

Supplementary data for article:

Veselinović, J. B.; Kocić, G. M.; Pavic, A.; Nikodinovic-Runic, J.; Senerovic, L.; Nikolić, G. M.; Veselinović, A. M. Selected 4-Phenyl Hydroxycoumarins: In Vitro Cytotoxicity, Teratogenic Effect on Zebrafish (*Danio Rerio*) Embryos and Molecular Docking Study. *Chemico-Biological Interactions* **2015**, *231*, 167–174.

<https://doi.org/10.1016/j.cbi.2015.02.011>

Supplementary Table S2. Effect percentages for abnormal morphological characteristics evaluated in the zebrafish teratogenicity assay after exposure to coumarin derivate 7C.

7C	Embryotoxicity ^a	Teratogenicity ^a	Growth retardation ^b	Notochord ^b	Eyes ^b	Otoliths ^b	Somites ^b	Tail detachment ^b	Pericardial oedema ^b	Yolk oedema ^b	Heart beat ^b	Blood circulation ^b	Head ^b	Scoliosis ^b	Tail ^b	Hatching ^b
24 hpf																
100 µg/ml	20.0	80.0	0.0	37.5	62.5	87.5	0.0	0.0	0.0	100.0						
10 µg/ml	20.0	80.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	100.0						
1 µg/ml	18.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0						
48 hpf																
100 µg/ml	25.0	75.0	0.0	80.0	100.0	100.0	0.0	0.0	53.3	100.0	20.0	26.7	100.0	0.0	0.0	
10 µg/ml	20.0	80.0	0.0	0.0	100.0	0.0	0.0	0.0	50.0	100.0	0.0	0.0	93.8	0.0	0.0	
1 µg/ml	18.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
72 hpf																
100 µg/ml	55.0	45.0	0.0	100.0	100.0	100.0	0.0	0.0	77.8	100.0	77.8	77.8	100.0	88.9	55.6	0.0
10 µg/ml	20.0	80.0	6.3	0.0	100.0	0.0	0.0	0.0	50.0	100.0	0.0	0.0	93.8	43.8	12.5	6.3
1 µg/ml	18.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
96 hpf																
100 µg/ml	55.0	45.0	0.0	100.0	100.0	100.0	0.0	0.0	77.8	100.0	77.8	77.8	100.0	88.9	55.6	
10 µg/ml	20.0	80.0	0.0	0.0	100.0	0.0	0.0	0.0	50.0	100.0	0.0	0.0	93.8	56.3	25.0	
1 µg/ml	18.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	

Supplementary Table S3. Effect percentages for abnormal morphological characteristics evaluated in the zebrafish teratogenicity assay after exposure to coumarin derivate 5,7C.

5,7C	Embryotoxicity ^a	Teratogenicity ^a	Growth retardation ^b	Notochord ^b	Eyes ^b	Otoliths ^b	Somites ^b	Tail detachment ^b	Pericardial oedema ^b	Yolk oedema ^b	Heart beat ^b	Blood circulation ^b	Head ^b	Scoliosis ^b	Tail ^b	Hatching ^b
24 hpf																
100 µg/ml	80.0	20.0	100.0	100.0	100.0	100.0	100.0	100.0	0.0	0.0						
10 µg/ml	25.0	65.0	0.0	0.0	86.7	86.7	33.3	33.3	0.0	0.0						
1 µg/ml	12.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0						
48 hpf																
100 µg/ml	100.0	0.0	-	-	-	-	-	-	-	-	-	-	-	-	-	-
10 µg/ml	55.0	45.0	0.0	0.0	100.0	77.8	0.0	0.0	77.8	77.8	0.0	0.0	100.0	0.0	100.0	
1 µg/ml	12.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
72 hpf																
100 µg/ml	100.0	0.0	-	-	-	-	-	-	-	-	-	-	-	-	-	-
10 µg/ml	65.0	35.0	0.0	0.0	100.0	100.0	0.0	0.0	100.0	100.0	0.0	14.3	100.0	0.0	100.0	14.3
1 µg/ml	31.3	12.5	0.0	9.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	9.1	0.0	0.0	10.0	-
96 hpf																
100 µg/ml	100.0	0.0	-	-	-	-	-	-	-	-	-	-	-	-	-	-
10 µg/ml	85.0	15.0	0.0	0.0	100.0	100.0	0.0	0.0	100.0	100.0	66.7	66.7	100.0	0.0	100.0	33.3
1 µg/ml	37.5	6.3	10.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	10.0	-

Abreviation used: (hpf) hours post fertilisation; (-) data not available due to 100% mortality.

