

In vivo bioconcentration, distribution and metabolization of benzophenone-3 (BP-3) by *Cyprinus carpio* (European carp)

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Table S1. Experimental condition used for identification of BP-3 and metabolites in fish tesue and organs

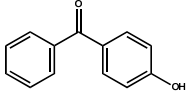
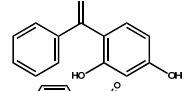
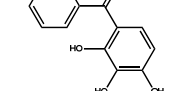
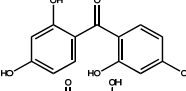
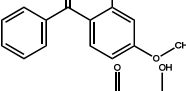
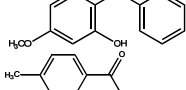
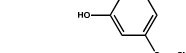
Compou nd	Chemical structure	tr	MRM	Fragment or Voltage (V)	Collizion Energy (V)	Cell Accelerated Voltage (V)	Dwell time (msec)	ESI
4HBP		3.6 1	197-92	150	40	5	165	Negativ
BP-1		4.5 1	213-135	130	20	4	250	Negativ
2,3,4HBP		3.1 6	229-151	135	25	0	165	Negativ
BP-2		2.5 6	245-91	110	30	5	165	Negativ
BP-3		8.0 9	229-151	135	20	1	250	Pozitiv
BP-8		5.0 8	245-121	150	20	5	250	Pozitiv
BP-10		8.9 6	243-151	130	20	2	250	Pozitiv

Table S2. Acquisition segments set for BP-3 and metabolite detection.

Time segment	Start Time (min)	Scan Type	Ionization mode	Div Valve	Store
1	0	MRM	ESI	To Waste	No
2	2.4	MRM	ESI	To MS	Yes
3	4.3	MRM	ESI	To MS	Yes
4	5.5	MRM	ESI	To MS	Yes
5	7.2	MRM	ESI	To MS	Yes
6	8.8	MRM	ESI	To MS	Yes
7	10	MRM	ESI	To Waste	No

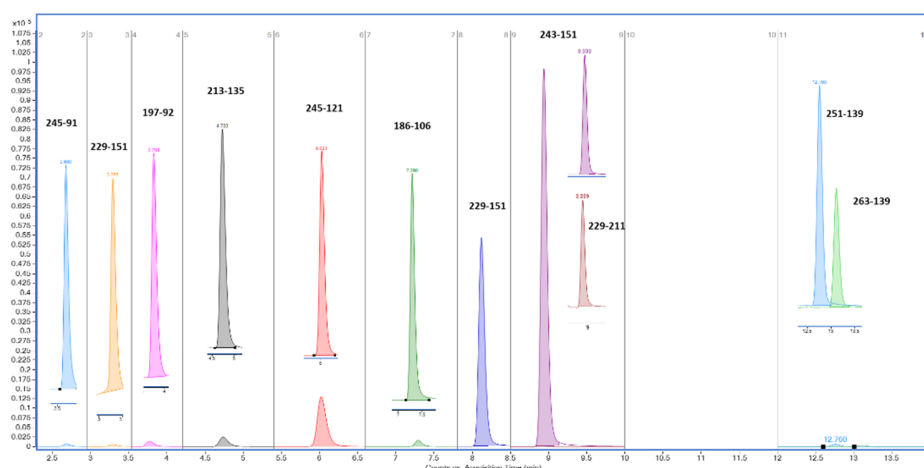


Figure S1 MRM chromatogram obtained for UV-Filters and IS (50ng/mL)

Table S3. Recoveries (R) and limits of quantification (LOQ) obtained for water and fish tissue

Analytes	R ^a	LOQ ^b	R ^c	LOQ ^d
BP-2	82.7	1.15	77.2	0.48
234HBP	81.4	0.92	75.4	0.12
4HBP	90.0	0.18	88.1	0.56
BP-1	101.2	0.81	115	0.33
BP-8	89.5	0.20	82.6	0.68
BP-3	108.7	1.22	112	0.26
BP-10	90.2	0.41	74	0.78

^a Recoveries obtained for water (%); ^b LOQ determined for water ng/L; ^c Recoveries obtained for fish tissue (%); ^d LOQ determined for fish tissue in ng/g d.w.

