

New parameter for simulation effect and its application in the prediction of hormetic effect for chemical mixtures

Table S1 Fitting parameters for hormetic effect of SAs on *E.coli* and their single simulation area

NO.	Chemicals	Exposure time	δ	α	β	γ	EC ₅₀	R ²	Area ^{Sim}
1	SDX	16h	80.31	-7.52	2.17	-1.37E+07	1.79E-06	0.99	2.57E-03
2		17h	79.78	-7.29	2.55	-2.41E+06	2.12E-06	0.99	2.56E-03
3		18h	79.33	-7.34	3.33	2.30E+06	2.47E-06	0.99	2.55E-03
4		19h	78.99	-6.47	4.21	8.37E+05	2.80E-06	0.99	2.52E-03
5		20h	78.94	-7.24	4.94	1.62E+06	3.06E-06	0.99	2.50E-03
6		21h	78.97	-6.18	5.88	1.76E+06	3.33E-06	0.99	2.49E-03
7		22h	79.05	-5.26	6.86	1.71E+06	3.60E-06	0.99	2.47E-03
8		23h	79.11	-4.67	7.25	1.59E+06	3.92E-06	0.99	2.45E-03
9	SCP	16h	73.36	-10.37	3.11	-6.63E+06	2.33E-06	0.97	7.91E-04
10		17h	83.43	-7.67	2.05	-2.92E+07	2.94E-06	0.97	7.65E-04
11		18h	126.61	-6.42	1.46	-7.25E+07	7.13E-06	0.97	6.89E-04
12		19h	214.67	-6.95	1.24	-1.03E+08	3.05E-05	0.96	5.85E-04
13		20h	82.87	-12.98	3.68	8.18E+05	5.95E-06	0.95	5.42E-04
14		21h	82.33	-4.10	3.95	-1.38E+07	1.33E-06	0.98	1.02E-03
15		22h	83.82	-3.59	3.44	-2.44E+07	1.44E-06	0.98	1.02E-03
16		23h	81.14	-6.55	10.54	-1.22E+06	1.54E-06	0.98	1.00E-03
17	smp	16h	83.73	-14.35	2.09	-2.45E+07	5.59E-06	0.97	3.94E-03
18		17h	80.05	-17.50	2.49	-1.32E+07	5.91E-06	0.98	3.85E-03
19		18h	78.25	-20.27	2.91	-6.55E+06	6.97E-06	0.98	3.70E-03
20		19h	75.86	-21.19	3.39	-4.29E+06	1.65E-06	0.97	3.56E-03
21		20h	73.93	-21.08	3.57	-4.38E+06	8.58E-06	0.96	3.36E-03
22		21h	74.56	-21.99	2.99	-4.86E+06	9.77E-06	0.95	3.17E-03

23		22h	76.08	-21.68	2.66	-4.54E+06	1.14E-05	0.94	2.98E-03
24		23h	75.67	-21.70	2.57	-4.77E+06	1.20E-05	0.94	2.86E-03
25	spy	16h	74.21	-10.24	3.02	-1.36E+06	7.58E-06	0.97	3.47E-03
26		17h	72.33	-9.73	3.56	-4.84E+06	8.27E-06	0.98	3.32E-03
27		18h	71.39	-10.16	3.71	-5.42E+06	9.33E-06	0.98	3.16E-03
28		19h	70.94	-10.68	3.72	-4.91E+06	1.06E-05	0.98	3.00E-03
29		20h	70.53	-10.11	3.58	-5.02E+06	1.21E-05	0.97	2.83E-03
30		21h	71.50	-10.54	3.47	-4.29E+06	1.37E-05	0.97	2.69E-03
31		22h	71.51	-10.54	3.47	-4.29E+06	1.37E-05	0.97	2.54E-03
32		23h	70.76	-10.54	4.04	-3.06E+06	1.55E-05	0.96	2.44E-03

Table S2 Fitting parameters for hormetic effect of chemicals on *p.p* and their single simulation area

NO.	Chemicals	δ	α	β	γ	EC ₅₀ (M)	R ²	Area ^{Sim}
1	SMZ	98.60	17.77	5.81	-1.77E+07	1.86E-05	0.99	9.22E-04
2	SMP	97.91	4.53	6.36	-3.59E+06	4.40E-05	0.99	5.05E-03
3	TMP	105.09	11.90	7.07	-2.45E+07	6.16E-06	0.98	1.65E-04
4	TTC	101.00	8.37	1.69		2.38E-08	0.97	0.00E+00
5	OTC	101.01	3.39	1.60		2.17E-08	0.97	0.00E+00

