

Probing the Differential Tissue Distribution and Bioaccumulation Behavior of Per- and Polyfluoroalkyl Substances of Varying Chain-Lengths, Isomeric Structures and Functional Groups in Crucian Carp

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Chemicals and reagents. All native and mass labelled standard solutions (PFAC-MXB, FOSA, TPFOA, br-PFOS and MPFAC-MXA) were purchased from Wellington Laboratories (Canada), except eight carbon chlorinated polyfluoroalkane ether sulfonic acid (C8 Cl-PFESA), which was purified from commercial product (Shanghai Synica Co., Ltd.). The full name and abbreviation for all compounds were listed in the Table S2. HPLC grade methanol was obtained from Fisher Scientific (Pittsburgh, PA, USA). Ammonium acetate (NH₄OAc, >97%), ammonium hydroxide (v/v, 50%), acetic acid (>99.8%), formic acid (>98%) were obtained from Alfa Aesar (Ward Hill, MA, USA). High purity water (> 18.2 MΩ cm⁻¹) was used in the present study, which was prepared using a Milli-Q Advantage A10 system (Millipore, USA). Oasis WAX cartridges (150mg, 6cc) and glass fiber filter membranes (0.7μm, 47mm i.d.) were obtained from Waters Co. (Milford, MA, USA) and Sartorius Stedim Biotech (Goettingen, Germany), respectively.

Instrumental analysis for confirmation of PFBA and PFPeA. The presence of PFBA and PFPeA was confirmed using HPLC with a dual pump, autosampler and column compartment (Ultimate 3000, Thermo Fisher Scientific) coupled with an Orbitrap Fusion MS system (Thermo Fisher Scientific, Waltham, MA) and *Xcalibur* software (Thermo Fisher). An Acclaim 120 C18 column (5 μm, 4.6 mm×150 mm) was used to separate targets with an injection volume of 10μL. The mixture of methanol (eluent A) and 50mM ammonium acetate in water (eluent B) was used as mobile phase in a gradient program described as follows. The composition of eluent B started at 28% and decreased to 5% within 4 min, and then held at 5% for 3 min, followed by increasing to 28% within 0.1 min, and held at 28% until 10 min to re-equilibrate the column. The flow rate was 1.0 ml/min. The Orbitrap MS was operated in negative ESI mode and full scan mode (50-700 m/z) with a resolution of 120000. Data were acquired using *Xcalibur* software. The operation parameters were as follows: the capillary voltage at 2500V, ion transfer tube and vaporizer temperatures at 350 and 200°C, the sheath,

aux, and sweep gas flow rates at 35, 10 and 1 Arb, the higher-energy collision dissociation (HCD) energy at 43%. Figure S1 shows the chromatogram of water and blood extract sample with extracting ion at $m/z=212.9780$ (PFBA) and 262.9760 (PFPeA) with a mass accuracy of 5 ppm.

Table S1. Length, weight, sex and organ weights of fish

	Sample	Length (cm)	Weight (g)	Gender	Measured after dissection								Literature values	
					Muscle (g)	Kidney (g)	Gill (g)	Heart (g)	Brain (g)	Bladder (g)	Gonad (g)	Liver (g)	Blood (g)	Muscle (g)
XR	1	11.2	35.38	male	12.15	0.11	0.38	0.02	0.06	0.06	1.08	1.18	1.59	17.69
	2	13	50.05	male	18.51	0.08	0.74	0.05	0.11	0.19	0.57	1.77	2.25	25.03
	3	12.3	34.57	female	11.36	0.04	0.54	0.03	0.03	0.11	1.27	0.54	1.56	17.29
	4	12.8	41.17	female	13.59	0.06	0.42	0.04	0.08	0.09	2.27	0.37	1.85	20.59
	5	11.3	26.9	female	9.62	0.07	0.20	0.02	0.07	0.04	2.07	0.40	1.21	13.45
	6	10.7	27.5	male	8.85	0.08	0.23	0.02	0.08	0.06	0.13	0.62	1.24	13.75
	7	13.5	58.82	female	19.68	0.48	0.86	0.17	0.14	0.20	2.37	1.51	2.65	29.41
	8	12.6	45.14	female	15.32	0.14	0.39	0.10	0.12	0.17	0.78	1.51	2.03	22.57
	9	13.2	43.7	female	16.58	0.17	0.22	0.09	0.18	0.18	1.63	0.32	1.97	21.85
	10	15.4	74.6	female	26.32	0.16	0.26	0.08	0.13	0.23	3.07	0.31	3.36	37.30
	11	13.6	47.72	female	18.59	0.18	0.24	0.05	0.08	0.15	2.18	0.30	2.15	23.86
	12	14.8	63.22	female	21.23	0.09	0.27	0.11	0.16	0.20	2.25	0.30	2.84	31.61
	13	17.8	130.84	female	48.95	0.25	1.59	0.62	0.43	0.33	4.79	1.03	5.89	65.42
	14	13.8	53.85	male	15.62	0.13	0.68	0.08	0.20	0.21	0.25	0.32	2.42	26.93
	15	15	67.87	female	20.65	0.14	0.23	0.18	0.18	0.32	2.91	0.35	3.05	33.94
	16	18.8	157.97	female	51.36	0.27	1.53	0.28	0.46	0.49	5.40	1.43	7.11	78.99
	17	15.3	81.27	female	23.58	0.64	0.60	0.12	0.19	0.23	4.82	1.44	3.66	40.64
	18	18.2	130.5	female	52.35	0.80	1.51	0.83	0.51	0.23	5.21	2.48	5.87	65.25
	19	15.1	81.46	female	24.62	0.47	1.34	0.12	0.19	0.21	5.80	1.70	3.67	40.73
	20	15.4	82.28	female	28.52	0.21	0.27	0.28	0.19	0.29	3.42	0.42	3.70	41.14
	21	13	34.86	male	12.67	0.11	0.26	0.06	0.14	0.08	0.24	0.31	1.57	17.43
	22	13.4	47.24	female	16.85	0.24	0.77	0.12	0.12	0.15	4.09	0.68	2.13	23.62
	23	14.8	78.8	female	32.12	0.54	1.30	0.11	0.20	0.21	4.96	1.81	3.55	39.40
	24	12	35.83	female	12.57	0.11	0.26	0.04	0.15	0.09	2.69	0.34	1.61	17.92
	25	12.6	45.15	female	15.69	0.19	0.93	0.19	0.12	0.11	3.36	0.39	2.03	22.58