Table S4. Matrix effect values determined for BP-3 and metabolites in the biological matrix

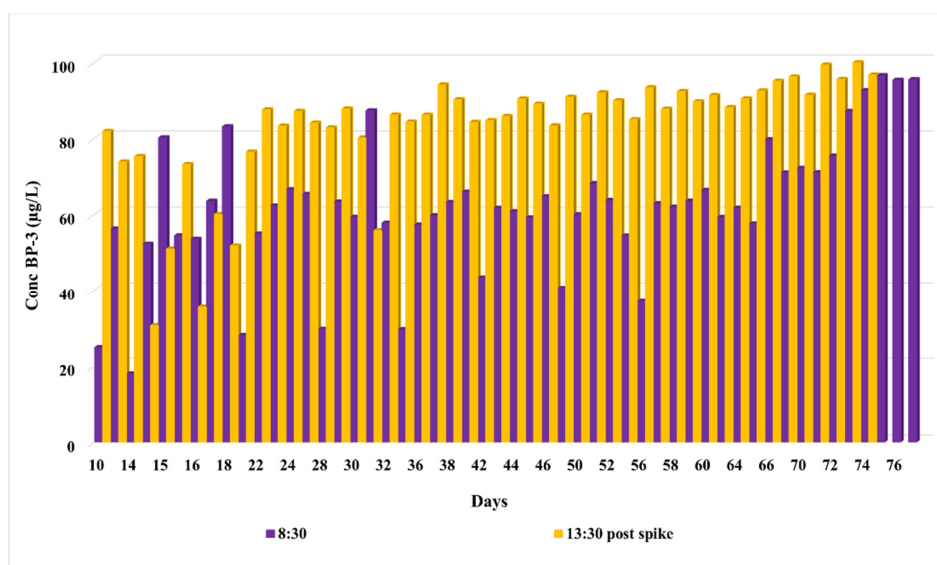
Analytes	Matrix effect, %
BP-2	42
234-HBP	70
4-HBP	1856
BP-1	1791
BP-8	78
BP-3	3464
BP-10	29

Table S5. Initial characteristics of the specimens selected for the bioconcentration test

	Test	Martor
Average weight	25.47 ± 11.08 g / fish	24.3 ± 6.28 g/fish
Total batch weight	501 g	486 g
Average length without caudal peduncle	9.16±1.2 cm	9.065±0.77 cm
Average total length (including caudal peduncle)	12.078 ±1.41 cm	11.93 ±0.92 cm
Average body height	3.34±0.57cm	3.44±0.35 cm

Table S6. Final characteristics of the specimens selected for the bioconcentration test

	Test	Martor
Average weight	27.66 ± 8.17 g / fish	24.76 ± 6.44 g/fish
Total batch weight	534 g	493 g
Average length without caudal peduncle	9.5 ± 1.09 cm	9.4 ± 0.70 cm
Average total length (including caudal peduncle)	12.03 ± 1.34 cm	12 ± 0.88 cm
Average body height	3.35 ± 0.52 cm	3.37 ± 0.43 cm