Table S3 Fitting parameters for hormetic effect of chemicals on *vibrio fischeri* and their single simulation area

NO.	Chemicals	δ	α	β	γ	EC ₅₀ (M)	R ²	Area ^{Sim}
1	B3O	67.88	99.55	20.29	-7.34E+05	5.35E-04	0.99	-4.34E-02
2	SMM	75.80	72.72	8.71	-2.52E+07	1.41E-05	0.98	-1.76E-04
3	SM	83.42	79.56	6.84	-5.95E+06	6.43E-05	0.99	-3.38E-04
4	SD	84.46	81.13	6.77	-4.65E+06	8.39E-05	0.99	-4.30E-04
5	SMP	76.11	53.73	5.96	-1.71E+07	1.49E-05	0.99	-1.42E-04
6	SDX	78.55	71.02	5.79	-5.08E+06	9.95E-05	0.95	-1.30E-03
7	SIX	78.43	59.35	7.52	-9.97E+06	2.40E-05	0.99	-2.65E-04
8	SMR	68.41	54.40	11.02	-7.01E+06	3.76E-05	0.99	-1.02E-03
9	SCP	90.46	33.03	6.74	-1.63E+07	1.18E-05	0.99	-2.25E-04
10	SMX	83.84	49.79	6.97	-1.68E+07	1.00E-05	0.99	-6.06E-05
11	SMZ	70.08	55.07	7.67	-5.53E+06	4.95E-05	0.96	-8.23E-04
12	SPY	63.44	36.90	9.68	-5.88E+06	2.10E-05	0.99	-1.69E-04
13	SQ	90.18	84.94	7.28	-2.79E+07	1.50E-05	0.99	-1.57E-04

Table S4 Fitting parameters for hormetic effect of chemicals on *E.coli* and their simulation area for mixture

NO.	Chemicals	Exposure time	δ	α	β	γ	EC ₅₀ (M)	R ²	Area ^{Sim}
1	SMP+SCP	16h	60.62	13.92	0.38	6.78E+07	1.19E-05	0.96	5.54E-04
2		17h	50.92	11.85	0.35	5.31E+07	9.52E-06	0.95	5.25E-04
3		18h	69.59	13.91	0.35	7.17E+07	1.57E-05	0.97	4.90E-04
4		19h	260.22	22.46	0.43	2.16E+08	1.29E-04	0.98	4.55E-04
5		20h	139.04	17.15	1.67	-8.13E+07	1.42E-05	0.98	5.18E-04
6		21h	58.76	11.45	0.38	5.48E+07	1.12E-05	0.97	5.20E-04
7		22h	62.37	11.48	0.38	5.71E+07	1.24E-05	0.99	5.19E-04
8		23h	63.90	12.67	0.41	6.17E+07	1.32E-05	0.99	5.04E-04
9	scp+sdx	16h	79.20	-4.53	3.44	-1.44E+07	1.88E-06	0.98	1.04E-03
10		17h	78.99	-5.17	4.04	-7.10E+06	2.03E-06	0.99	1.03E-03
11		18h	78.76	-5.64	4.82	-3.52E+06	2.20E-06	0.99	1.02E-03
12		19h	78.39	-4.95	5.67	-3.24E+06	2.35E-06	0.99	1.01E-03
13		20h	78.47	-6.19	6.13	-1.63E+06	2.48E-06	0.99	9.99E-04
14		21h	78.60	-5.31	6.43	-1.06E+06	2.63E-06	0.99	9.92E-04
15		22h	78.85	-4.87	6.65	-1.04E+05	2.91E-06	0.99	9.83E-04
16		23h	79.07	-5.01	6.95	1.23E+06	3.06E-06	0.99	9.64E-04
17	spy+sdx	16h	74.42	-18.11	11.75	3.29E+06	1.27E-05	0.97	1.14E-03
18		17h	76.14	-18.18	15.54	2.64E+06	1.43E-05	0.97	1.06E-03
19		18h	74.62	-20.21	53.83	2.76E+06	1.52E-05	0.97	1.03E-03
20		19h	74.31	-19.97	56.29	2.53E+06	1.54E-05	0.97	9.98E-04
21		20h	71.46	-22.20	39.33	3.23E+06	1.44E-05	0.96	9.97E-04
22		21h	138.41	41.43	1.57	-5.82E+07	4.80E-05	0.96	1.05E-03

