	1.888(13)
W7-O28	2.029(13)	W7-O30	2.008(12)	W7-O45	2.219(10)
W8-O15	1.927(13)	W8-O21	1.713(12)	W8-O26	1.944(12)
W8-O29	1.863(13)	W8-O35	1.977(12)	W8-O39	2.237(11)
W9-O13	1.742(13)	W9-O15	1.966(12)	W9-O22	2.019(12)
W9-O19	1.963(13)	W9-O24	1.808(13)	W9-O39	2.215(10)
W10-O6	1.849(14)	W10-O8	1.894(18)	W10-O18	2.093(12)
W10-O25	2.119(12)	W10-O29	1.967(13)	W10-O32	2.009(12)
Co1-O3	2.037(16)	Co1-O4	2.101(16)	Co1-O5	2.148(17)
Co1-O17	2.092(12)	Co1-O24	2.040(12)	Co1-O37	2.071(12)
Co1-O24	2.040(12)	Co1-O17	2.092(12)	Bi1-O39	2.127(10)
Bi1-O40	2.128(11)	Bi1-O45	2.143(10)	Na1-O20	2.294(15)
Na1-O31	2.294(15)	Na1-O9	2.428(18)	Na1-O10	2.410(18)
Na1-O11	2.477(17)	Na1-O1	2.34(3)	Na2-O2	2.38(3)
Na2-O7	2.382(16)	Na2-O9	2.451(18)	Na2-O10	2.344(16)
Na2-O11	2.448(17)	Na2-O14	2.417(17)	N1-C3	1.26(4)
N1-C1	1.28(4)	N2-C2	1.29(4)	N2-C1	1.35(4)
C3-C2	1.33(5)	O38-W1-O40	71.6(4)	O37-W1-O40	164.0(5)
O28-W2-O45	72.7(5)	O20-W2-O45	170.0(5)	O38-W3-O40	73.1(4)
O31-W3-O40	168.3(5)	O30-W4-O45	75.2(4)	O12-W4-O45	173.8(5)
O44-W5-O40	73.8(4)	O33-W5-O40	170.5(5)	O22-W6-O39	73.6(4)
O23-W6-O39	171.2(5)	O28-W7-O45	72.0(4)	O16-W7-O45	163.0(5)
O15-W8-O39	74.4(4)	O21-W8-O39	170.9(5)	O22-W9-O39	73.6(4)
O13-W9-O39	166.7(6)	O18-W10-O25	81.0(5)	O6-W10-O25	173.1(7)
O4-Co1-O5	84.9(8)	O3-Co1-O24	179.1(6)	O39-Bi1-O45	85.2(4)
O40-Bi1-O45	89.1(4)	O10-Na1-O9	77.9(6)	O20-Na1-O10	176.9(6)
O10-Na2-O9	78.7(6)	O2-Na2-O11	169.9(8)	N2-C2-C3	106(3)

N1-C3-C2	111(3)	N1-C1-N2	108(3)	C2-N2-C1	107(3)
C3-N1-C1	108(3)	W2-O20-Na1	170.3(8)	W3-O31-Na1	139.1(7)