	26	17	110.94	female	40.23	0.55	1.56	0.80	0.20	0.32	5.05	2.53	4.99	55.47
	27	19.8	173.74	female	58.94	0.25	0.27	0.25	0.25	0.66	5.49	1.08	7.82	86.87
	28	15.8	75.98	female	28.53	0.50	1.16	0.14	0.14	0.23	1.18	2.12	3.42	37.99
	29	20.3	161.23	male	60.26	1.18	4.83	0.26	0.41	0.44	0.43	3.08	7.26	80.62
	30	19.3	169.67	female	68.53	0.26	3.37	0.67	0.51	0.43	4.67	1.41	7.64	84.84
mean		14.73	75.61		26.79	0.28	0.91	0.20	0.19	0.22	2.81	1.07	3.40	37.80
median		14.30	61.02		20.16	0.18	0.57	0.11	0.15	0.20	2.53	0.86	2.75	30.51
min		10.70	26.90		8.85	0.04	0.20	0.02	0.03	0.04	0.13	0.30	1.21	13.45
max		20.30	173.74		68.53	1.18	4.83	0.83	0.51	0.66	5.80	3.08	7.82	86.87
TL	1	24.5	354.02	male	123.62	1.87	5.51	0.54	0.44	2.11	18.55	6.43	15.93	177.01
	2	25.5	396.43	female	126.54	1.41	6.63	0.45	0.22	2.51	10.36	4.89	17.84	198.22
	3	25	333.76	female	115.83	0.86	5.32	0.19	0.29	1.39	60.46	2.98	15.02	166.88
	4	28.5	521.4	female	185.60	1.91	10.36	0.34	0.49	4.93	128.42	6.74	23.46	260.70
	5	26.5	384.38	female	132.77	2.62	12.39	0.53	0.41	3.64	94.24	9.15	17.30	192.19
	6	22	225.57	male	78.48	0.87	4.08	0.21	0.34	0.98	3.03	3.11	10.15	112.79
	7	19.5	185.12	female	67.25	1.08	3.21	0.19	0.26	0.79	25.30	3.81	8.33	92.56
	8	26.5	413.47	male	137.89	1.02	7.75	0.30	0.50	2.62	1.07	3.54	18.61	206.74
	9	19	182.82	female	62.51	0.83	5.21	0.20	0.37	1.10	11.37	2.95	8.23	91.41
	10	26	394	female	138.25	2.31	10.77	0.43	0.56	3.02	91.04	7.94	17.73	197.00
	11	25.5	431.98	female	136.73	1.18	8.81	0.47	0.50	2.93	23.10	4.11	19.44	215.99
	12	26	340.49	female	123.86	0.88	4.99	0.32	0.45	2.28	55.94	2.99	15.32	170.25
	13	26	289.56	male	89.83	1.18	5.25	0.00	0.50	2.03	15.67	3.99	13.03	144.78
mean		24.65	342.54		116.86	1.39	6.95	0.32	0.41	2.33	41.43	4.82	15.41	171.27
median		25.5	354.02		123.86	1.18	5.51	0.32	0.44	2.28	23.10	3.99	15.93	177.01
min		19	182.82		62.51	0.83	3.21	0.00	0.22	0.79	1.07	2.95	8.23	91.41
max		28.5	521.4		185.61	2.62	12.39	0.54	0.56	4.93	128.42	9.15	23.46	260.70

Table S2. Full name and abbreviations of PFASs

Brand name	Full name	Abbreviation
PFCA-MXB	perfluorobutanoic acid	PFBA
	perfluoropentanoic acid	PFPeA
	perfluorohexanoic acid	PFHxA
	perfluoroheptanoic acid	PFHpA
	perfluorooctanoic acid	PFOA
	perfluorononanoic acid	PFNA
	perfluorodecanoic acid	PFDA
	perfluoroundecanoic acid	PFUnDA
	perfluorododecanoic acid	PFDoDA
	perfluorotridecanoic acid	PFTTrDA
	perfluorotetradecanoic acid	PFTeDA
	perfluorobutanesulfonic acid	PFBS
	perfluorohexanesulfonic acid	PFHxS
	perfluorooctanesulfonic acid	PFOS
T-PFOA	perfluoro-1-octanoic acid	n-PFOA (79%)
	6-trifluoromethylperfluoroheptanoic acid	iso-PFOA (9%)
	5- trifluoromethylperfluoroheptanoic acid	5m-PFOA (4.5%)
	4-trifluoromethylperfluoroheptanoic acid	4m-PFOA (4%)
	3-trifluoromethylperfluoroheptanoic acid	3m-PFOA (3%)
br-PFOSK	perfluoro-1-octane sulfonic acid	n-PFOS (78.8%)
	6-trifluoromethylperfluoroheptane sulfonic acid	iso-PFOS (10%)
	5-trifluoromethoylperfluoroheptane sulfonic acid	5m-PFOS (4.5%)
	4-trifluoromethylperfluoroheptane sulfonic acid	4m-PFOS (2.2%)
	3-trifluoromethylperfluoroheptane sulfonic acid	3m-PFOS (1.9%)

	1-trifluoromethylperfluoroheptane sulfonic acid	1m-PFOS (1.2%)
FOSA	perfluorooctane sulfonamide	FOSA
F-53B	6:2 Chlorinated polyfluoroalkyl ether sulfonic acids	C8 Cl-PFESA
MPFCA-MXA	perfluoro [1,2,3,4- ¹³ C] butanoic acid	¹³ C ₄ -PFBA
	perfluoro [1,2,3,4- ¹³ C] octanoic acid	¹³ C ₄ -PFOA
	perfluoro [1,2- ¹³ C]dodecanoic acid	¹³ C ₂ -PFDoA
	perfluoro [1,2,3,4- ¹³ C] octanesulfonic acid	¹³ C ₄ -PFOS

Table S3. Experimental conditions used for electrospray tandem mass spectrometry.

Curtain gas pressure: 10 psi; collision gas pressure: 6 psi; ion spray voltage: -2000 V; Source temperature: 350°C; gas 1: 40 psi; and gas 2: 40 psi, Dwell time: 15 ms						
Compound	Parent ion (Q1)	Daughter ion (Q3)	Declustering Potential (V)	Entrance Potential (V)	Collision Energy (eV)	Collision Cell Exit Potential (V)
PFBA	212.8	168.8	-20	-10	-12	-8
PFPeA	262.8	218.9	-20	-10	-11	-9
PFHxA	312.8	269.0	-25	-10	-11	-13
PFHpA	362.8	319.0	-25	-10	-11	-13
n-PFOA	412.8	369.0	-22	-4.0	-21	-15
iso-PFOA	412.8	369.0	-22	-4.0	-21	-15
5m-PFOA	412.8	219.0	-22	-4.5	-21	-6
4m-PFOA	412.8	119.0	-18	-4.5	-32	-5
3m-PFOA	412.8	169.0	-19	-4.5	-25	-6.0
PFNA	462.8	419.1	-25	-10	-14	-15
PFDA	512.8	469.1	-30	-10	-15	-15
PFUnDA	562.8	519.1	-30	-10	-16	-20
PFDoDA	612.8	569.0	-30	-10	-17	-20
PFTTrDA	662.8	619.0	-40	-10	-18	-10
PFTeDA	712.8	669.0	-40	-10	-18	-10

PFBS	298.8	79.9*	-80	-6	-63	-5
	298.8	99.0	-80	-10	-55	-7
PFHxS	398.8	79.9*	-80	-10	-80	-6
	398.8	99.0	-80	-10	-75	-6
n-PFOS	498.8	79.9	-79	-10	-105	-7
iso-PFOS	498.8	79.9	-79	-10	-105	-7
5m-PFOS	498.8	79.9*	-79	-10	-105	-7
5m-PFOS	498.8	130.0	-80	-10	-60	-7
4m/3m-PFOS	498.8	79.9*	-79	-10	-105	-7
4m/3m-PFOS	498.8	130.0	-80	-10	-60	-7
1m-PFOS	498.8	419.0	-60	-10	-35	-15
C8 Cl-PFESA	530.6	351.0*	-85	-10	-36	-12
	530.6	83.0	-85	-10	-70	-6
n-FOSA	497.9	169.0*	-110	-10	-36	-8
	497.7	77.9	-100	-10	-85	-6
13C4 PFBA	216.9	171.9	-20	-6	-12	-13
13C4 PFOA	416.8	372.1	-50	-10	-13	-15
13C2PFDoDA	614.8	570.0	-60	-8	-15	-13
13C4 PFOS	502.8	79.9	-100	-10	-105	-7

*quantification ion

Table S4. Recoveries and Method Limit of Quantifications (MLQs) for PFASs and isomers in different matrix