23	spy+smp	22h	118.75	48.62	1.64	-6.18E+07	5.12E-05	0.94	9.84E-04
24		23h	180.98	38.03	1.35	-7.90E+07	1.00E-05	0.95	9.82E-04
25		16h	195.21	-3.76	1.29	-1.86E+07	4.95E-06	0.96	7.74E-04
26		17h	74.27	-3.87	1.78	-9.67E+06	9.59E-06	0.97	7.24E-04
27		18h	740.25	-2.79	1.08	-7.64E+07	3.20E-02	0.98	5.53E-04
28		19h	709.11	-3.24	1.14	-3.08E+07	8.61E-04	0.97	5.86E-04
29		20h	1275.01	0.55	1.06	-9.66E+07	3.30E-01	0.95	5.16E-04
30		21h	1200.57	-3.59	1.08	-4.55E+07	4.20E-02	0.96	5.16E-04
31		22h	219.89	-7.45	0.90	5.90E+06	2.92E-05	0.97	4.42E-04
32		23h	65.00	-8.43	40.89	1.85E+06	1.73E-05	0.97	4.83E-04

Table S5 Fitting parameters for hormetic effect of chemicals on *p.p* and their simulation area for mixture

NO.	Chemicals	Toxic Ratio	δ	α	β	γ	EC₅₀(M)	R²	Area^{Sim}
1	SMZ+SMP	1:320	95.00	16.87	7.02	-4.43E-06	4.86E-05	0.94	-1.48E-03
2		1:100	95.00	8.71	7.05	-3.66E-06	4.50E-05	0.98	-1.82E-03
3		1:32	100.00	6.95	6.08	-4.32E-07	4.81E-05	0.97	-1.93E-03
4		1:10	100.00	7.01	5.72	-5.15E-06	4.70E-05	0.97	-2.14E-03
5		1:3	100.00	6.86	5.70	-6.00E-06	4.44E-05	0.97	-2.22E-03
6		1:1	96.61	2.74	6.15	-9.47E-06	3.05E-05	0.98	-2.30E-03

7	TMP+OTC	10:1	100.00	7.98	4.22	-2.13E-07	2.30E-05	0.99	-2.29E-03
8		32:1	100.00	2.79	4.16	-2.42E-07	2.10E-05	0.99	-2.28E-03
9		100:1	100.00	12.89	4.16	-2.57E-07	2.04E-05	0.98	-1.99E-03
10		320:1	100.00	5.62	4.29	-2.27E-07	2.04E-05	0.98	-2.08E-03
11		1:320	100.00	2.21	1.57	—	4.23E-08	0.97	0.00E+00
12		1:100	100.00	7.65	1.39	—	8.86E-08	0.96	0.00E+00
13		1:32	100.00	-0.50	1.30	—	5.42E-07	0.92	0.00E+00
14		1:10	100.00	1.62	1.26	—	1.07E-06	0.90	0.00E+00
15		1:3	100.00	6.75	1.40	—	3.53E-06	0.91	0.00E+00
16		1:1	99.13	7.77	4.43	-5.71E-07	8.43E-06	0.93	-1.72E-05
17		1:3	99.78	8.64	5.03	-1.27E-07	8.68E-06	0.98	-7.75E-05
18		10:1	100.00	6.71	5.89	-1.78E-07	8.60E-06	0.99	-1.53E-04
19		32:1	100.00	12.40	7.29	-1.47E-07	8.53E-06	0.93	-1.16E-04
20		100:1	100.00	7.51	13.11	-1.11E-07	7.26E-06	0.90	-1.01E-04
21		320:1	99.29	15.02	9.04	-2.31E-07	7.94E-06	0.88	-1.18E-04
22	TMP+SMP	1:320	92.23	4.77	13.11	-3.38E-06	3.71E-05	0.98	-1.43E-03