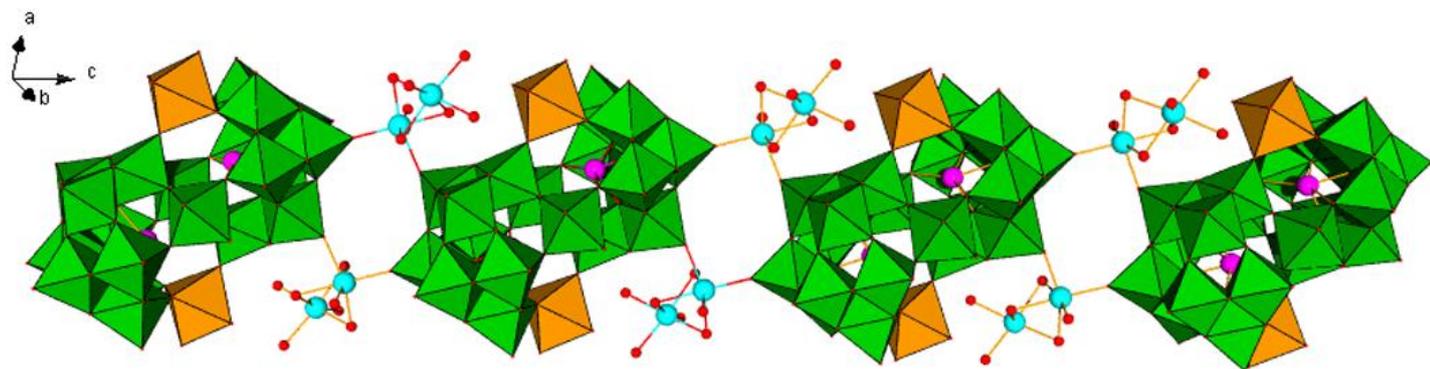


Figure S1. 1-D chain of BWCN was made by sandwiched POM units and $[Na_2]$ linkers (green octahedra, W; yellow octahedra, Co; purple ball, Bi; green ball, Na).

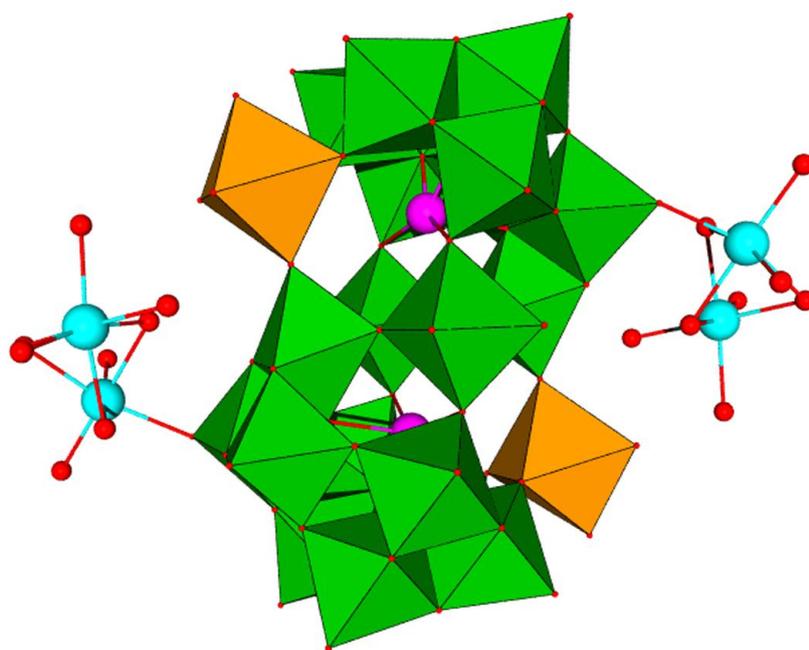


Figure S2. View of the molecule structure of compound BWCN. Elements show green octahedra, W, yellow octahedra, Co, purple ball, Bi, and green ball, Na in the picture.

