Supplementary materials

The Degradation of Sulfamethoxazole via the Fe^{2+}/Ultraviolet/Sodium Percarbonate Advanced Oxidation Process: Performance, Mechanism, and Back-Propagate–Artificial Neural Network Prediction Model

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Figure lists:

Table lists:

Figure S1. The calibration curve of SMX used in this study.

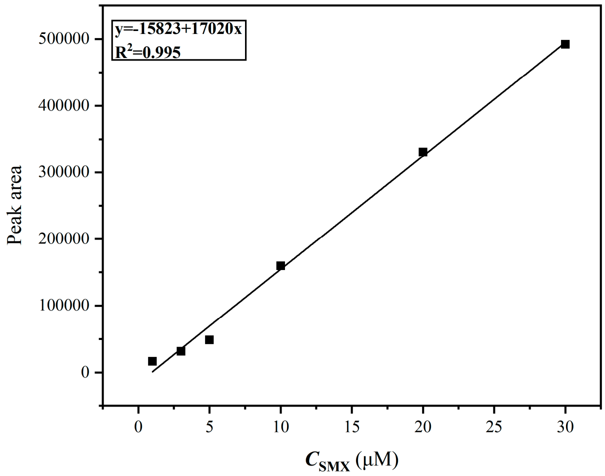
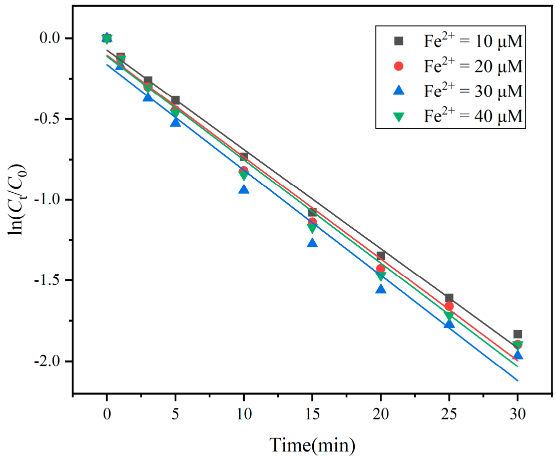
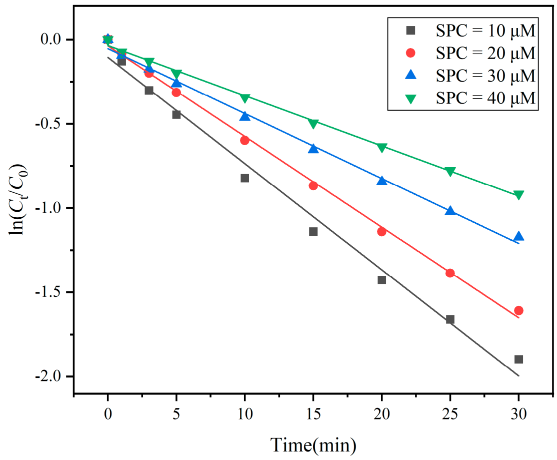


Figure S2. Based on pseudo-first-order kinetic model, the fitting curves of ln(C_t/C_0) of SMX (section 3.1.2 in main-text), under the effect of Fe^{2+} dosage (a), SPC concentration (b), solution pH (c).



(a)



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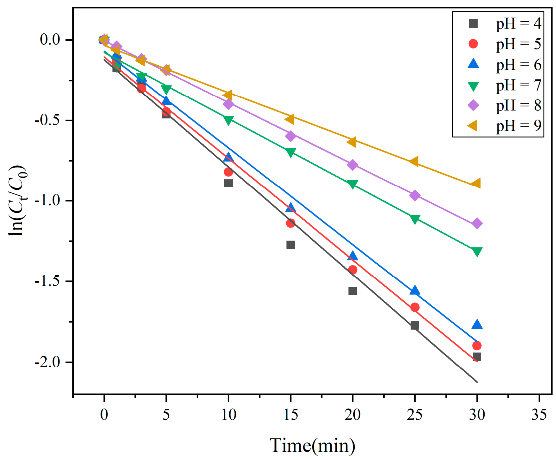

(c)

Figure S3. Based on the pseudo-first-order kinetic model, the fitting curves of the ln(C_t/C_0) of SMX (section 3.1.3 in main-text), at the pH of 4 (a), 6 (b), and 8 (c).