23		1:100	99.58	2.55	9.26	-3.74E-06	3.02E-05	0.96	-9.20E-04
24		1:32	98.34	13.71	12.78	-5.73E-06	2.20E-05	0.98	-6.74E-04
25		1:10	97.50	11.50	10.34	-6.05E-06	1.69E-05	0.98	-3.72E-04
26		1:3	99.65	11.31	15.74	-9.01E-06	9.31E-06	0.98	-1.94E-04
27		1:1	100.00	18.55	11.04	-1.19E-07	9.64E-06	0.98	-2.06E-04
28		1:3	99.01	24.05	14.70	-3.75E-07	3.21E-06	0.98	-7.39E-05
29		10:1	97.11	16.51	13.16	-4.21E-07	2.86E-06	0.99	-7.76E-05
30		32:1	98.88	13.90	17.80	-3.27E-07	2.55E-06	0.97	-5.49E-05
31		100:1	100.00	0.03	12.78	-1.88E-07	3.09E-06	0.93	-5.95E-05
32		320:1	99.89	2.93	11.71	-1.86E-07	3.93E-06	0.96	-8.25E-05
33	TMP+SMZ	1:320	98.08	3.87	7.55	-1.57E-07	1.66E-05	1.00	-9.81E-04
34		1:100	99.10	6.91	8.90	-2.17E-07	1.36E-05	0.99	-1.00E-03
35		1:32	94.93	13.68	8.02	-2.88E-07	9.39E-06	0.96	-4.72E-04
36		1:10	98.05	18.31	12.63	-2.89E-07	7.61E-06	0.99	-4.30E-04
37		1:3	98.86	32.14	33.03	-5.02E-07	3.61E-06	0.98	-1.73E-04

38		1:1	99.71	24.15	21.32	-6.96E-07	2.20E-06	0.98	-8.63E-05
39		1:3	98.82	25.00	13.02	-9.64E-07	1.68E-06	0.96	-5.63E-05
40		10:1	99.35	13.32	88.71	-6.05E-07	1.87E-06	0.98	-7.54E-05
41		32:1	99.00	10.55	16.62	-4.66E-07	2.27E-06	0.98	-6.60E-05
42		100:1	98.17	14.42	109.99	-3.13E-07	2.99E-06	0.96	-9.21E-05
43		320:1	94.65	2.57	18.74	-2.27E-07	3.80E-06	0.94	-1.18E-04
44	TMP+TTC	1:320	95.00	10.19	1.87	—	5.41E-08	0.94	0.00E+00
45		1:100	98.89	13.86	1.79	—	1.11E-07	0.98	0.00E+00
46		1:32	100.00	5.21	1.37	—	2.23E-07	0.99	0.00E+00
47		1:10	100.00	-0.23	1.20	—	3.59E-07	0.97	0.00E+00
48		1:3	95.00	-5.15	0.68	—	3.36E-06	0.83	0.00E+00
49		1:1	100.00	6.31	3.80	-6.73E-06	1.02E-05	0.92	-4.17E-05
50		1:3	95.00	8.48	4.55	-1.26E-07	7.11E-06	0.94	-5.96E-05
51		10:1	99.45	11.34	6.47	-1.73E-07	6.08E-06	0.97	-9.26E-05
52		32:1	96.37	3.68	10.70	-1.03E-07	6.25E-06	0.97	-1.05E-04
53		100:1	98.06	-2.44	14.82	-1.06E-07	6.13E-06	0.94	-1.38E-04

54		320:1	99.72	6.68	7.72	-1.77E-07	6.13E-06	0.97	-1.39E-04
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Table S6 Fitting parameters for hormetic effect of chemicals on *Vibrio fischeri* and their simulation area for mixture

NO.	Chemicals	Toxic Ratio	δ	α	β	γ	EC ₅₀ (M)	R ²	Area ^{Sim}
1	SIX+B3O	1:100	105.38	106.63	12.90	-9.32E+05	8.94E-04	0.99	-6.45E-02
2		1:10	89.73	106.22	10.65	-7.30E+05	8.12E-04	0.96	-5.49E-02
3		1:05	100.72	102.17	18.52	-7.66E+05	7.13E-04	0.99	-4.58E-02
4		5:01	61.76	84.82	6.11	-1.83E+06	2.20E-04	0.98	-4.06E-03
5		10:01	62.90	78.93	7.05	-2.66E+06	1.14E-04	0.95	-1.61E-03
6		100:1	42.26	60.87	8.28	-6.44E+06	3.09E-05	0.94	-4.54E-04
7	SPY+B3O	1:100	34.38	121.76	6.92	-4.38E+05	9.79E-04	0.96	-6.58E-02
8		1:10	161.33	164.03	3.85	-1.49E+06	4.37E-03	0.97	4.37E-03
9		1:05	111.14	112.35	8.65	-8.26E+05	1.49E-03	0.97	-8.35E-02
10		5:01	367.97	398.39	1.36	-3.03E+07	1.57E+00	0.98	-2.75E-03
11		10:01	56.23	71.55	5.50	-3.66E+06	9.45E-05	1.00	-9.66E-04
12		100:1	83.76	91.42	3.03	-2.29E+07	6.89E-05	0.97	-9.95E-05
13	SDX+B3O	1:100	89.52	148.58	5.08	-6.23E+05	1.81E-03	0.97	-1.40E-01
14		1:10	97.30	99.64	6.11	-7.16E+05	2.40E-03	0.94	-1.10E-01
15		1:05	128.42	132.09	5.15	-8.56E+05	2.93E-03	0.98	-1.22E-01
16		5:01	65.17	70.08	3.45	-2.12E+06	9.33E-04	0.88	-9.60E-03
17		10:01	27.68	55.41	4.50	-1.45E+06	2.72E-04	0.95	-6.79E-03
18		100:1	39.57	40.27	12.48	-3.83E+06	8.53E-05	0.96	-2.70E-03
19	SCP+B3O	1:100	117.12	120.06	7.90	-8.40E+05	1.70E-03	0.96	-1.20E-01
20		1:10	85.67	103.91	12.27	-6.30E+05	9.43E-04	0.98	-8.08E-02