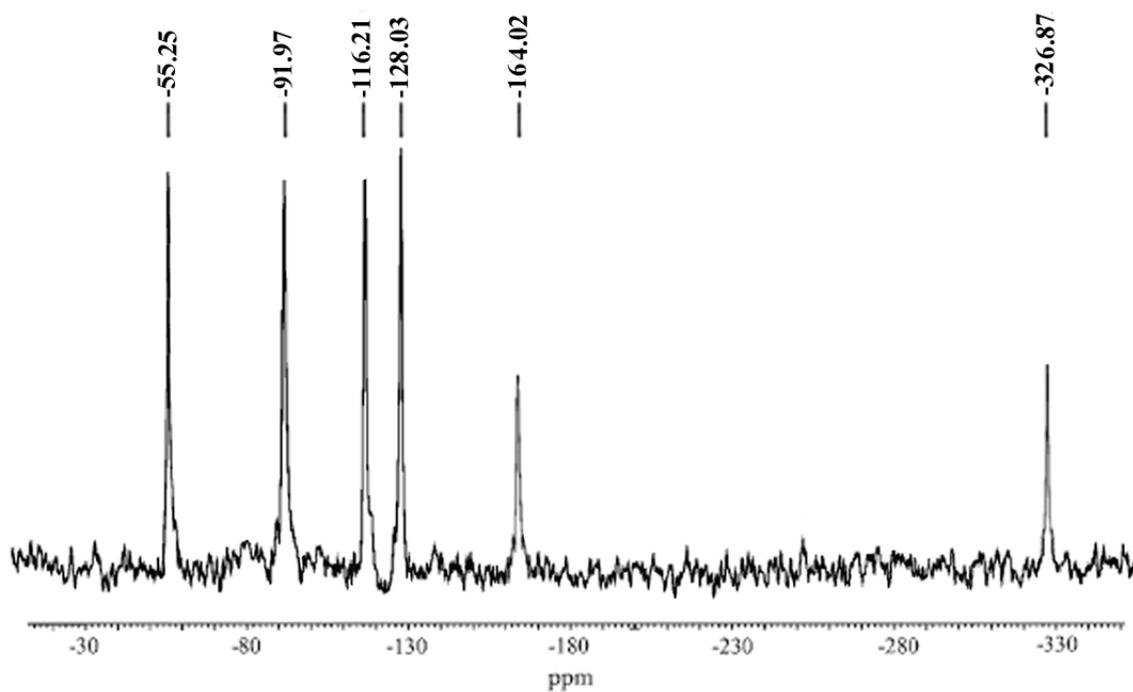


Figure S3. Tungsten-183 NMR spectra of compound BWCN at 293 K.