**Figure S2.** BP-3 variation in water aquarium during the bioaccumulation experiment

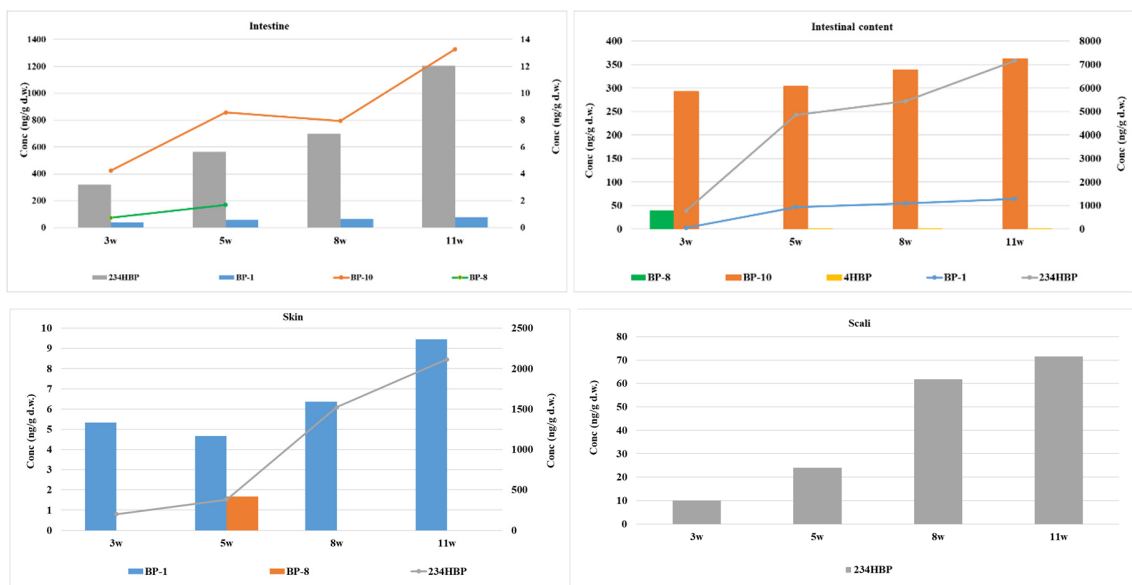


Figure S4. Occurrence of BP-3 biotransformation products in fish organs and tissue.

Table S7. Concentration values of BP-3 and major biotransformation products (ng/g d.w.) identified in organs and tissue.

Tissue	Amalytes	3w	5w	8w	11w
Brain	234HBP	1207±42.2	1031±36.1	1815±63.5	1762±61.7
	BP-1	9.01±0.32	44.7±1.56	13.4±0.47	16.7±0.58
	BP-3	7.32±0.26	138±4.83	225±7.88	229±8.02
Gonads	234HBP	369±12.9	509±17.8	647±22.6	955±33.4
	4HBP	ND	0.79±0.03	ND	ND
	BP-1	16.8±0.59	19.0±0.67	25.8±0.90	24.8±0.87
	BP-8	ND	0.83±0.03	ND	ND
	BP-3	3.18±0.11	226±7.91	364±12.7	468±16.4
Intestine	234HBP	321±11.2	563±19.7	698±24.4	1206±42.2
	BP-1	38±1.33	57.6±2.02	65.5±2.29	75.3±2.64
	BP-8	0.74±0.03	1.69±0.06	ND	ND
	BP-3	41.9±1.47	77.8±2.72	80.2±2.81	96.5±3.38
	BP-10	4.25±0.15	8.58±0.30	7.95±.28	13.3±0.47
Intestinal contents	234HBP	785±27.5	4859±170	5442±191	7172±251
	4HBP	ND	0.72±0.03	0.7±0.02	0.57±0.02
	BP-1	48±1.68	931±32.6	1097±28.4	1281±44.8
	BP-8	40±1.40	ND	ND	ND
	BP-3	71.8±2.51	583±20.4	717±25.1	782±27.4
	BP-10	292±10.2	304±10.6	339±11.9	363±12.7
Kidney	234HBP	297±10.4	296±10.4	1126±39.4	1193±41.8
	BP-1	53.8±1.88	51.8±1.81	102±3.57	142±4.97
	BP-3	63.5±2.22	55.3±1.94	83.7±2.93	114±3.99