	Blood	Liver	Gonad	Bile	Gill	Bladder	Heart	Brain	Kidney	Muscle	Water
	Recoveries (n=4, mean±SD%)										
PFBA	113.1±6.5	105.4±4.6	109.0±4.9	99.7±9.5	120.1±13.6	127.2±1.8	130.5±5.2	110.0±9.6	117.5±11.8	97.2±7.3	96.9±5.8
PFPeA	75.4±5.0	73.8±6.8	76.5±7.9	76.8±10.0	78.5±2.4	77.8±2.9	71.5±4.7	89.5±6.5	80.3±8.0	92.8±7.5	82.3±5.7
PFHxA	111.2±7.4	96.3±7.0	101.4±7.2	103.5±13.2	100.2±4.5	107.4±3.0	108.9±5.1	109.6±5.9	119.9±5.9	96.4±5.0	103.4±6.0
PFHpA	106.8±8.5	94.9±8.7	96.1±6.6	82.9±9.8	97.0±3.2	91.5±4.6	100.3±5.7	113.1±2.0	102.5±3.8	95.2±6.5	92.9±8.8
n-PFOA	83.3±2.8	87.9±4.6	74.9±3.0	75.7±2.4	85.4±4.0	84.5±3.5	78.6±5.6	89.6±1.9	75.8±2.8	82.4±7.5	96.4±8.9
iso-PFOA	80.8±6.2	81.2±2.4	71.5±2.3	72.0±3.6	74.9±4.0	72.0±2.5	75.5±6.4	81.4±5.1	80.8±2.6	95.0±2.0	92.0±6.6
5m-PFOA	71.4±4.0	71.5±2.9	80.4±4.6	76.7±4.4	72.4±2.1	78.4±0.9	73.7±1.1	77.0±3.4	73.4±2.6	94.9±3.9	105.9±7.8
4m-PFOA	83.5±5.6	72.3±3.1	80.0±6.1	78.4±2.4	74.8±5.0	78.4±3.4	73.0±3.1	77.4±4.0	71.0±4.3	99.0±4.3	109.2±4.1
3m-PFOA	75.6±8.0	87.4±10.8	91.2±2.6	109.2±10.5	72.2±7.5	79.8±9.1	79.2±5.2	72.2±8.0	80.1±6.9	83.2±2.0	94.4±5.0
PFNA	85.2±6.2	105.1±11.1	109.2±6.8	110.7±13.3	102.9±5.9	95.0±8.4	90.9±7.3	115.6±4.5	105.6±8.5	100.2±3.5	99.9±8.4
PFDA	48.8±5.9	71.1±10.8	85.4±6.5	67.4±5.7	74.7±6.7	70.5±7.1	85.3±6.6	108.5±8.6	89.4±8.0	95.0±7.0	90.0±6.8
PFUnDA	89.5±2.9	104.4±17.4	98.8±10.1	115.5±9.2	96.9±11.9	84.1±7.9	100.7±10.6	105.5±3.9	97.5±8.7	98.0±8.7	87.9±9.0
PFDoDA	84.2±7.5	75.9±7.5	88.9±7.4	92.2±8.0	79.5±4.9	83.8±9.0	82.3±7.3	94.3±6.8	73.8±8.9	97.3±7.9	98.5±5.1
PFTTrDA	77.2±8.9	68.3±13.6	87.9±5.5	111.0±10.6	70.8±6.7	82.4±11.7	81.6±6.1	87.2±10.0	72.9±7.8	89.2±10.1	75.9±5.7
PFTeDA	82.2±9.0	75.2±7.1	65.8±5.4	90.4±10.9	68.5±5.8	76.5±6.8	73.5±7.6	61.9±4.3	61.9±5.3	87.2±8.5	70.4±8.7
PFBS	107.1±7.4	89.2±8.4	103.0±5.6	84.8±2.9	107.5±4.2	114.6±8.1	95.3±5.4	97.9±3.9	105.8±4.0	114.8±5.8	106.4±6.7
PFHxS	105.2±5.9	84.1±7.7	92.1±4.2	73.1±8.9	91.1±1.5	85.1±2.8	94.3±6.1	92.6±4.1	90.9±4.4	107.8±4.7	105.6±9.9
n-PFOS	87.6±3.2	88.0±1.5	80.8±7.8	72.9±1.5	75.1±3.9	73.9±5.7	76.8±1.5	74.7±0.9	79.5±4.6	103.9±4.2	99.1±6.9
iso-PFOS	75.9±6.0	79.6±3.9	80.6±2.3	79.2±3.4	78.3±3.4	85.0±10.5	79.7±6.5	79.4±3.5	84.1±6.3	83.4±5.3	89.3±5.4
5m-PFOS	81.1±2.8	73.3±7.5	77.4±5.6	81.9±7.0	75.3±5.6	78.2±4.2	79.9±6.5	72.9±1.7	73.3±3.6	87.6±6.2	88.7±7.1
4m/3m-PFOS	80.9±4.9	70.0±3.8	75.3±8.7	71.4±2.7	75.1±3.0	73.5±5.9	70.8±2.6	75.1±2.6	77.4±3.3	98.3±5.6	87.2±6.2
1m-PFOS	86.6±8.8	79.5±3.2	89.3±14.9	73.0±5.5	79.9±9.6	78.6±6.0	100.4±13.6	77.5±4.8	76.0±8.1	89.8±4.6	96.7±5.8
C8 Cl-PFESA	103.0±9.7	77.1±7.6	97.2±10.6	71.0±9.9	96.8±6.9	87.7±10.1	109.2±5.1	94.0±1.6	86.1±9.6	98.9±8.0	92.9±6.2
FOSA	100.0±6.5	82.6±5.8	96.5±6.8	68.2±2.3	54.2±2.0	79.3±5.8	75.6±4.0	87.8±7.5	77.3±2.5	81.2±4.5	85.2±3.8

MLQ (unit: ng/L for water, ng/ml for blood and bile, ng/g ww for tissue samples)											
PFBA	0.32	0.61	0.50	0.62	0.18	0.45	0.50	0.46	0.59	0.04	0.19
PFPeA	0.07	0.17	0.39	0.22	0.52	0.24	0.15	0.26	0.25	0.02	0.10
PFHxA	0.17	0.33	0.23	0.29	0.51	0.41	0.31	0.34	0.60	0.04	0.20
PFHpA	0.15	0.38	0.27	0.13	0.24	0.22	0.21	0.30	0.26	0.04	0.19
n-PFOA	0.16	0.31	0.21	0.15	0.40	0.32	0.37	0.29	0.29	0.02	0.10
iso-PFOA	0.10	0.25	0.18	0.13	0.30	0.27	0.19	0.27	0.22	0.02	0.09
5m-PFOA	0.10	0.27	0.18	0.13	0.34	0.27	0.32	0.24	0.21	0.02	0.09
4m-PFOA	0.15	0.27	0.17	0.13	0.33	0.27	0.23	0.26	0.24	0.02	0.09
3m-PFOA	0.13	0.24	0.20	0.14	0.33	0.28	0.28	0.25	0.25	0.02	0.09
PFNA	0.10	0.24	0.13	0.13	0.24	0.19	0.15	0.16	0.18	0.01	0.07
PFDA	0.06	0.14	0.13	0.08	0.12	0.06	0.12	0.15	0.15	0.02	0.10
PFUnDA	0.04	0.11	0.08	0.16	0.19	0.19	0.12	0.10	0.19	0.02	0.09
PFDoDA	0.03	0.07	0.13	0.07	0.12	0.14	0.13	0.11	0.17	0.01	0.07
PFTTrDA	0.05	0.12	0.07	0.14	0.08	0.08	0.12	0.13	0.12	0.01	0.05
PFTeDA	0.07	0.17	0.16	0.13	0.19	0.18	0.12	0.11	0.12	0.01	0.03
PFBS	0.18	0.34	0.41	0.38	0.44	0.34	0.36	0.39	0.43	0.08	0.07
PFHxS	0.24	0.23	0.24	0.31	0.28	0.21	0.21	0.23	0.24	0.05	0.08
n-PFOS	0.17	0.59	0.48	1.04	0.66	0.39	0.51	0.51	0.68	0.01	0.02
iso-PFOS	0.10	0.46	0.40	0.94	0.49	0.33	0.27	0.46	0.51	0.003	0.02
5m-PFOS	0.11	0.51	0.41	0.89	0.56	0.33	0.45	0.41	0.49	0.003	0.02
4m/3m-PFOS	0.16	0.50	0.38	0.92	0.54	0.33	0.32	0.44	0.57	0.003	0.02
1m-PFOS	0.13	0.45	0.45	0.96	0.54	0.34	0.39	0.42	0.59	0.003	0.02
C8 Cl-PFESA	0.10	0.24	0.41	0.26	0.53	0.37	0.50	0.26	0.55	0.003	0.06
FOSA	0.07	0.16	0.25	0.22	0.21	0.19	0.27	0.22	0.28	0.002	0.01