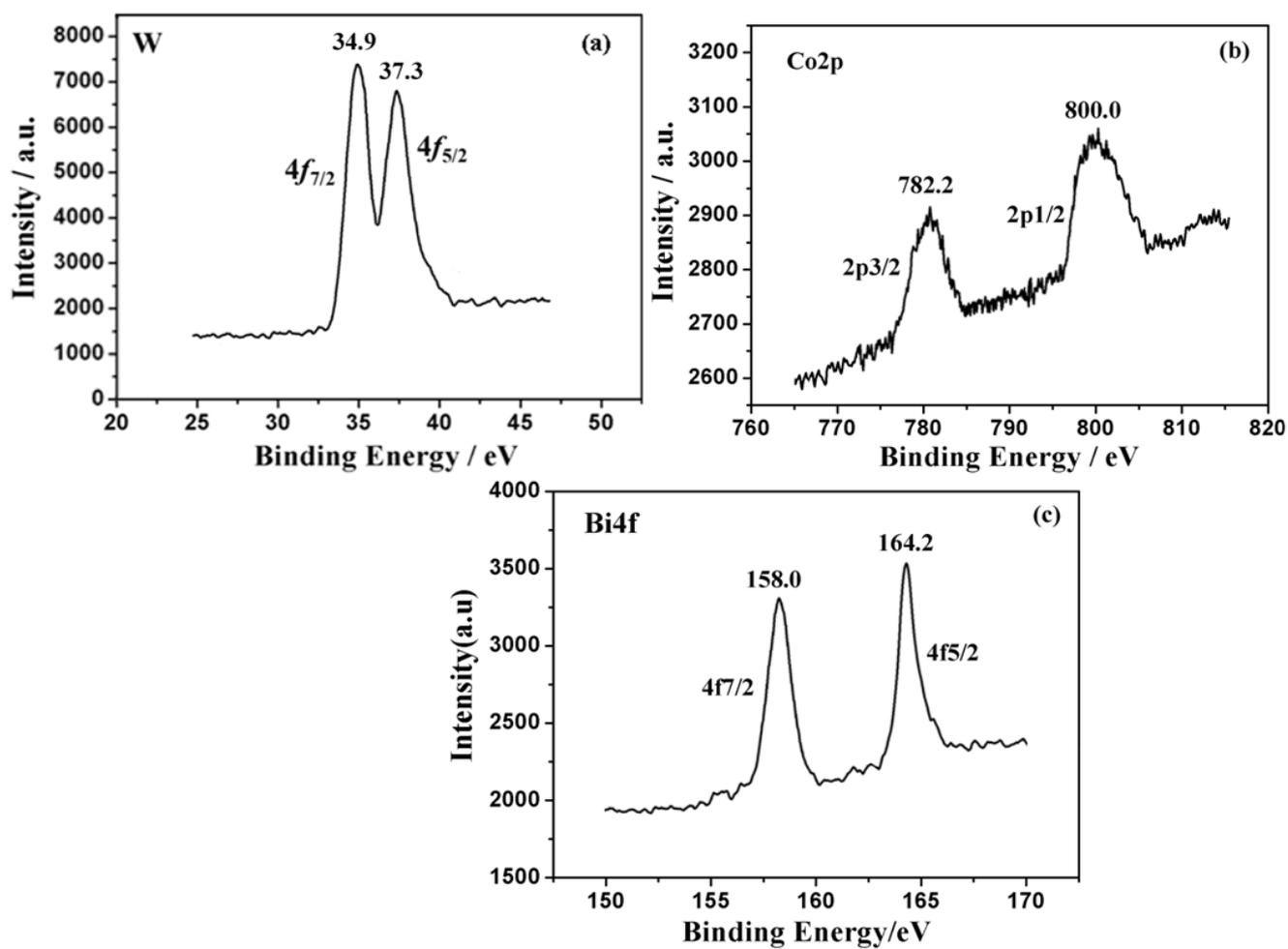


Figure S4. XPS spectra of compound BWCN.

