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Supplemental Material

Characterization of tryptanthrin as an antibacterial reagent inhibiting *Vibrio splendidus*

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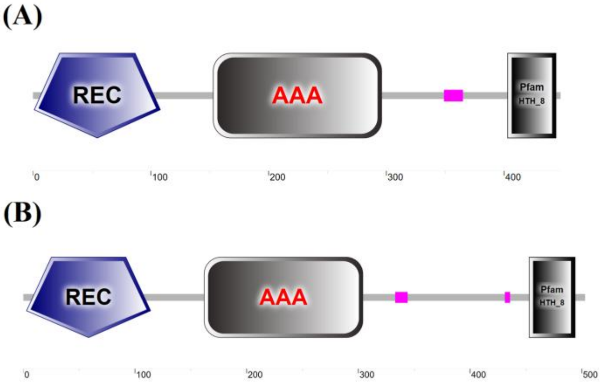

Fig. S1 The SMART analysis of LuxO$_1$ and LuxO$_2$.

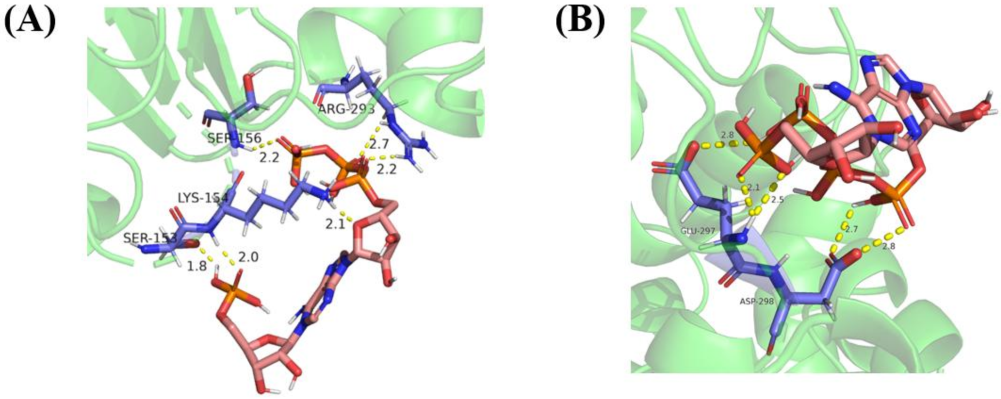

Fig. S2 One representative molecular binding prediction of LuxO$_1$ (A) and LuxO$_2$ (B) with ATP

Table S1 Prediction of the binding sites between ATP and LuxO by autodock 4. The binding sites were sorted according to the binding energy from low to high, and the lower the binding energy value, the more stable the binding ability.

	LuxO$_1$		**LuxO$_2$**	
	Binding sites	**Binding energy**	**Binding sites**	**Binding energy**
ATP	Lys154, Arg293	2.42	Gln297	3.83
	Gln218	4.13	Arg296	5.22
	Lys279	4.62	Arg204	5.57
	Lys179, Lys183	4.95		
	Arg217	5.03		
	Gln282, Trp278	5.33		
	Ser152, Lys179	5.46		
	Lys179	5.6		

Table S2 Prediction of the binding sites between tryptanthrin and LuxO calculated by autodock 4. The binding sites were sorted according to the binding energy from low to high, and the lower the binding energy value, the more stable the binding ability.

	LuxO$_1$		**LuxO$_2$**	
	Binding sites	**Binding energy**	**Binding sites**	**Binding energy**
Tryptanthrin	Ser121	-6.21	Lys253	-4.88
	Val69	-5.55	Asp191	-4.81
	Thr146	-5.46	Arg360	-4.77
	Lys195	-5.12	Lys338	-4.66
	Ala101	-4.39	Phe194	-4.51
	Arg293	-4.88	Lys227	-3.97
	Glu288	-4.88	Arg119	-3.92
	Arg88	-4.81	Arg2	-3.77
	Leu118	-4.63	Gln131	-3.49
	Leu288	-4.59	Lys154	-3.46
	Asn120, Gln218	-4.58	Thr348	-3.27
	Gln218	-4.55		
	Lys207, Lys261	-4.36		
	Asn364	-4.29		
	Lys119	-4.28		
	Asp22	-4.23		
	Tyr316	-4.12		
	Arg105	-4.02		
	Leu239	-3.96		
	Asn364	-3.92		
	Lys195	-3.8		
	Thr370	-3.71		