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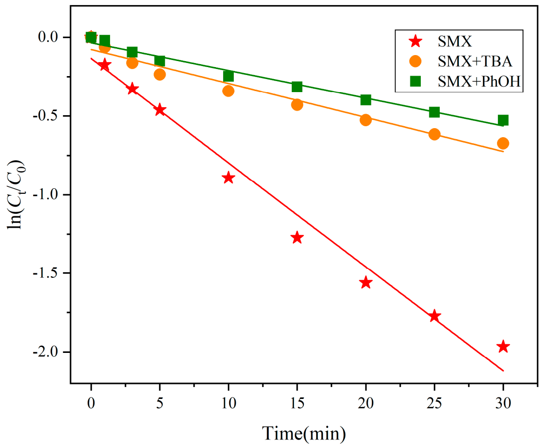
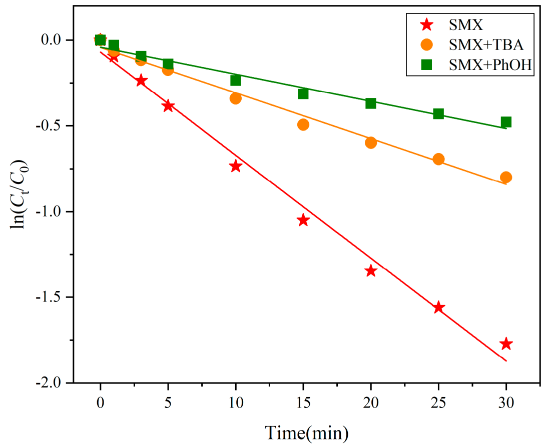


(a)



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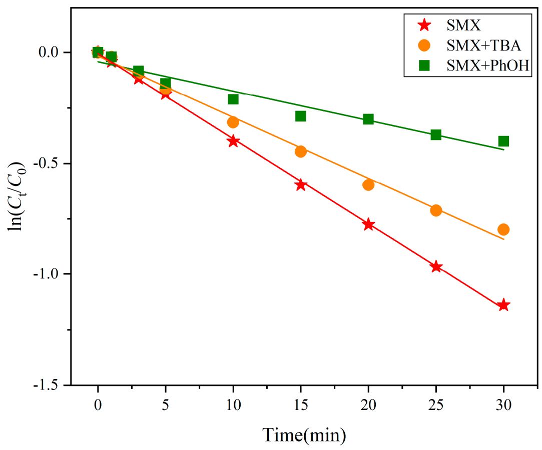
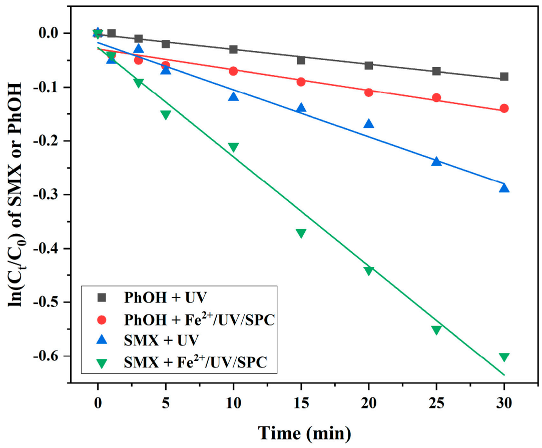
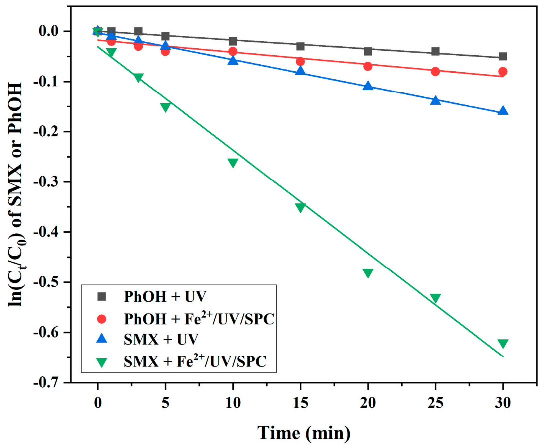


(c)

Figure S4. Based on the chemical reaction kinetics, the ln(C_t/C_0) of SMX or PhOH (section 3.1.3 in main-text), at the pH of 4 (a), 6 (b), and 8 (c).



