

Supplementary Materials

Different antibacterial modes of plant flavonoids to gram-negative from to -positive bacteria

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Figure S1. Chemical structure of fifty-two plant flavonoids reported.

Figure S2. Another effective regression curve for equation (6) established from the LogP of reported plant flavonoids and their $\log_{10}(\text{MIC})$ values.

Figure S3. The Polynomial regression analyses for the LogP (x) of plant flavonoids in Table S2 and the $\log_{10}(\text{IC}_{50})$ (y) to DNA gyrase.

Table S1. Comparison for the tested and reported MIC values of nine compounds.

Table S2. The ACD/LogP values and IC_{50} to DNA gyrase of fourteen flavonoids reported, together with their MICs to *E. coli*_{ss} [35].

Table S3. Regression equations established from the LogP (x) values of flavonoids and the IC_{50} or $\log_{10}(\text{IC}_{50})$ (μM) values (y) of these flavonoids to DNA gyrase.

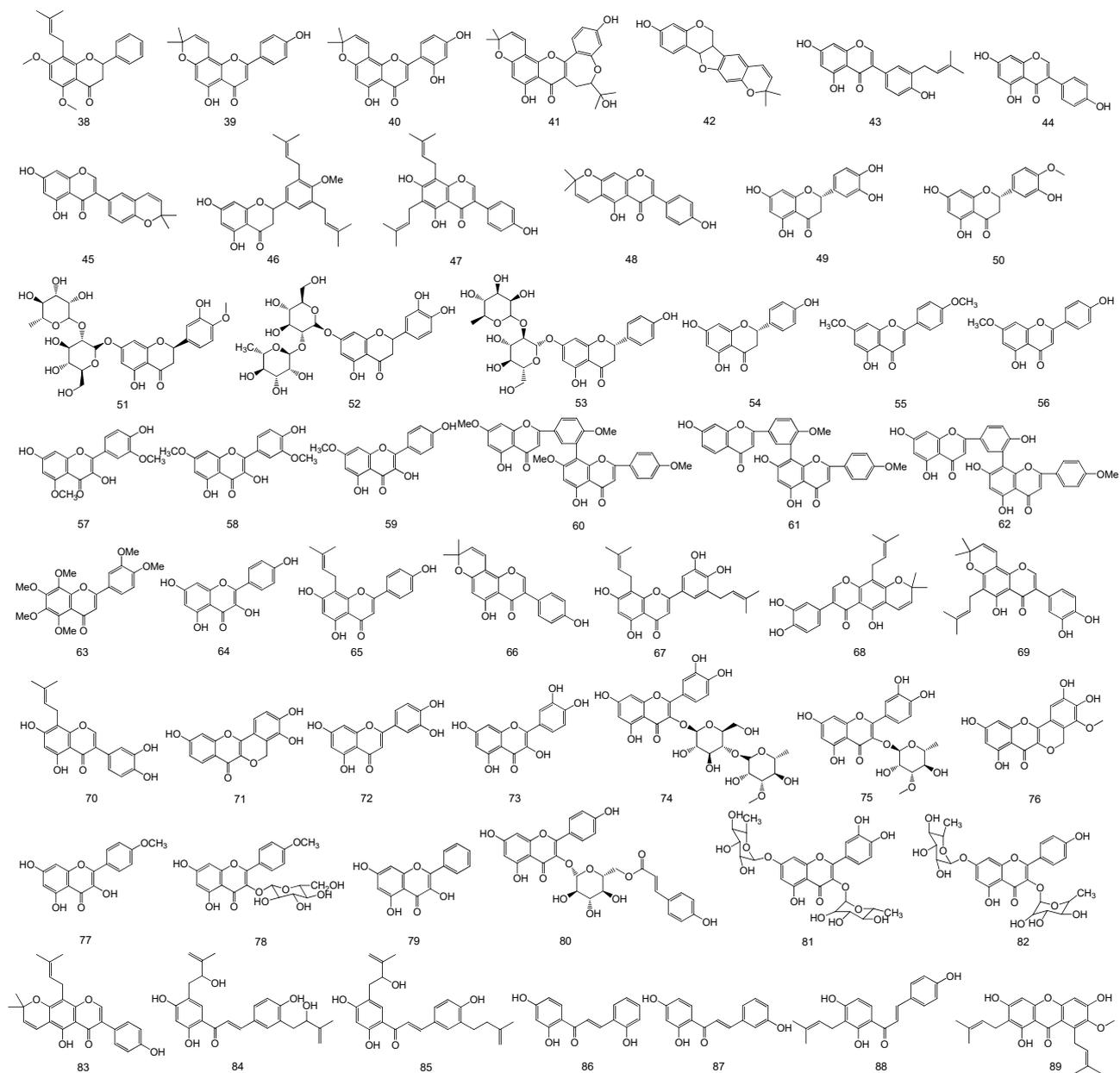


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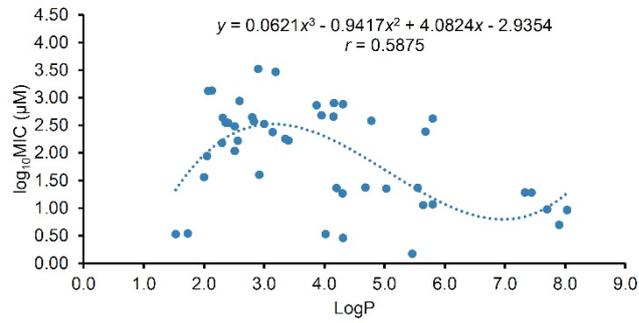


Figure S2. Another effective regression curve for equation (6) established from the LogP of reported plant flavonoids and their log₁₀(MIC) values.