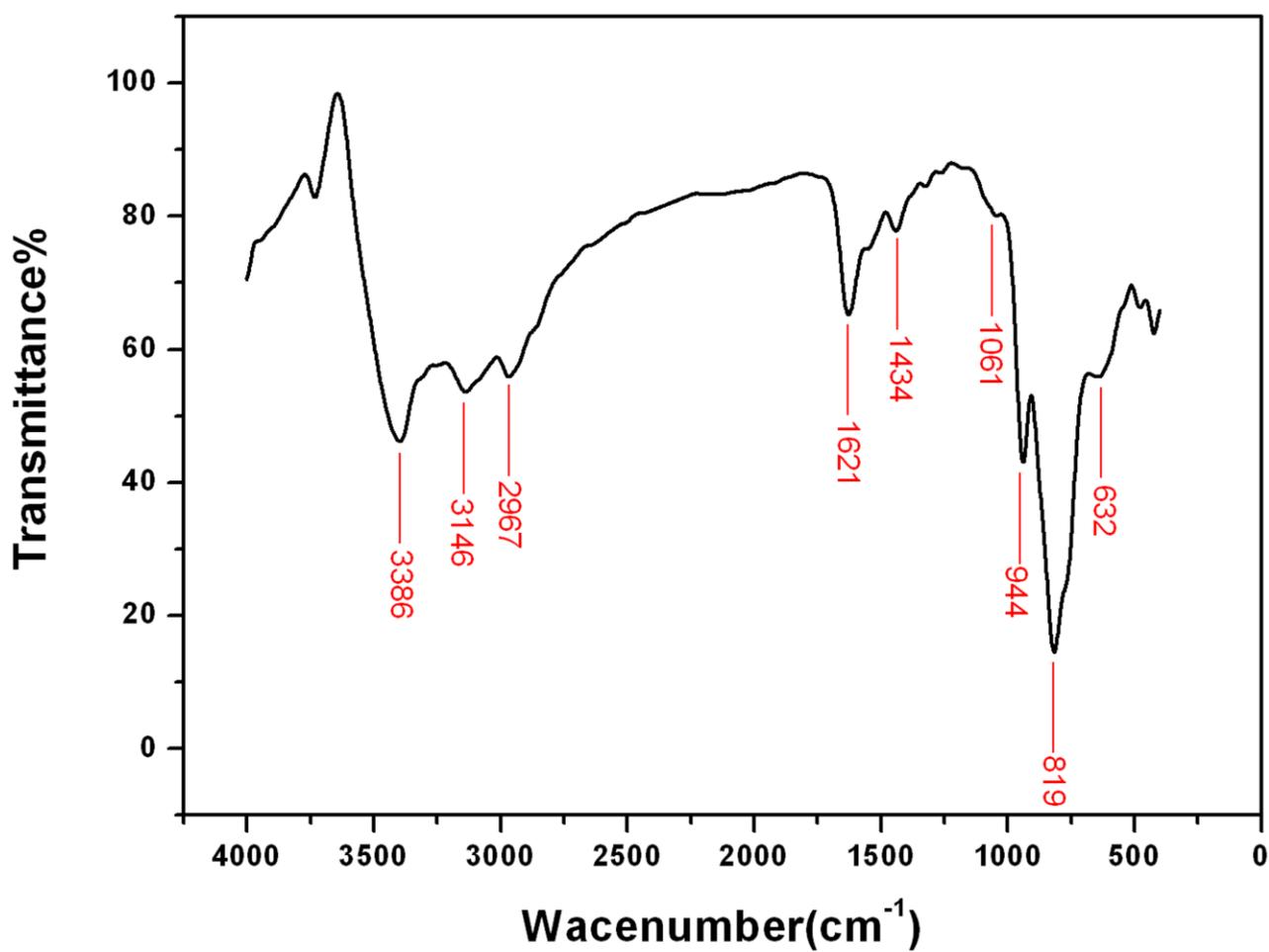


Figure S5. IR spectra of compound BWCN.