21	SMX+B3O	1:05	110.73	109.81	12.24	-8.59E+05	1.10E-03	0.96	-8.20E-02
22		5:01	81.11	164.59	2.16	-3.48E+06	5.51E-04	0.97	-3.42E-03
23		10:01	403.25	824.29	1.19	-9.07E+07	1.14E-01	0.95	-1.21E-03
24		100:1	106.33	112.67	3.03	-3.27E+07	6.83E-05	0.96	-1.08E-04
25		1:100	80.96	114.91	7.56	-6.48E+05	1.00E-03	0.95	-6.60E-02
26		1:10	53.09	100.47	43.66	-4.49E+05	5.82E-04	0.99	-3.90E-02
27		1:05	115.83	153.31	4.53	-7.49E+05	1.54E-03	0.95	-5.82E-02
28		5:01	26.97	60.56	7.50	-8.79E+05	1.81E-04	0.93	-3.07E-03
29		10:1	49.63	55.53	9.03	-2.19E+06	8.99E-05	0.94	-6.32E-04
30		100:1	48.79	49.35	10.75	-7.67E+06	2.32E-05	0.85	-3.73E-05
31	SIX+SD	1:1	68.41	66.23	8.77	-7.30E+06	4.69E-05	0.94	-5.61E-04
32	SIX+SQ	1:1	81.92	77.67	8.05	-2.33E+07	2.02E-05	0.98	-4.00E-04
33	SD+SMP	1:1	66.24	58.27	7.36	-7.86E+06	4.64E-05	0.98	-8.87E-04
34	SD+SMR	1:1	66.30	57.16	6.70	-5.93E+06	6.65E-05	0.96	-1.30E-03
35	SD+SMZ	1:1	73.98	66.41	5.89	-6.21E+06	7.59E-05	0.97	-1.06E-03
36	SIX+SMP	1:1	66.53	64.30	8.25	-1.42E+07	2.45E-05	0.95	-2.93E-04
37	SIX+SMR	1:1	74.66	52.16	7.51	-9.60E+06	2.97E-05	0.98	-5.91E-04
38	SIX+SMZ	1:1	72.76	68.80	6.58	-1.06E+07	4.62E-05	0.93	-6.46E-04
39	SCP+SQ	1:1	60.85	27.34	16.97	-2.28E+07	9.02E-06	0.97	-4.11E-04
40	SCP+SD	1:1	65.64	51.90	5.53	-5.81E+06	5.02E-05	0.99	-4.43E-04
41	SCP+SMZ	1:1	81.38	34.52	6.18	-6.86E+06	2.36E-05	0.99	-8.08E-04
42	SCP+SM	1:1	70.60	29.13	8.74	-5.05E+06	2.69E-05	0.97	-3.96E-04
43	SCP+SMP	1:1	53.56	11.77	11.75	-1.28E+07	1.10E-05	0.97	-3.54E-04
44	SCP+SMR	1:1	32.60	31.75	12.67	-1.25E+07	2.13E-05	0.91	-5.96E-04
45	SD+SQ	1:1	78.72	75.72	5.32	-1.25E+07	7.87E-05	0.97	-1.27E-03

