

Supplementary Materials

**Table 1.** Antioxidant activity of the 70% MeOH root extract of *V. rigida* using DPPH, ABTS, and ORAC assays.

Sample	TE (μmol Trolox equivalents per μg extract)		
	DPPH	ABTS	ORAC
Extract	0.75 ± 0.05	0.82 ± 0.05	2.60 ± 0.08

Note: the antioxidant activity is expressed as Trolox equivalent antioxidant capacity (TE) (μmol Trolox equivalents/μg extract). Data was presented as mean ± SD (*n* ≥ 3).

**Table 2.** Partition coefficients ( $K_{\text{upper/lower}}$ ) of target compounds **1–7** in different solvent systems.

Scheme 1.	$K_{\text{(upper/lower) value}}$						
	1	2	3	4	5	6	7
<i>n</i> -Hexane/EtOAc/MeOH/H <sub>2</sub> O, 2:5:2:5	0.01	0.00	0.01	0.01	0.05	0.03	0.07
<i>n</i> -Hexane/EtOAc/MeOH/H <sub>2</sub> O, 1:5:1:5	0.00	0.02	0.03	0.16	0.46	0.34	2.69
EtOAc/H <sub>2</sub> O, 5:5	0.00	0.01	0.02	0.53	2.36	2.17	35.91
<i>n</i> -Hexane/EtOAc/MeOH/H <sub>2</sub> O, 0.8:5:1.2:5	0.00	0.00	0.01	0.24	0.71	0.51	4.13
<i>n</i> -Hexane/EtOAc/MeOH/H <sub>2</sub> O, 0.5:5:1.5:5	0.00	0.01	0.02	0.30	1.29	0.89	5.16
<i>n</i> -Hexane/EtOAc/MeOH/H <sub>2</sub> O, 0.8:5:1.2:5	0.00	0.02	0.02	0.39	1.14	0.73	5.62
<i>n</i> -Hexane/EtOAc/MeOH/H <sub>2</sub> O, 0.8:5:1.2:5+17.4 mM acetic acid	0.04	0.20	0.18	2.49	3.26	3.58	8.40
<i>n</i> -Hexane/EtOAc/MeOH/H <sub>2</sub> O, 0.5:5:1.5:5+17.4 mM acetic acid	0.11	0.26	0.32	1.79	4.28	5.10	8.94
<i>n</i> -Hexane/EtOAc/MeOH/H <sub>2</sub> O, 0.8:5:1.2:5+17.4 mM acetic acid	0.33	0.46	0.58	3.00	4.60	5.18	14.82

**Table S3.** <sup>1</sup>H-NMR chemical shifts ( $\delta_{\text{H}}$  in ppm) and coupling constants ( $J$  in Hz) of the compounds **1–8** separated from the 70% MeOH extract of *V. rigida* root.

[illegible]

Note: the field strengths (MHz) and solvents used for  $^1\text{H}$ -NMR checking are 600 MHz ( $\text{DMSO}-d_6$ ) for 3-*O*-caffeoylquinic acid (3-CQA), 4-*O*-caffeoylquinic acid (4-CQA), 5-*O*-caffeoylquinic acid (5-CQA), 3,4-*O*-di-caffeoylquinic acid (3,4-diCQA), 3,5-*O*-di-caffeoylquinic acid (3,5-diCQA), and 3,4,5-*O*-tri-caffeoylquinic acid (3,4,5-triCQA); 600 MHz ( $\text{MeOD}-d_4$ ) for 4,5-*O*-di-caffeoylquinic acid (4,5-diCQA); 400 MHz ( $\text{DMSO}-d_6$ ) for acacetin. “-” means no signals appeared.