(a)



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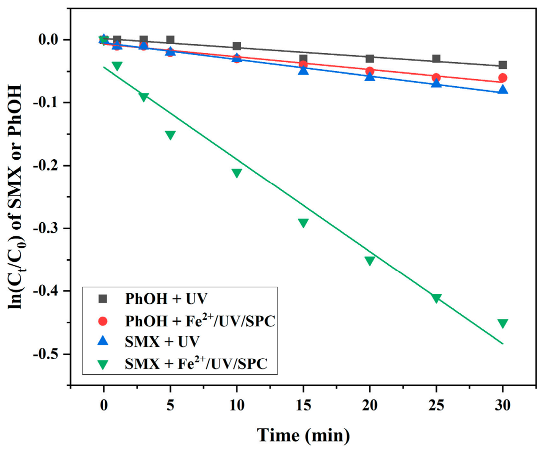
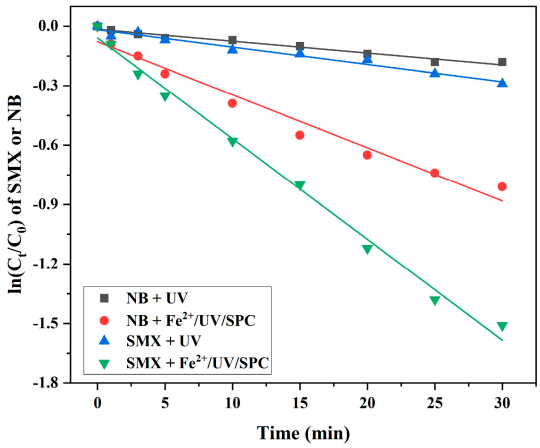
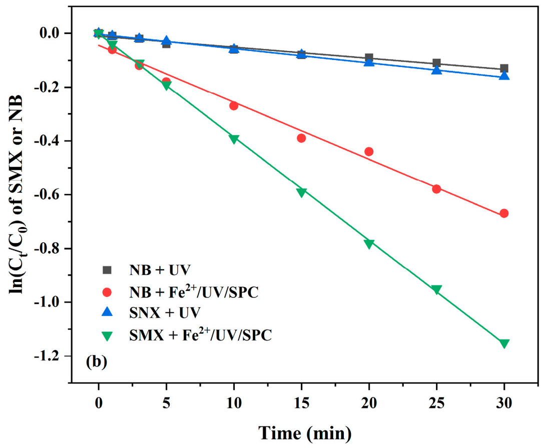


(c)

Figure S5. Based on the chemical reaction kinetics, the ln(C_t/C_0) of SMX or NB (section 3.1.3 in main-text), at the pH of 4 (a), 6 (b), and 8 (c).



(a)



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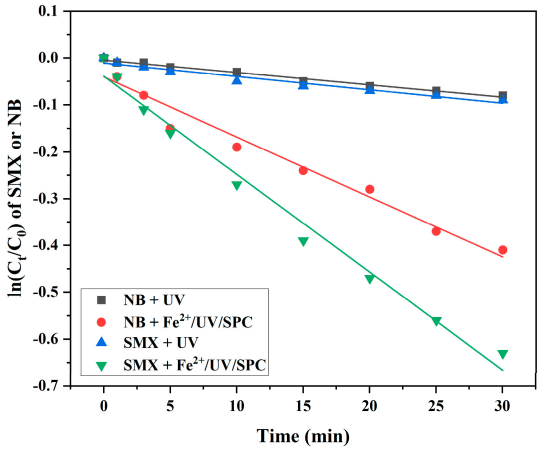

(c)

Figure S6. During experiments of negative effect of inorganic anions on SMX degradation by Fe^{2+}/UV/SPC process (section 3.1.4 in main-text), the fitting curves based on pseudo-first-order kinetic model under the effect of Cl^{-} dosage (a); HCO_3^{-} dosage (b); CO_3^{2-} dosage (c); SO_4^{2-} dosage (d).

