Supplementary

Structure-Dependent Eco-Toxicity of Vegetable Tannin

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Section S1. Method for culturing *P. phosphoreum*

Freeze-dried *P. phosphoreum* was purchased from Shenzhen Langshi Biological Instrument Co., Ltd.. The reagent was stored at −20 °C and rehydrated before inoculation. The complete culture medium was listed in Table S1. The 100 mL liquid culture medium was contained in 250 mL conical flasks which were occluded with a cotton plug and paper and then sterilized with a high-pressure steam for 20 min at 120 °C. Precultured *P. phosphereum* was inoculated in the complete medium, then maintained at 20°C with a shaking speed of 200 rpm. Bacteria were grown in the liquid medium up to the logarithmic growth stage after 18 h, which could be used for toxicity assay [22,28].

**Table S1.** Culture medium of *P. phosphoreum*.

Name	Purity	Mass (g)
Tryptone		5.00
Yeast extract		5.00
NaCl	AR	30.00
$Na_2HPO_4·12H_2O$	AR	12.61
$K_2HPO_4·3H_2O$	AR	6.55
Glycerin	AR	3.00
Distilled water		1000.00

Section S2. The fitting equations

Table S2. Regression models describing the concentration-response curves of vegetable tannin and model compounds.

| Materials and Chemicals		The Regression Model	R
Hydrolyzed tannin	Tara tannin	$y=\dfrac{121.64}{1+e^{-8.23\times(x-0.21)}}$	0.9813
	Valonia tannin	$y=-1.70+\dfrac{371.15}{1+10^{-0.67\times(-0.47-x)}}$	0.9981
Condensed tannin	Larch tannin	$y=1.22+\dfrac{120.29-1.22}{1+10^{-1.24\times(0.68-x)}}$	0.9990
	Wattle tannin	$y=-9.79+\dfrac{139.89-9.79}{1+10^{-0.61\times(0.71-x)}}$	0.9942
	Baberry tannin	$y=-104.60+\dfrac{101.69-104.60}{1+(\frac{x}{7.12})^{0.78}}$	0.9995
	Acacia mangium tannin	$y=-31.34+\dfrac{116.56-31.34}{1+(\frac{x}{2.96})^{1.23}}$	0.9989
Model compounds	GA	$y=-9.17+\dfrac{146.69-9.17}{1+10^{-0.0020\times(288.52-x)}}$	0.9901
	CAT	$y=7.37+\dfrac{128.61-7.37}{1+10^{-0.0012\times(570.11-x)}}$	0.9986
	EGC	$y=-24.96+\dfrac{141.56-24.96}{1+10^{-0.00025\times(1921.62-x)}}$	0.9891

Section S3. The binding site of luciferase
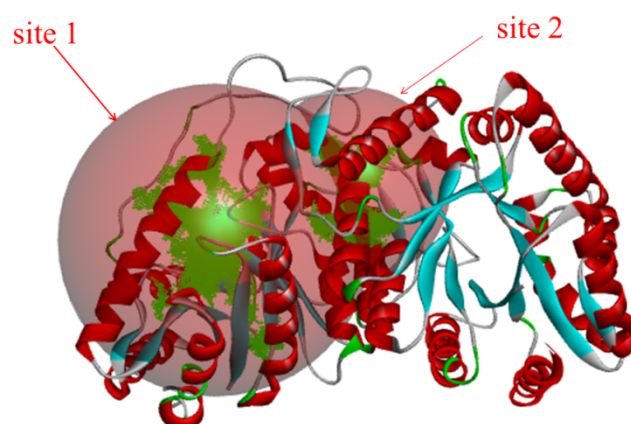
Figure S1. The binding site of luciferase.