Muscle	234HBP	182±6.37	327±11.4	333±11.7	369±12.9
	BP-1	3.67±0.13	6.74±0.24	7.64±0.27	9.83±0.34
	BP-3	19.1±0.67	96.3±3.37	116±4.06	128±4.48
Liver	234HBP	262±9.17	517±17.1	157±5.50	75.7±2.65
	BP-1	40.9±1.43	54±1.89	20.2±0.71	1.08±0.04
	BP-8	ND	0.67±0.02	ND	ND
	BP-3	50.4±1.76	186±6.51	40.9±1.43	5.72±0.20
Gills	234HBP	93.7±3.28	313±11.0	258±9.03	22.7±0.79
	BP-1	ND	ND	7.90±0.28	2.20±0.08
	BP-8	ND	ND	0.93±0.03	ND
	BP-3	21.1±0.74	177±6.20	21.6±0.76	15.0±0.53
	BP-10	ND	ND	25.5±0.89	ND
Skin	234HBP	199±6.97	379±13.3	1523±53.3	2113±74.0
	BP-1	5.33±0.19	4.67±0.16	6.37±0.22	9.45±0.33
	BP-8	ND	1.67±0.06	ND	ND
	BP-3	47.3±1.66	327±11.4	414±14.5	453±15.9
Scaly	234HBP	10.0±0.35	24.0±0.84	61.8±2.16	71.5±2.50
	BP-3	37.7±1.32	55.3±1.94	117±4.10	156±5.46

results expressed as averages of 3 replicates ± SD

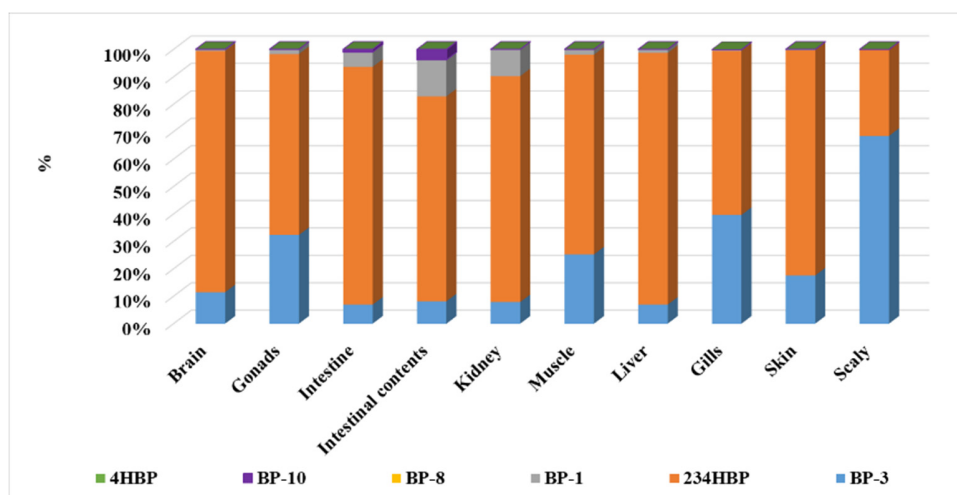


Figure S5. Percentage distribution of BP-3 UV filter and its metabolites in fish organs

Table S8. Concentration values of BP-3 and major biotransformation products ($\mu\text{g/L}$) identified in water

Analytes	3w	5w	8w	11w
234HBP	2177 \pm 32.2	2757 \pm 40.8	3328 \pm 49.3	4050 \pm 59.5
4HBP	ND	ND	ND	ND
BP-1	25 \pm 0.37	112 \pm 1.66	125 \pm 1.85	152 \pm 2.25
BP-3	371 \pm 5.48	41 \pm 0.61	58.3 \pm 0.86	92.4 \pm 1.37

results expressed as averages of 3 replicates \pm SD

Table S9. Pearson correlation and p-values determined between BP-3 and metabolites in gills