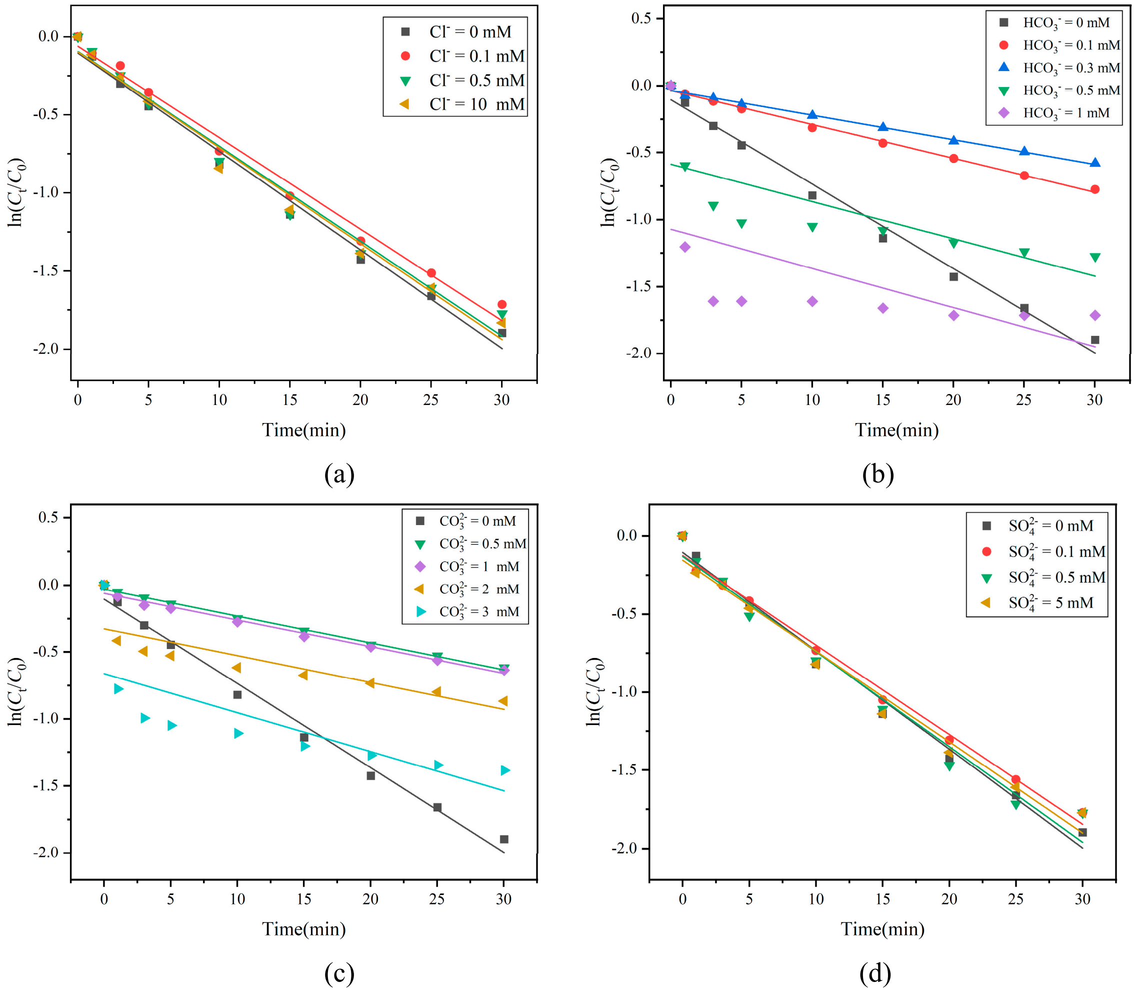

Table S1. The supplier information of chemicals used in this study.