Table S5. Table with p-values from Wilcoxon rank sum test for concentrations in XR and TL

Compound	Blood XR	Blood TL
PFBA	NA	NA
PFPeA	NA	NA
PFHxA	NA	NA
PFHpA	NA	NA
n-PFOA	0.7	0.41
PFNA	0.41	0.71
PFDA	0.08	0.71
PFUnDA	0.11	0.5
PFDoDA	0.46	0.83
PFTTrDA	0.86	0.71
PFTeDA	0.82	0.6
iso-PFOA	0.63	0.83
5m-PFOA	0.74	1
4m-PFOA	0.98	0.33
3m-PFOA	0.46	0.83
PFBS	0.08	1
PFHxS	0.02	0.5
n-PFOS	0.02	0.41
iso-PFOS	0.06	0.83
5m-PFOS	NA	0.94
4m/3m-PFOS	NA	0.5
1m-PFOS	NA	0.41
C8 Cl-PFESA	NA	0.83
br-FOSA	NA	0.83
n-FOSA	NA	0.6

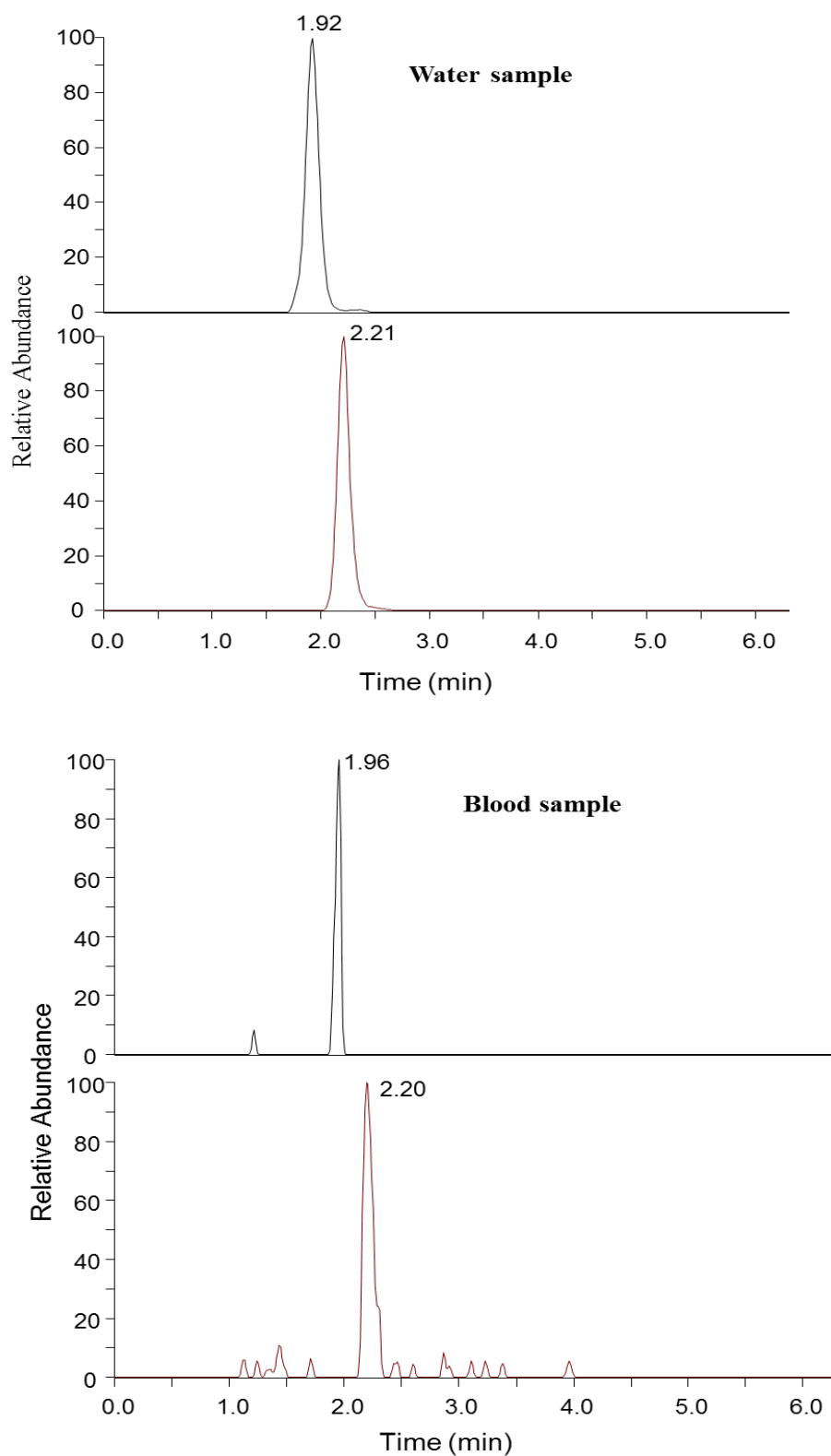


Figure S1. Chromatograms of water and blood extract samples in HR-MS at $m/z=212.9780$ (PFBA, in black) and 262.9760 (PFPeA, in red) with a mass accuracy of 5 ppm (C18 column)