Gills		BP-1	BP-8	BP-3	BP-10
234HBP	Pearson Corr.	-0.211	0.258	1.000	0.258
	p value	0.789	0.742	0.000	0.742
BP-1	Pearson Corr.		0.816	0.789	0.816
	p value		0.018	0.022	0.184
BP-8	Pearson Corr.			0.258	1.000
	p value			0.742	0.001
BP-3	Pearson Corr.				0.724
	p value				0.016

Table S10. Pearson correlation and p-values determined between BP-3 and metabolites in liver

Liver		BP-1	BP-8	BP-3
234HBP	Pearson Corr.	1.000	0.775	1.000
	p value	0.000	0.225	0.000
BP-1	Pearson Corr.		0.775	1.000
	p value		0.225	0.000
BP-8	Pearson Corr.			0.775
	p value			0.025

Table S11. Pearson correlation and p-values determined between BP-3 and metabolites in muscle

Muscle		BP-1	BP-3
234HBP	Pearson Corr.	1.000	1.000
	p value	0.000	0.000
BP-1	Pearson Corr.		1.000
	p value		0.000

Table S12. Pearson correlation and p-values determined between BP-3 and metabolites in kidney

Kidney		BP-1	BP-3
234HBP	Pearson Corr.	1.000	1.000
	p value	0.000	0.000
BP-1	Pearson Corr.		1.000
	p value		0.000

Table S13. Pearson correlation and p-values determined between BP-3 and metabolites in brain

Brain		BP-1	BP-3
234HBP	Pearson Corr.	-0.400	0.760
	p value	0.184	0.040
BP-1	Pearson Corr.		0.400
	p value		0.184

Table S14. Pearson correlation and p-values determined between BP-3 and metabolites in gonads

Gonads		4HBP	BP-1	BP-8	BP-3
234HBP	Pearson Corr.	-0.258	0.800	-0.258	1.000
	p value	0.184	0.020	0.184	0.000
4-HBP	Pearson Corr.		-0.258	1.000	-0.258
	p value		0.184	0.038	0.184
BP1	Pearson Corr.			-0.258	0.800
	p value			0.184	0.020
BP-8	Pearson Corr.				-0.258
	p value				0.184

Table S15. Pearson correlation and p-values determined between BP-3 and metabolites in intestine

Intestine		BP-1	BP-8	BP-3	BP-10
234HBP	Pearson Corr.	1.000	-0.738	1.000	0.823
	p value	0.000	0.262	0.000	0.017
BP-1	Pearson Corr.		-0.738	1.000	0.844
	p value		0.262	0.000	0.025
BP-8	Pearson Corr.			-0.738	-0.211
	p value			0.262	-0.714
BP-3	Pearson Corr.				0.873
	p value				0.012

Table S16. Pearson correlation and p-values determined between BP-3 and metabolites in the intestinal content

Intestinal content		4HBP	BP-1	BP-8	BP-3	BP-10
234HBP	Pearson Corr.	0.200	1.000	-0.775	1.000	1.000
	p value	0.800	0.000	0.225	0.000	0.000
4HBP	Pearson Corr.		0.200	-0.775	0.200	0.200
	p value		0.800	0.225	0.800	0.800
BP-1	Pearson Corr.			-0.775	1.000	1.000
	p value			0.225	0.000	0.000
BP-8	Pearson Corr.				-0.844	-0.775
	p value				0.025	0.225
BP-3	Pearson Corr.					1.000
	p value					0.000

Table S17. Pearson correlation and p-values determined between BP-3 and metabolites in skin

Skin		BP-1	BP-8	BP-3
234HBP	Pearson Corr.	0.800	0.000	1.000
	p value	0.020	1.000	0.000
BP-1	Pearson Corr.		-0.775	0.800
	p value		0.225	0.013
BP-8	Pearson Corr.			-0.258
	p value			0.742

Table S18. Pearson correlation and p-values determined between BP-3 and metabolites in scaly

Scaly		BP-3
234HBP	Pearson Corr.	1.000
	p value	0.000