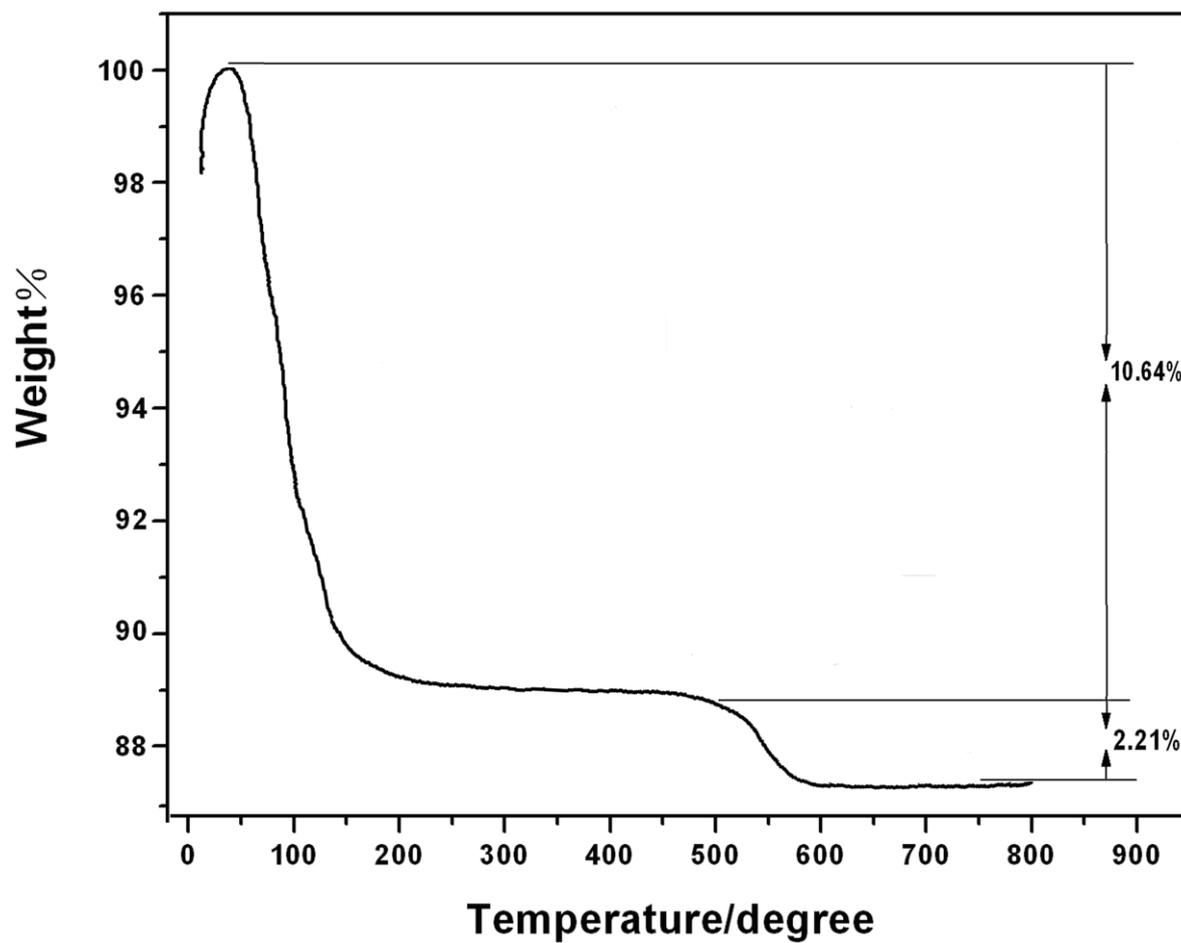


Figure S6. TG curve of compound BWCN.