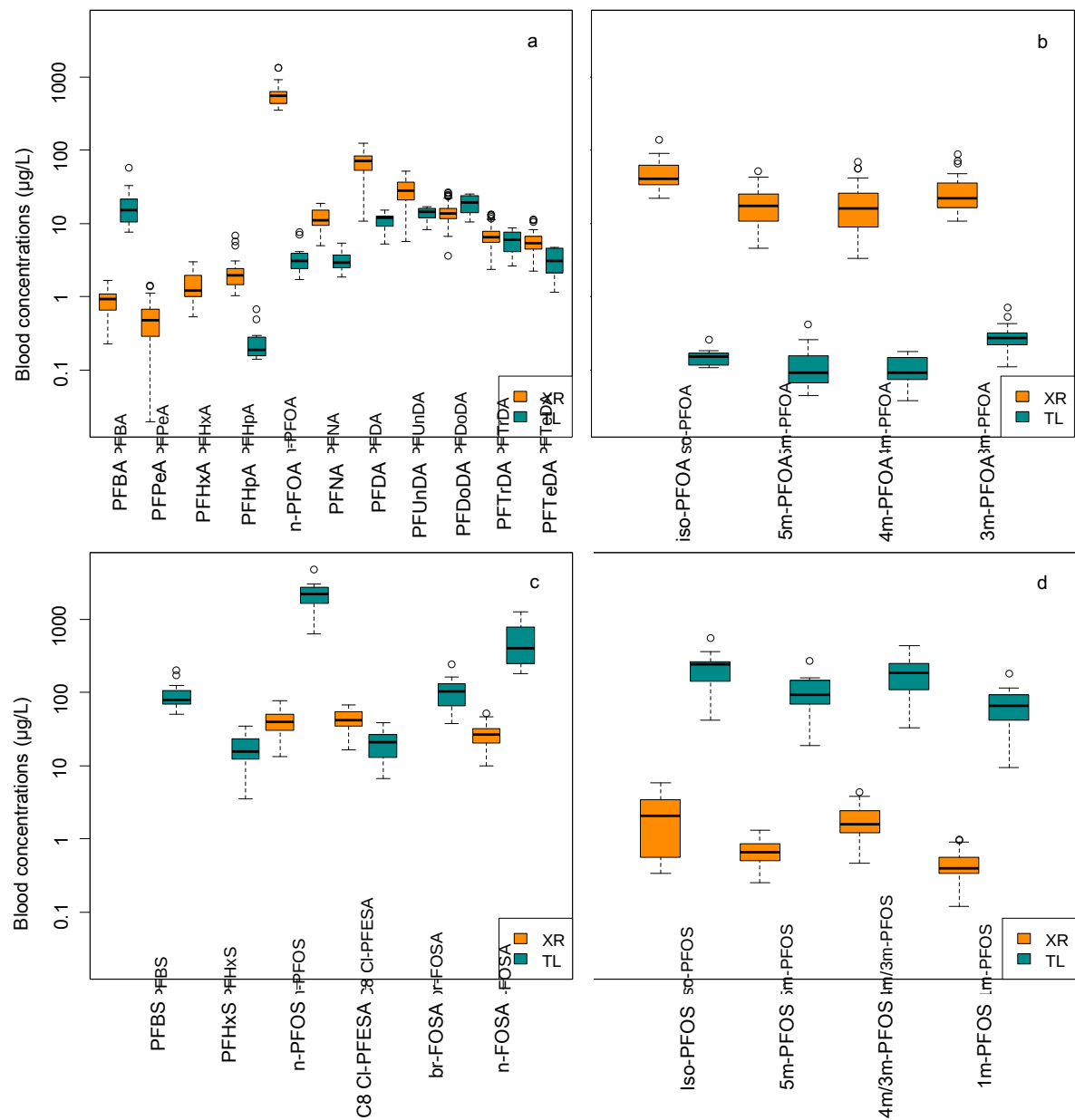


Figure S2a–d. Box-whisker plots of PFAS concentrations in blood of fish from XR (orange) and TL (blue). Boxes indicate 25th, 50th and 75th percentiles and whiskers indicate 5th and 95th percentiles. Extreme values are indicated as circles. a: PFCAs; b: br-PFOA isomers; c: PFSA, FOSA and C8 Cl-PFESA; d: br-PFOS isomers

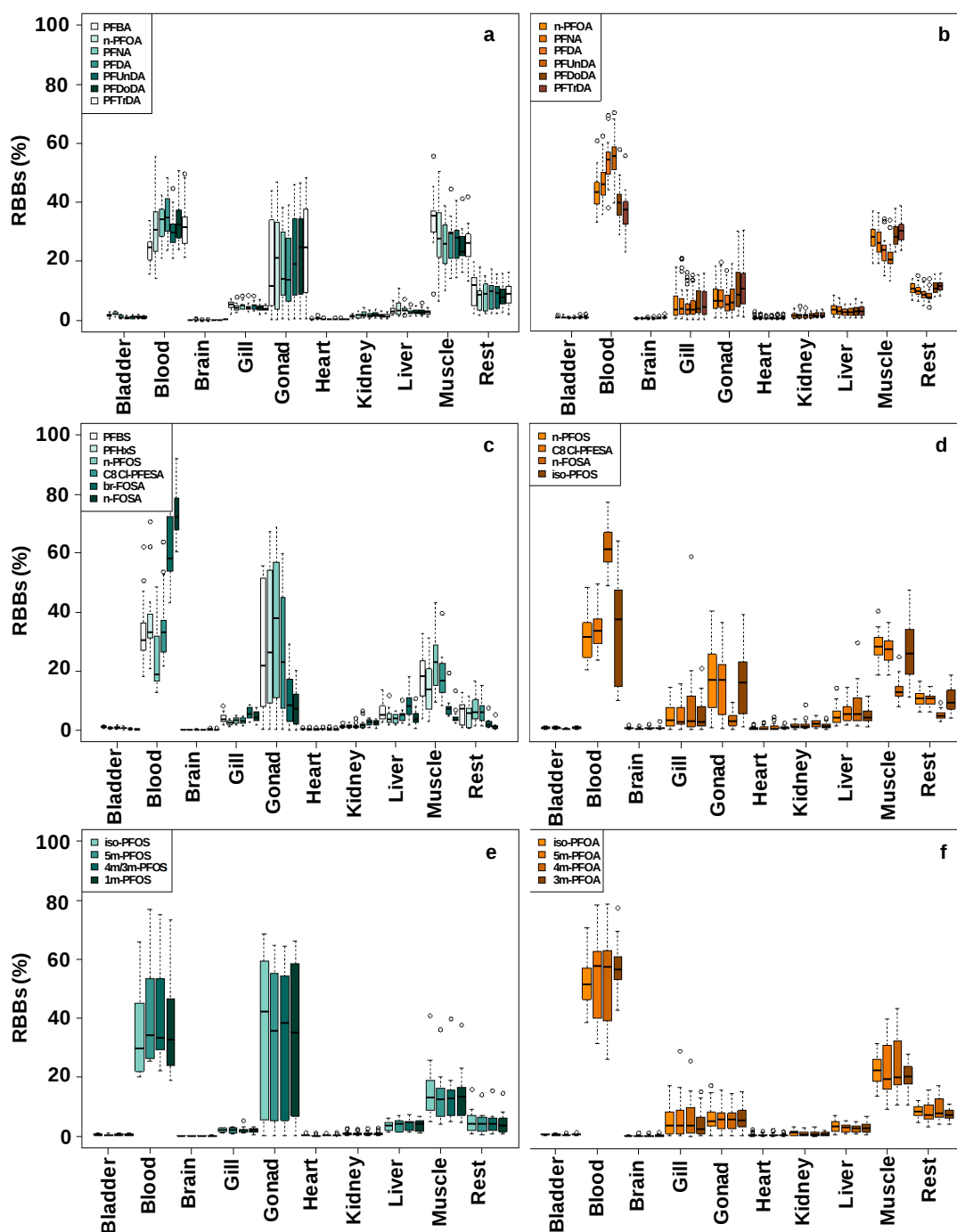


Figure S4a-f. RBBs of PFASs in TL (blue) and XR (orange). Data with <80% detected concentrations in all tissues were excluded. Boxes indicate 25th, 50th and 75th percentiles and whiskers indicate 5th and 95th percentiles. Extreme values in the data sets are indicated as circles. a and b: C3, C7-C13 PFCAs; c and d: PFBS, PFHxS, n-PFOS, C8 Cl-PFESA, br-FOSA and n-FOSA; e and f: br-PFOS and br-PFOA isomers.