46	SMM+SMP	1:1	78.94	46.75	6.43	-1.60E+07	1.49E-05	0.99	-2.13E-04
47	SMM+SMR	1:1	85.35	29.87	7.53	-7.78E+06	2.28E-05	0.98	-4.70E-04
48	SMM+SM	1:1	81.54	73.75	7.25	-1.27E+07	3.38E-05	0.96	-5.86E-04
49	SMM+SMZ	1:1	83.55	41.94	6.44	-8.63E+06	2.68E-05	0.98	-4.78E-04
50	SMM+SIX	1:1	60.26	41.88	11.25	-1.30E+07	1.51E-05	0.97	-2.30E-04
51	SMP+SMZ	1:1	74.47	14.64	5.27	-7.84E+06	3.12E-05	0.99	-9.49E-04
52	SMP+SQ	1:1	75.78	24.54	5.19	-2.32E+07	1.30E-05	0.98	-3.93E-04
53	SMP+SM	1:1	67.50	23.96	7.42	-7.62E+06	2.71E-05	0.99	-4.23E-04
54	SMP+SMR	1:1	65.43	35.36	11.03	-8.34E+06	2.58E-05	0.97	-8.43E-04
55	SQ+SMR	1:1	82.75	77.68	5.75	-1.19E+07	4.25E-05	0.97	-3.52E-04
56	SQ+SM	1:1	77.49	74.65	8.08	-1.29E+07	3.30E-05	0.94	-4.71E-04
57	SCP+SIX	1:1	66.35	61.66	10.75	-1.43E+07	2.00E-05	0.97	-3.83E-04

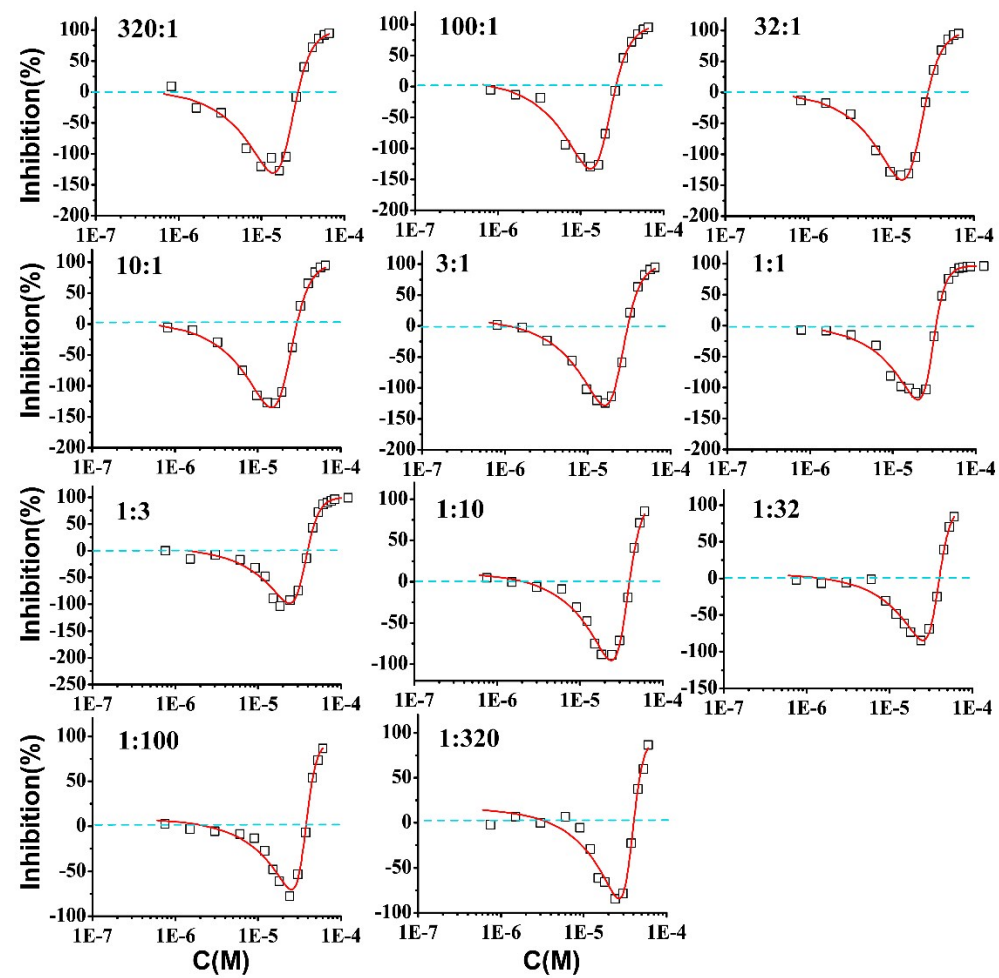


Figure S1 The hormetic effect of SAs on *p.p.* under different toxic ratios