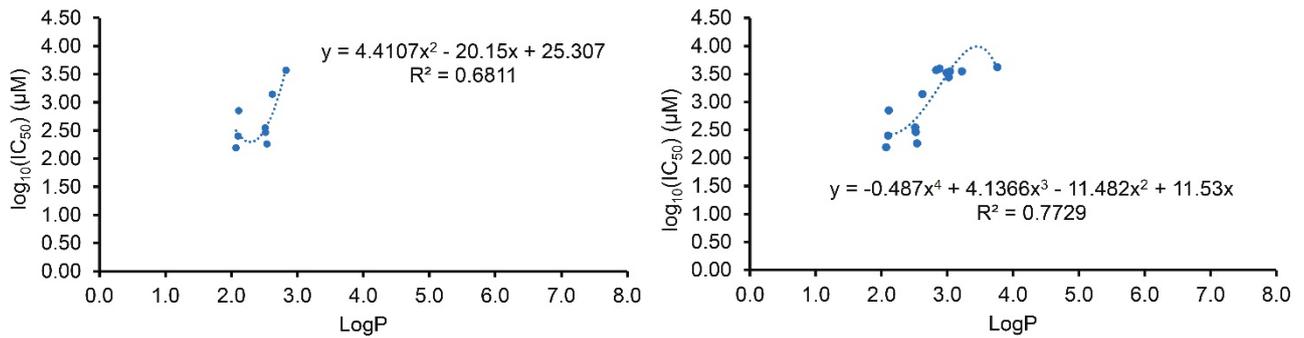


Figure S3. The Polynomial regression analyses for the LogP (x) of plant flavonoids in Table S2 and the log₁₀(IC₅₀) (y) to DNA gyrase. Left and right panels presented the regression curves respectively for equations (2) and (4) in Table S3.

Table S1. Comparison for the tested and reported MIC values of nine compounds.

Compound Number ^a	Compounds	Tested MIC (μM)	Reported MIC (μM)	References
3 (53)	Naringin	1763.88	>1722.53	3
6 (49)	Eriodictyol	7104.7	867.27	3
8 (50)	Hesperetin	6775.18	3308.19	3
9 (54)	Naringenin	7527.47	2938.37	3
13 (65)	Licoflavone C	3026.36	23.08	7
15 (63)	Nobiletin	2544.73	439.86	6
27 (73)	Quercetin	>3388.04	1323.45	10
28 (79)	Galangin	3789.22	370.04	12
37 (89)	α -mangostin	2494.7	>311.84	16

^a: The number out of bracket is the number of tested flavonoids in Table 1, while that in bracket is the number of reported flavonoids in Table 2.

Table S2. The ACD/LogP values and IC₅₀ to DNA gyrase of fourteen flavonoids reported, together with their MICs to *E. coli*_{ss} [35].^a

Compounds	LogP ^b	IC ₅₀ (µg/mL)	IC ₅₀ (µM)	Log ₁₀ (IC ₅₀) (µM) ^c	MIC (µg/mL)
5a	2.07	47	155.51	2.192	31.25
5f	2.10	67.6	250.15	2.398	>125
5d	2.11	225	707.01	2.849	62.5
5n	2.51	89.2	350.85	2.545	125
5h	2.52	83.3	291.01	2.464	62.5
5k	2.54	55	181.97	2.260	62.5
5c	2.62	418	1383.01	3.141	125
5g	2.83	>500	>1850.21	>3.568	>125
5b	2.88	>500	>1966.65	>3.595	>125
5j	2.99	>500	>1665.17	>3.522	>125
5l	3.02	>500	>1387.66	>3.443	>125
5i	3.04	>500	>1758.89	>3.546	>125
5m	3.22	>500	>1758.89	>3.546	>125
5e	3.76	>500	>2098.72	>3.623	>125

^a: The structures, IC₅₀ (µg/mL), and MIC (µg/mL) of designed flavonoids were reported by Ohemeng, *et al.*, and their MICs to *E. coli*_{ss} were determined using half dilution method [35].

^b: The LogP values were calculated using software ACD/Labs 6.0.

^c: log₁₀(IC₅₀) means Log₁₀ of IC₅₀.

Table S3. Regression equations established from the LogP (x) values of flavonoids and the IC₅₀ or Log₁₀(IC₅₀) (µM) values (y) of these flavonoids to DNA gyrase.^a

Equation number	Sample numbers (n) ^b	Regression equation (r^c)	Coefficient of determination (R^2)
(1)	8	$y = 15268x^3 - 99002x^2 + 212413x - 150519$ (0.9777) ^d	0.9559
(2)		$y = 4.4107x^2 - 20.15x + 25.307$ (0.8253) ^e	0.6811
(3)	14	$y = -4709.9x^3 + 40214x^2 - 108812x + 95023$ (0.9175) ^d	0.8418
(4)		$y = -0.487x^4 + 4.1366x^3 - 11.482x^2 + 11.53x$ (0.8791) ^e	0.7729

^a: The LogP (x) values, and IC₅₀ and Log₁₀(IC₅₀) (µM) were shown in Table S2.

^b: According to half dilution method, the IC₅₀ of compound 5g was set as 1000 µg/mL and used for the regression analyses in equations (1) and (2), and while all compounds with the IC₅₀ more than 500 µg/mL were set as 1000 µg/mL and used for those in equations (3) and (4), together with compounds 5a, 5f, 5d, 5n, 5h, 5k and 5c.

^c: r , correlation coefficient; the significant level α was set as 0.05, and the critical values of $r_{0.975}(6)$ and $r_{0.975}(12)$ were equal to 0.707 and 0.532, respectively.

^d: Regression equations were established from the LogP (x) and the IC₅₀ (µM) (y) values.

^e: Regression equations were established from the LogP (x) and the Log₁₀(IC₅₀) (µM) (y) values.