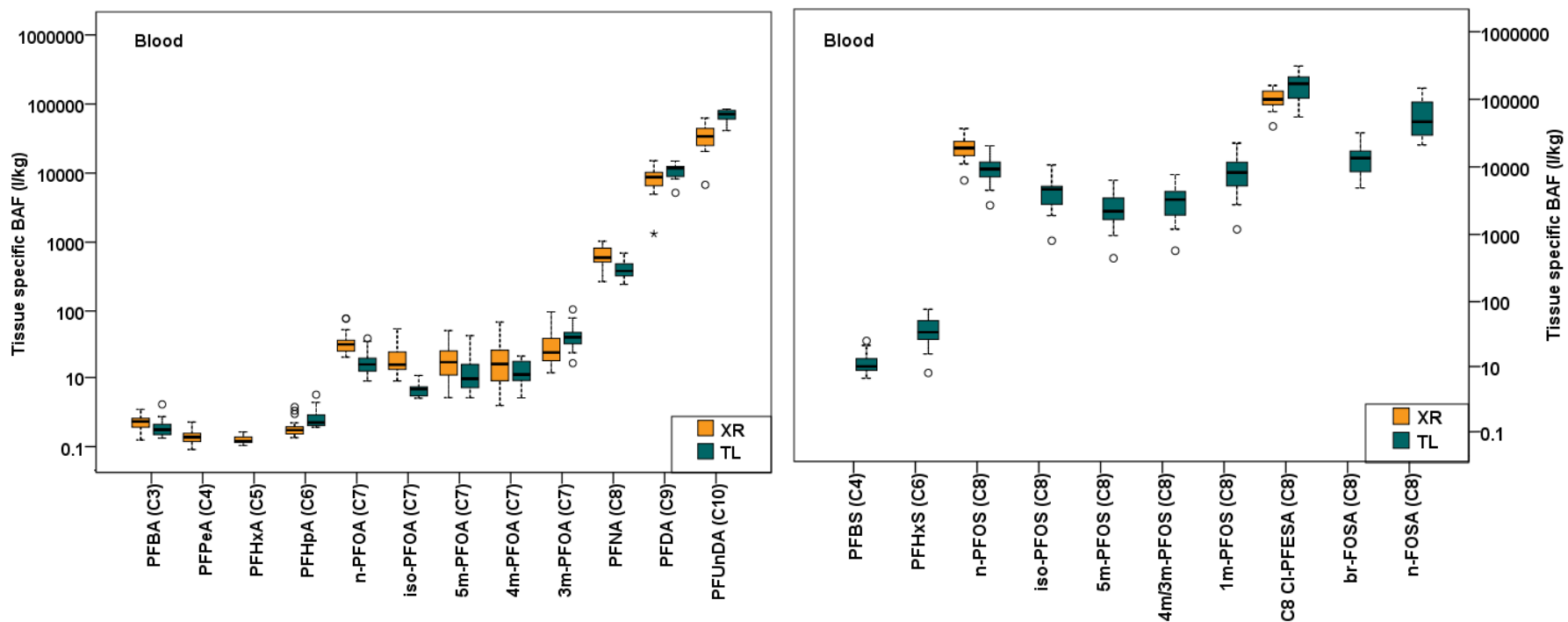


Figure S5. Tissue-specific BAF for blood with varying chain-length, isomeric structures and functional groups for XR (orange) and TL (blue). Data with <80% detected concentrations in all tissues were excluded. Boxes indicate 25th, 50th and 75th percentiles and whiskers indicate 5th and 95th percentiles. Extreme values in the data sets are indicated as circles.

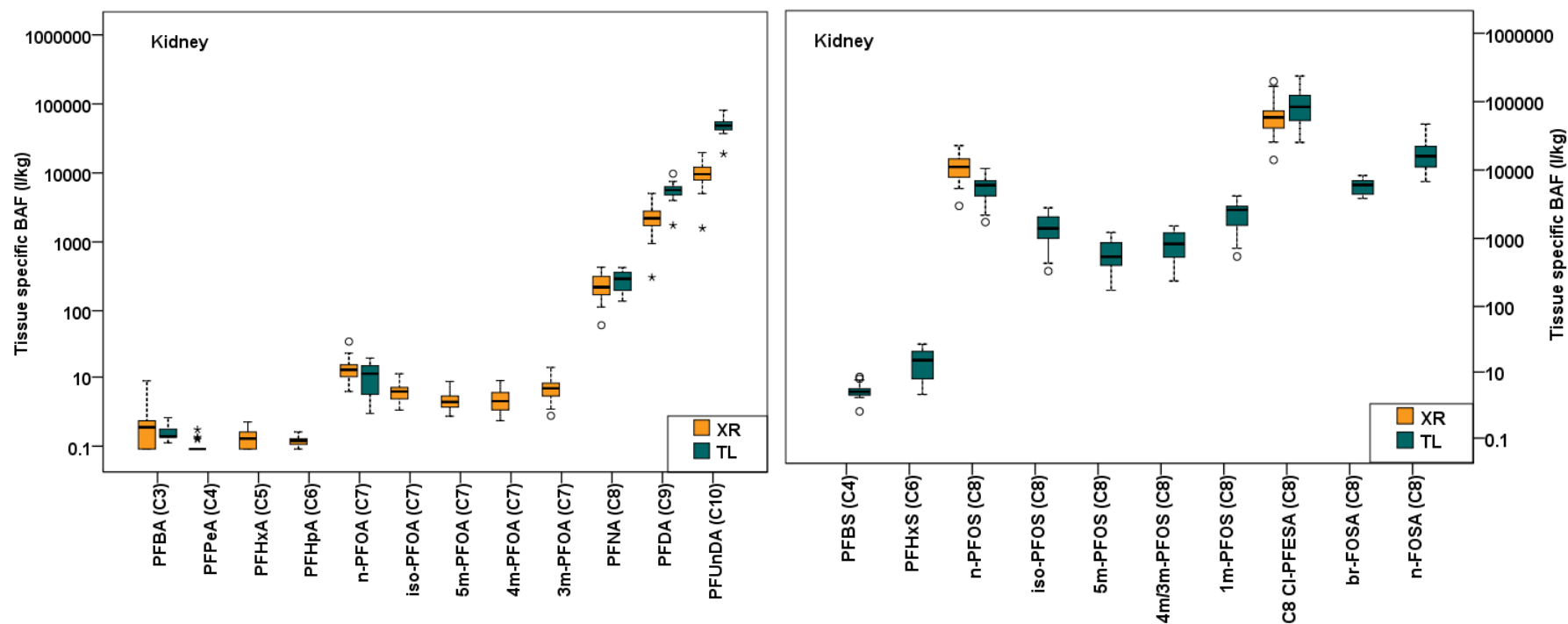


Figure S6. Tissue-specific BAF for kidney with varying chain-length, isomeric structures and functional groups for XR (orange) and TL (blue). Data with <80% detected concentrations in all tissues were excluded. Boxes indicate 25th, 50th and 75th percentiles and whiskers indicate 5th and 95th percentiles. Extreme values in the data sets are indicated as circles.

