

# Supplementary Materials: Evaluation of Tanshinone IIA Developmental Toxicity in Zebrafish Embryos

Table S1. Crystal data and structure refinement for (Tanshinone IIA).

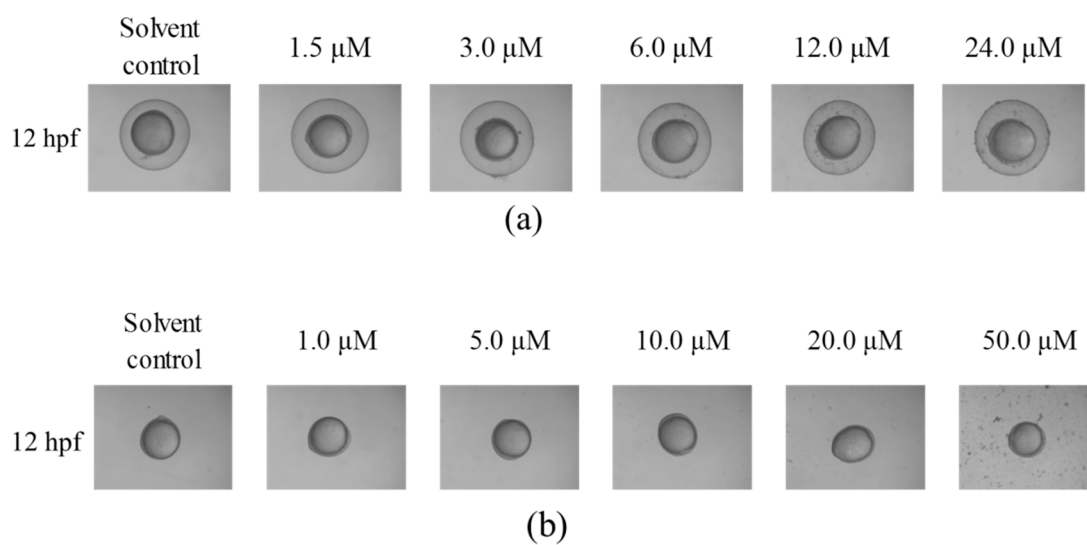
Empirical formula	C <sub>19</sub> H <sub>18</sub> NO <sub>3</sub>
Formula weight	294.33
Temperature/K	100(2)
Crystal system	N/A
Space group	Pmna
a/Å	6.646(3)
b/Å	9.193(4)
c/Å	24.468(10)
α/°	90.00
β/°	90.00
γ/°	90.00
Volume/Å <sup>3</sup>	1494.9(11)
Z	4
ρ <sub>calc</sub> /cm <sup>3</sup>	1.308
μ/mm <sup>-1</sup>	0.088
F(000)	624.0
Crystal size/mm <sup>3</sup>	0.21 × 0.20 × 0.19
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	4.74 to 50
Reflections collected	7233
Data/restraints/parameters	1429/2/136
Goodness-of-fit on F <sup>2</sup>	1.051
Final R indexes [I>=2σ (I)]	R <sub>1</sub> = 0.0529, wR <sub>2</sub> = 0.1679
Final R indexes [all data]	R <sub>1</sub> = 0.0605, wR <sub>2</sub> = 0.1753
Largest diff. peak/hole / e Å <sup>-3</sup>	0.27/-0.23

**Table S2.** Lethality (%) of dechorionated embryos exposed to Tan-IIA at 12 hpf.

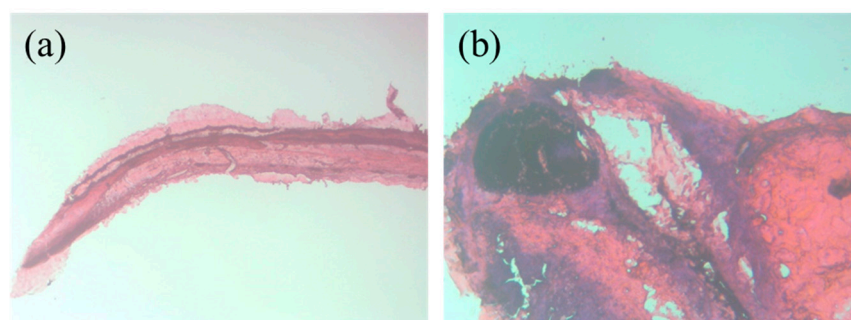
	Solvent control	1.0 $\mu\text{M}$	5.0 $\mu\text{M}$	10.0 $\mu\text{M}$	20.0 $\mu\text{M}$	50.0 $\mu\text{M}$
12 hpf	1.7	5.2	5.0	8.3	10.0	21.0

**Table S3.** Lethality (%) of chorionic embryos exposed to Tan-IIA at 12 hpf.

	Solvent control	1.5 $\mu\text{M}$	3.0 $\mu\text{M}$	6.0 $\mu\text{M}$	12.0 $\mu\text{M}$	24.0 $\mu\text{M}$
24 hpf	0.0	0.0	3.3	8.3	10.0	6.7



**Figure S1.** Morphology of zebrafish embryos exposed to Tan-IIA at 12 hpf. (a) Morphology of chorionic embryos; (b) Morphology of dechorionated embryos.



**Figure S2.** Longitudinal sections of scoliosis (a,  $\times 10$ ) and pericardial edema (b,  $\times 40$ ) with HE staining.

**Table S4.** Observations of teratogenic effects of dechorionated embryos at 48 hpf depending on concentration of Tan-IIA.

	Solvent control	1 $\mu$ M	5 $\mu$ M	10 $\mu$ M	20 $\mu$ M	50 $\mu$ M
Scoliosis				+	+	+
Tail autolysis				+	+	+
Pericardial edema					+	+
Malformation of head					+	+
Malformation of eyes					+	+
Yolk sac edema					+	+
Growth retardation						+

**Table S5.** Observations of acute toxicity in dechorionated embryos exposed to Tan-IIA.

	Exposure times			
	24 hrs	48 hrs	72 hrs	96 hrs
Coagulated embryos	+	+	+	
Lack of somite formation	+	+		
Non-detachment of the tail	+	+		
Lack of heartbeat		+	+	+