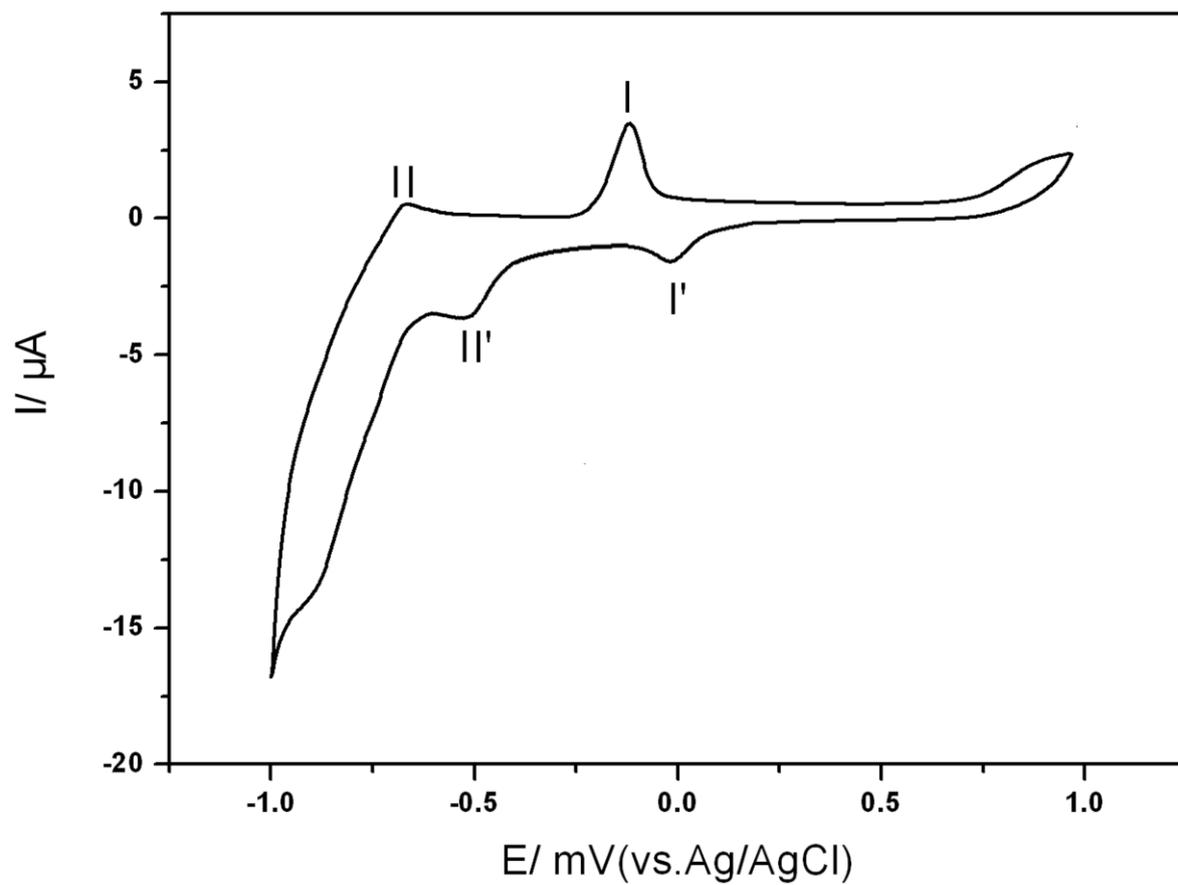


Figure S7. Cyclic voltammograms of compound BWCN.