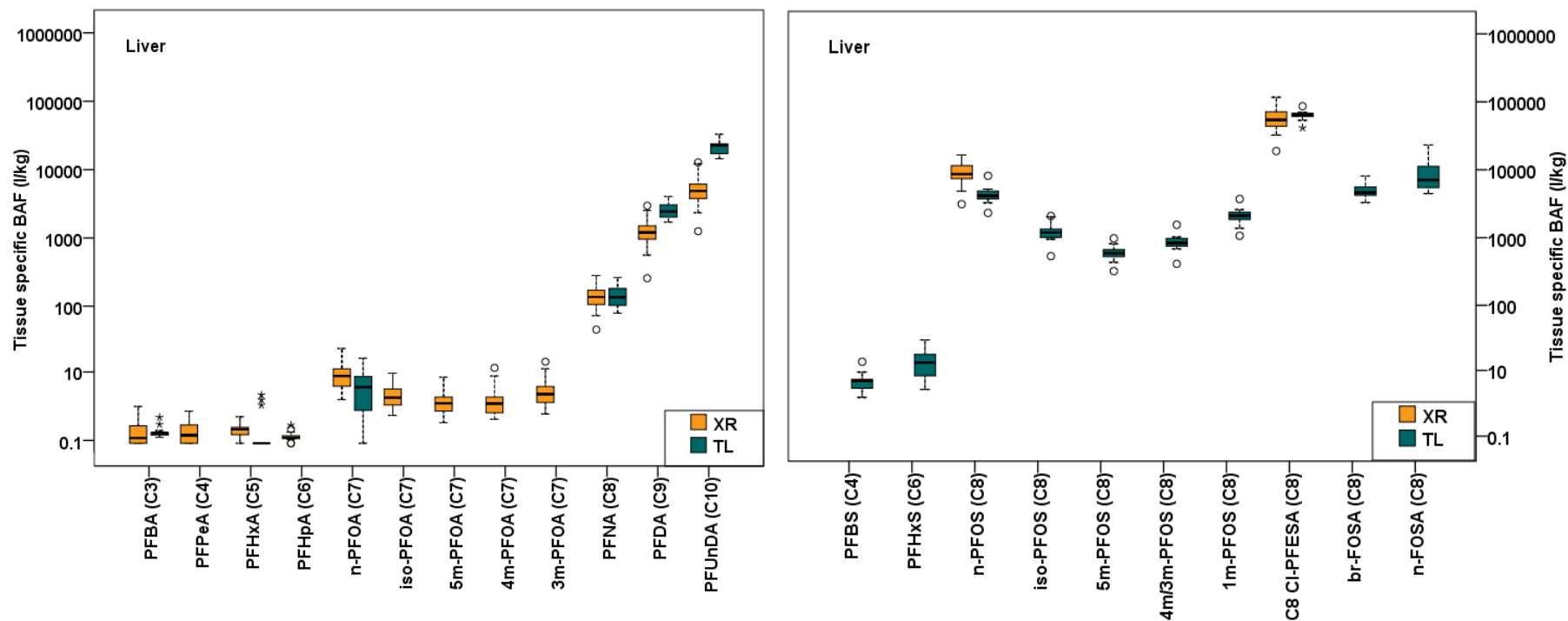


Figure S7. Tissue-specific BAF for liver with varying chain-length, isomeric structures and functional groups for XR (orange) and TL (blue). Data with <80% detected concentrations in all tissues were excluded. Boxes indicate 25th, 50th and 75th percentiles and whiskers indicate 5th and 95th percentiles. Extreme values in the data sets are indicated as circles.

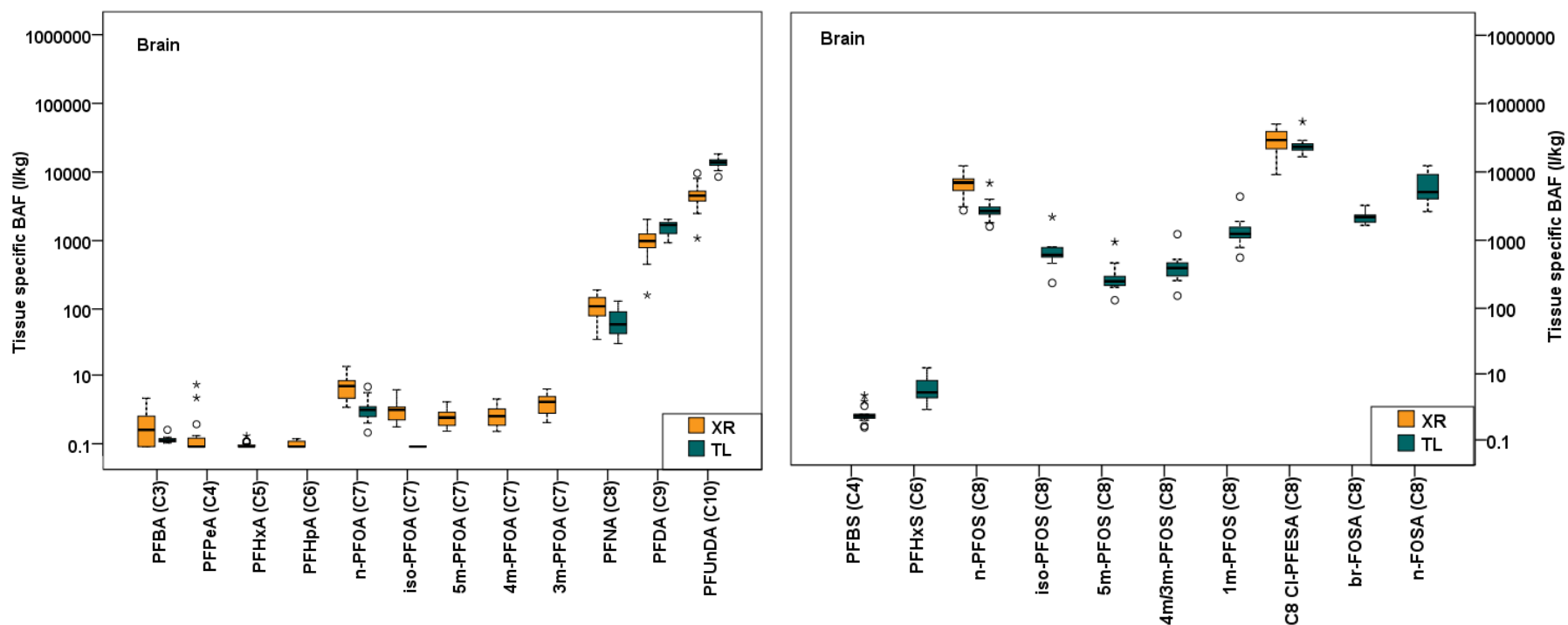


Figure S8. Tissue-specific BAF for brain with varying chain-length, isomeric structures and functional groups for XR (orange) and TL (blue). Data with <80% detected concentrations in all tissues were excluded. Boxes indicate 25th, 50th and 75th percentiles and whiskers indicate 5th and 95th percentiles. Extreme values in the data sets are indicated as circles.

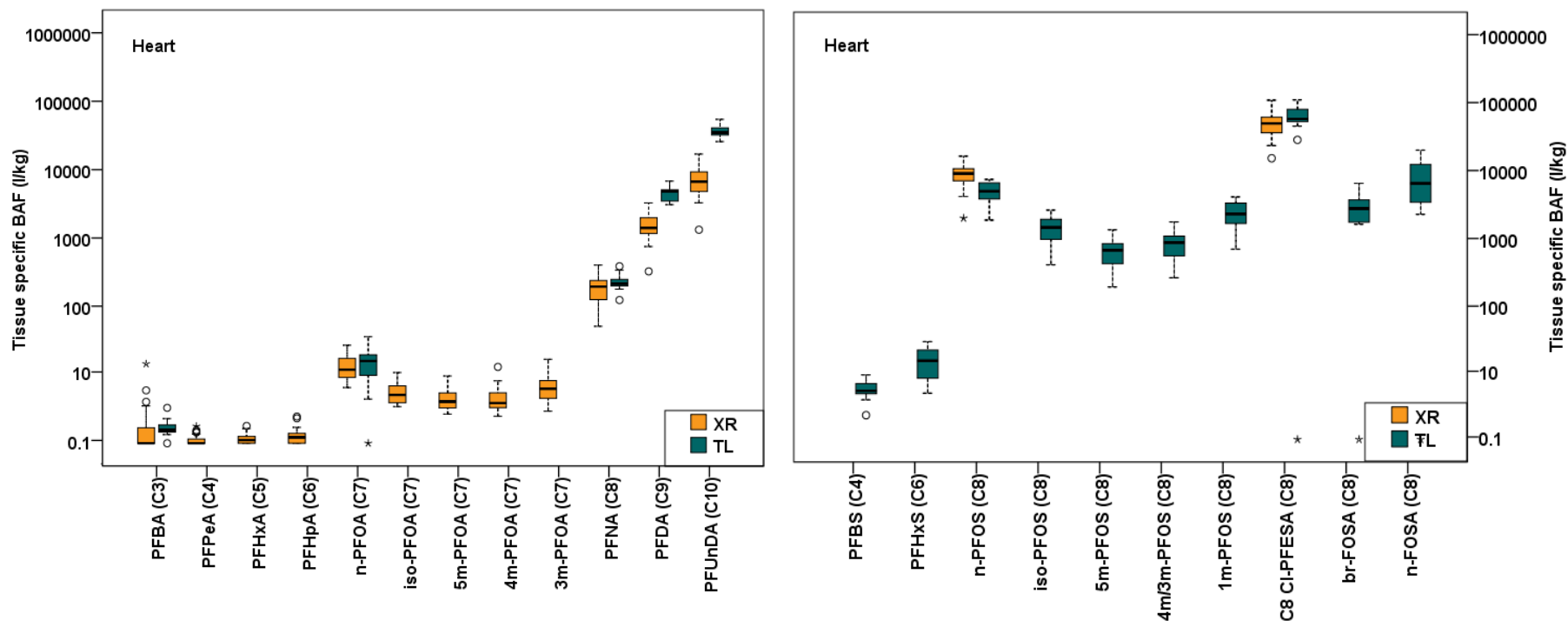


Figure S9. Tissue-specific BAF for heart with varying chain-length, isomeric structures and functional groups for XR (orange) and TL (blue). Data with <80% detected concentrations in all tissues were excluded. Boxes indicate 25th, 50th and 75th percentiles and whiskers indicate 5th and 95th percentiles. Extreme values in the data sets are indicated as circles.