^a Percentage of mortality and teratogenicity based on all eggs.^b Percentage of teratogenic effect based on all alive embryos at the time of assessment.

Supplementary Table S4. Effect percentages for abnormal morphological characteristics evaluated in the zebrafish teratogenicity assay after exposure to coumarin derivate 7,8C.

7,8C	Embryotoxicity ^a	Teratogenicity ^a	Growth retardation ^b	Notochord ^b	Eyes ^b	Otoliths ^b	Somites ^b	Tail detachment ^b	Pericardial oedema ^b	Yolk oedema ^b	Heart beat ^b	Blood circulation ^b	Head ^b	Scoliosis ^b	Tail ^b	Hatching ^b
24 hpf																
100 µg/ml	100.00	0.0	-	-	-	-	-	-	-	-	-	-	-	-	-	-
10 µg/ml	90.00	10.0	100.0	100.0	0.0	100.0	100.0	100.0	0.0	0.0	-	-	-	-	-	-
1 µg/ml	30.00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
48 hpf																
100 µg/ml	100.00	0.0	-	-	-	-	-	-	-	-	-	-	-	-	-	-
10 µg/ml	100.00	0.0	-	-	-	-	-	-	-	-	-	-	-	-	-	-
1 µg/ml	30.00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
72 hpf																
100 µg/ml	100.00	0.0	-	-	-	-	-	-	-	-	-	-	-	-	-	-
10 µg/ml	100.00	0.0	-	-	-	-	-	-	-	-	-	-	-	-	-	-
1 µg/ml	30.00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
96 hpf																
100 µg/ml	100.00	0.0	-	-	-	-	-	-	-	-	-	-	-	-	-	-
10 µg/ml	100.00	0.0	-	-	-	-	-	-	-	-	-	-	-	-	-	-
1 µg/ml	30.00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Supplementary Table S5. Effect percentages for abnormal morphological characteristics evaluated in the zebrafish teratogenicity assay after exposure to coumarin.

Coumarin	Embryotoxicity ^a	Teratogenicity ^a	Growth retardation ^b	Notochord ^b	Eyes ^b	Otoliths ^b	Somites ^b	Tail detachment ^b	Pericardial oedema ^b	Yolk oedema ^b	Heart beat ^b	Blood circulation ^b	Head ^b	Scoliosis ^b	Tail ^b	Hatching ^b
24 hpf																
100 µg/ml	55.0	30.0	33.3	0.0	33.3	33.3	33.3	44.4	0.0	0.0	-	-	-	-	-	-
10 µg/ml	43.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-	-	-	-	-	-
1 µg/ml	25.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-	-	-	-	-	-
48 hpf																
100 µg/ml	60.0	40.0	12.5	87.5	0.0	100.0	0.0	0.0	100.0	100.0	25.0	37.5	100.0	0.0	12.5	-
10 µg/ml	43.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1 µg/ml	25.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
72 hpf																
100 µg/ml	60.0	40.0	50.0	87.5	0.0	100.0	0.0	0.0	100.0	100.0	37.5	50.0	100.0	25.0	50.0	50.0
10 µg/ml	43.8	37.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	66.7	0.0
1 µg/ml	35.0	5.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	7.7	0.0	7.7	0.0	0.0
96 hpf																
100 µg/ml	85.0	15.0	0.0	100.0	0.0	100.0	0.0	0.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	0.0
10 µg/ml	43.8	37.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	66.7	0.0
1 µg/ml	55.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Abreviation used: (hpf) hours post fertilisation; (-) data not available due to 100% mortality.

^a Percentage of mortality and teratogenicity based on all eggs.

^b Percentage of teratogenic effect based on all alive embryos at the time of assessment.