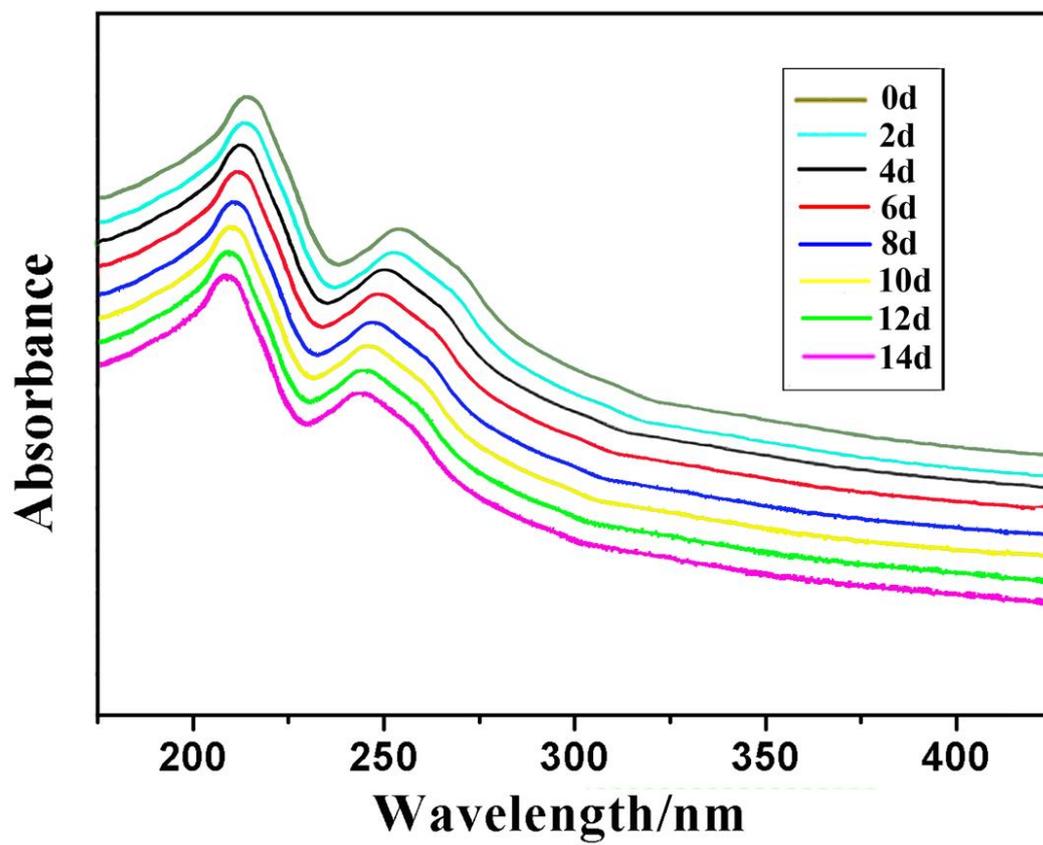


Figure S8. The influence of time on the stability of compound BWCN in the aqueous solution.

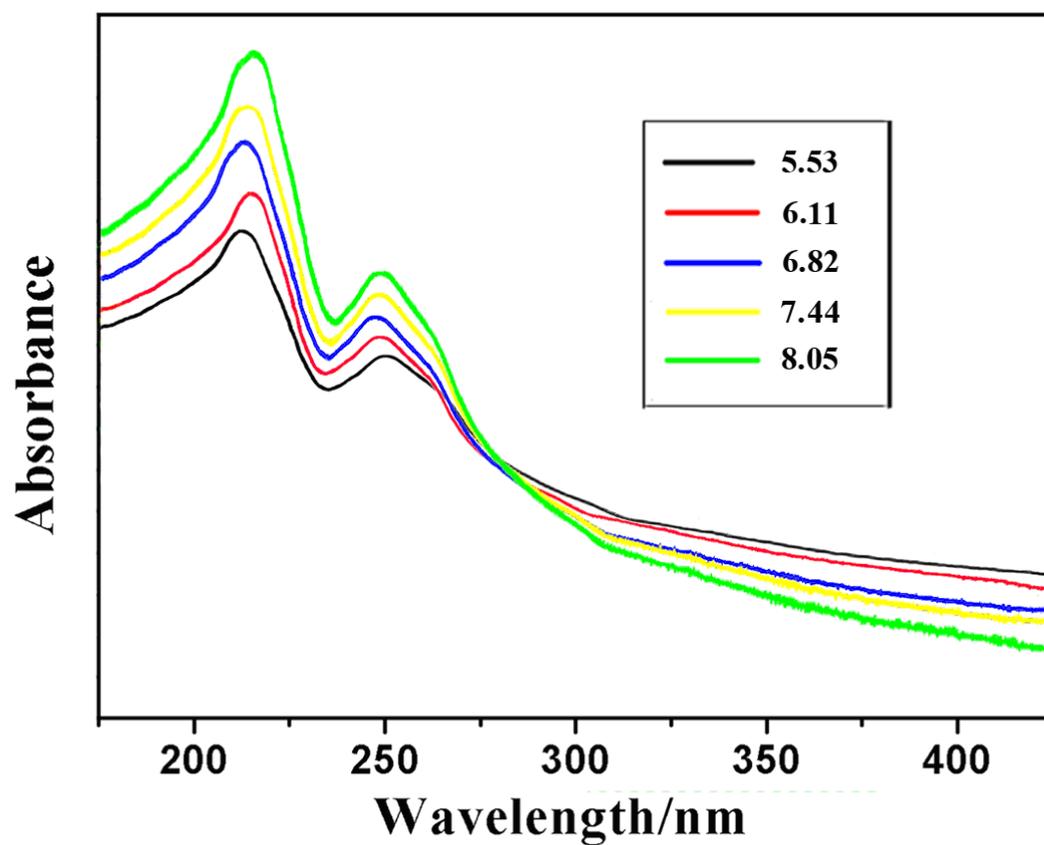


Figure S9. The influence of the pH value on the stability of compound BWCN in the aqueous solution. the pH values of the acidic direction and alkaline direction were adjusted using diluted HCl solution and NaOH solution, respectively.