Chemicals	**Supplier**
Sulfamethoxazole, SMX	Shanghai Aladdin Biochemical Technology Co., Ltd., China
$FeSO_4 \cdot 7H_2O$	Shanghai Macklin Biochemical Technology Co., Ltd., China
$Na_2CO_3 \cdot 1.5H_2O_2$, SPC	Shanghai Aladdin Biochemical Technology Co., Ltd., China
NaOH	Guangfu Technology Development Co. Ltd., China
HCl	Sigma-Aldrich (Shanghai) Trading Co. Ltd., China
Na_2CO_3	Guangfu Technology Development Co. Ltd., China
$NaHCO_3$	Guangfu Technology Development Co. Ltd., China
Na_2SO_4	Sinopharm Chemical Reagent Co. Ltd., China
$(CH_3)_3COH$, TBA	Sinopharm Chemical Reagent Co. Ltd., China
C_6H_6O, PhOH	Shanghai Aladdin Biochemical Technology Co. Ltd., China
$C_6H_5NO_2$, NB	Shanghai Macklin Biochemical Technology Co. Ltd., China
KI	Shanghai Aladdin Biochemical Technology Co. Ltd., China
KIO_3	Shanghai Macklin Biochemical Technology Co. Ltd., China
$Na_2S_2O_3$	Zigaoxin Chemical Co. Ltd., China
NaCl	Zigaoxin Chemical Co. Ltd., China
CH_3OH	Sigma-Aldrich (Shanghai) Trading Co. Ltd., China
CH_3CN	Sigma-Aldrich (Shanghai) Trading Co. Ltd., China
$Na_2B_4O_7 \cdot 5H_2O$	Zigaoxin Chemical Co. Ltd., China

Table S2. During experiments of influence factors, the fitting equations and K_{obs} values of SMX degradation by Fe^{2+}/UV/SPC process.

Figure name	Experimental Condition	Fitting equation	K_{obs} ($\times 10^{-2}$ min^{-1})	R^2
Fig. S2a	Fe^{2+}=10 μm/L	Y= − 0.06146X − 0.07403	6.146	0.9935
	Fe^{2+}=20 μm/L	Y= − 0.06304X − 0.10553	6.304	0.9890
	Fe^{2+}=30 μm/L	Y= − 0.06523X − 0.16401	6.523	0.9769
	Fe^{2+}=40 μm/L	Y= − 0.06403X − 0.112	6.403	0.9855
Fig. S2b	SPC=10 mg/L	Y= − 0.06304X − 0.10553	6.304	0.9890
	SPC=20 mg/L	Y= − 0.05381X − 0.03688	5.381	0.9982
	SPC=30 mg/L	Y= − 0.03855X − 0.05344	3.855	0.9958
	SPC=40 mg/L	Y= − 0.02978X − 0.0353	2.978	0.9977
Fig. S2c	pH=4	Y= − 0.06674X − 0.1222	6.674	0.9803
	pH=5	Y= − 0.06304X − 0.10553	6.304	0.9890
	pH=6	Y= − 0.0601X − 0.06986	6.010	0.9907
	pH=7	Y= − 0.04117X − 0.07736	4.117	0.9946
	pH=8	Y= − 0.03837X − 0.00482	3.837	0.9994
	pH=9	Y= − 0.02924X − 0.03408	2.924	0.9967

Table S3. During experiments of identifying major free radicals, the fitting equations and K_{obs} values of SMX degradation by Fe^{2+}/UV/SPC process.

Figure name	Experimental Condition	Fitting equation	K_{obs} ($\times 10^{-2}$ min^{-1})	R^2
Fig. S3a	SMX	Y= − 0.06623X − 0.13439	6.623	0.9806
	SMX + TBA (TBA=2 mM/L)	Y= − 0.02158X − 0.07754	2.158	0.9643
	SMX + PhOH (PhOH=2 mM/L)	Y= − 0.01761X − 0.03507	1.761	0.9798
Fig. S3b	SMX	Y= − 0.0601X − 0.06986	6.010	0.9907
	SMX + TBA (TBA=2 mM/L)	Y= − 0.02658X − 0.04238	2.658	0.9879
	SMX + PhOH (PhOH=2 mM/L)	Y= − 0.01581X − 0.04123	1.581	0.9715
Fig. S3c	SMX	Y= − 0.03837X − 0.00482	3.837	0.9994
	SMX + TBA (TBA=2 mM/L)	Y= − 0.02755X − 0.01611	2.755	0.9936
	SMX + PhOH (PhOH=2 mM/L)	Y= − 0.0132X − 0.04171	1.320	0.9490

Table S4. During experiments of inorganic anions, the fitting equations and K_{obs} values of SMX degradation by Fe^{2+}/UV/SPC process.