Section S4. 3D-diagrams and 2D-diagrams of CDOCKER results
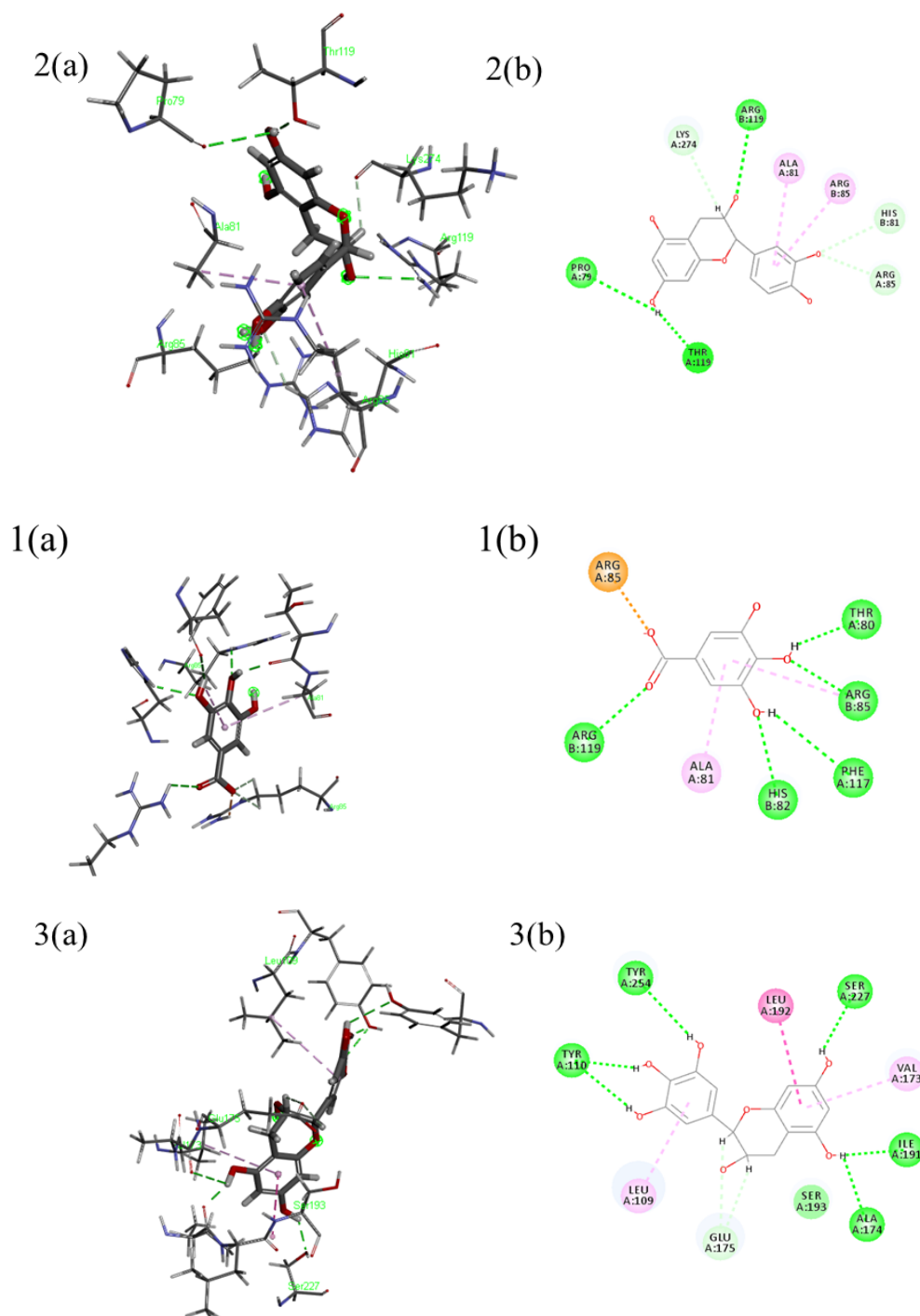
Figure S2. The preferential conformations of complex formed by luciferase with model compounds from CDOCKER (1: GA, 2: CAT, 3: EGC. (a): 3D-diagram (b): 2D-diagram. For the interaction, Pi bond was set as purple line, the hydrogen bond was set as green line, the van der Waals was set as light green and salt bridge was set as orange.).

Section S5. Molecular dynamics
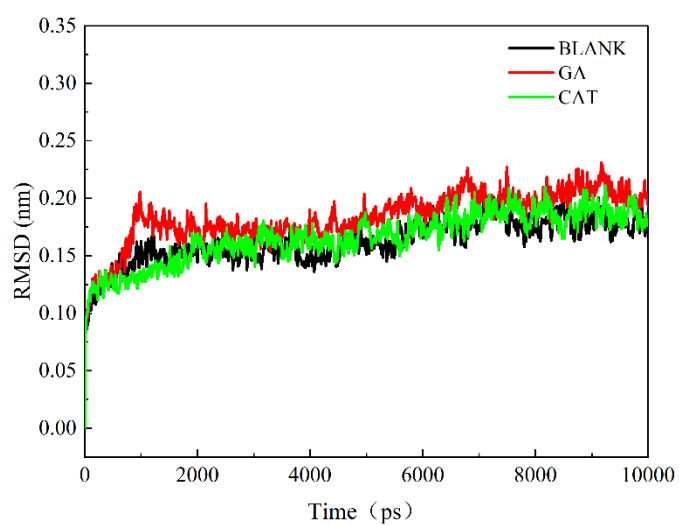
Figure S3. Times dependence of root-mean-square deviations (RMSD).