Figure name	Experimental Condition	Fitting equation	K_{obs} ($\times 10^{-2}$ min^{-1})	R^2
Fig. S6a	Cl^-=0 mM	Y=-0.06304X-0.10553	6.304	0.9890
	Cl^-=0.1 mM	Y=-0.05857X-0.06196	5.857	0.9888
	Cl^-=0.5 mM	Y=-0.06074X-0.09536	6.074	0.9811
	Cl^-=10 mM	Y=-0.06141X-0.09786	6.141	0.9856
Fig. S6b	HCO_3^-=0 mM	Y=-0.06304X-0.10553	6.304	0.9890
	HCO_3^-=0.1 mM	Y=-0.02535X-0.03666	2.535	0.9957
	HCO_3^-=0.3 mM	Y=-0.01845X-0.03583	1.845	0.9940
	HCO_3^-=0.5 mM	Y=-0.02781X-0.58781	2.781	0.5777
	HCO_3^-=1 mM	Y=-0.02925X-1.07217	2.925	0.3316
Fig. S6c	CO_3^{2-}=0 mM	Y=-0.06304X-0.10553	6.304	0.9890
	CO_3^{2-}=0.5 mM	Y=-0.0201X-0.03062	2.010	0.9951
	CO_3^{2-}=1 mM	Y=-0.01994X-0.06156	1.994	0.9839
	CO_3^{2-}=2 mM	Y=-0.02008X-0.3265	2.008	0.7247
	CO_3^{2-}=3 mM	Y=-0.02921X-0.66168	2.921	0.5688
Fig. S6d	SO_4^{2-}=0 mM	Y=-0.06304X-0.10553	6.304	0.9890
	SO_4^{2-}=0.1 mM	Y=-0.05734X-0.12548	5.734	0.9907
	SO_4^{2-}=0.5 mM	Y=-0.06099X-0.1307	6.099	0.9769
	SO_4^{2-}=5 mM	Y=-0.05821X-0.15509	5.821	0.9803

Table S5. During RSM experiments, the experimental design matrix and the corresponding response values.

Experimental number	Range and levels				Code value				Experimental values	Response values
	Z_1	Z_2	Z_3	Z_4	x_1 (C_{SPC})	x_2 ($C_{Fe^{2+}}$)	x_3 (pH)	x_4 (t)	y* (%)	y (%)
1	0	-1	0	1	30	10	6	30	60.4	61.2
2	-1	0	1	0	20	20	8	20	65.4	69.0
3	0	1	0	1	30	30	6	30	74.5	74.7
4	0	0	-1	1	30	20	4	30	89.4	90.6
5	1	0	-1	0	40	20	4	20	86.1	84.1
6	-1	0	0	1	20	20	6	30	80.6	77.8
7	0	1	1	0	30	30	8	20	62.8	65.6
8	0	0	1	-1	30	20	8	10	35.1	31.8
9	0	0	0	0	30	20	6	20	65.0	65.2
10	1	0	1	0	40	20	8	20	47.2	44.3
11	-1	1	0	0	20	30	6	20	82.1	76.8
12	0	0	0	0	30	20	6	20	63.0	65.2
13	0	-1	-1	0	30	10	4	20	84.4	82.1
14	0	-1	0	-1	30	10	6	10	30.9	32.4
15	0	-1	1	0	30	10	8	20	46.2	44.6
16	1	0	0	1	40	20	6	30	62.3	61.4
17	0	0	1	1	30	20	8	30	66.7	68.2
18	1	-1	0	0	40	10	6	20	45.2	48.4
19	0	1	0	-1	30	30	6	10	45.1	45.9

Experimental number	Range and levels				Code value				Experimental values	Response values
	Z_1	Z_2	Z_3	Z_4	x_1 (C_{SPC})	x_2 ($C_{Fe^{2+}}$)	x_3 (pH)	x_4 (t)	y* (%)	y (%)
20	0	0	0	0	30	20	6	20	69.0	65.2
21	-1	0	-1	0	20	20	4	20	84.6	89.2
22	-1	0	0	-1	20	20	6	10	46.1	47.5
23	-1	-1	0	0	20	10	6	20	60.0	58.5
24	0	0	0	0	30	20	6	20	65.0	65.2
25	0	0	0	0	30	20	6	20	64.0	65.2
26	1	1	0	0	40	30	6	20	57.7	57.1
27	0	1	-1	0	30	30	4	20	86.0	88.1
28	1	0	0	-1	40	20	6	10	30.8	34.0
29	0	0	-1	-1	30	20	4	10	72.9	69.4