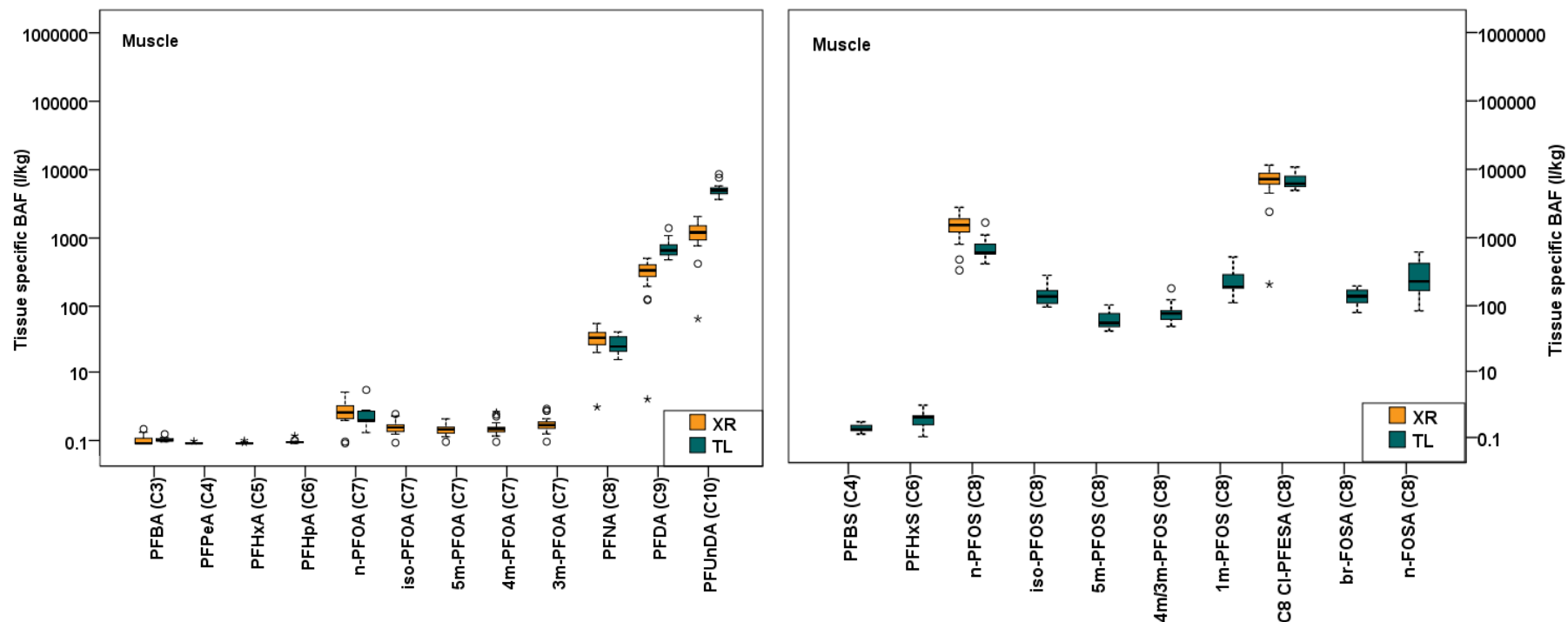


Figure S10. Tissue-specific BAF for muscle with varying chain-length, isomeric structures and functional groups for XR (orange) and TL (blue). Data with <80% detected concentrations in all tissues were excluded. Boxes indicate 25th, 50th and 75th percentiles and whiskers indicate 5th and 95th percentiles. Extreme values in the data sets are indicated as circles.

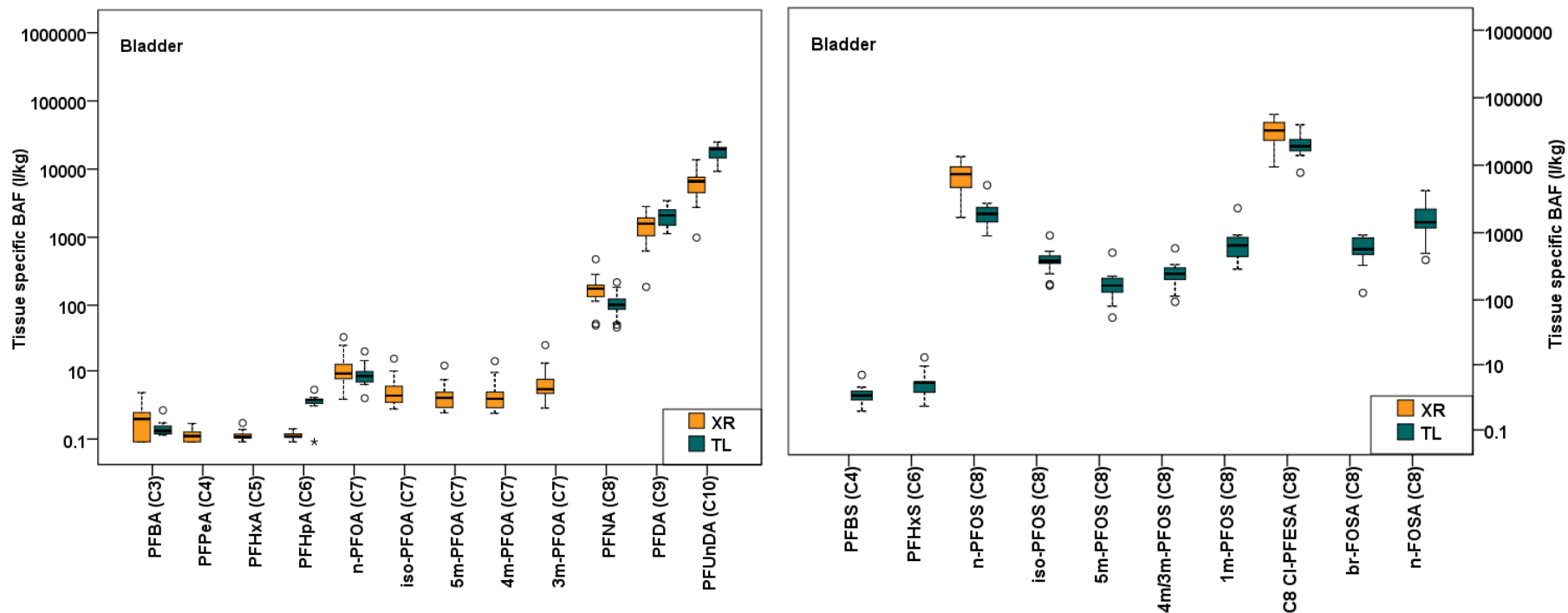


Figure S11. Tissue-specific BAF for bladder with varying chain-length, isomeric structures and functional groups for XR (orange) and TL (blue). Data with <80% detected concentrations in all tissues were excluded. Boxes indicate 25th, 50th and 75th percentiles and whiskers indicate 5th and 95th percentiles. Extreme values in the data sets are indicated as circles.

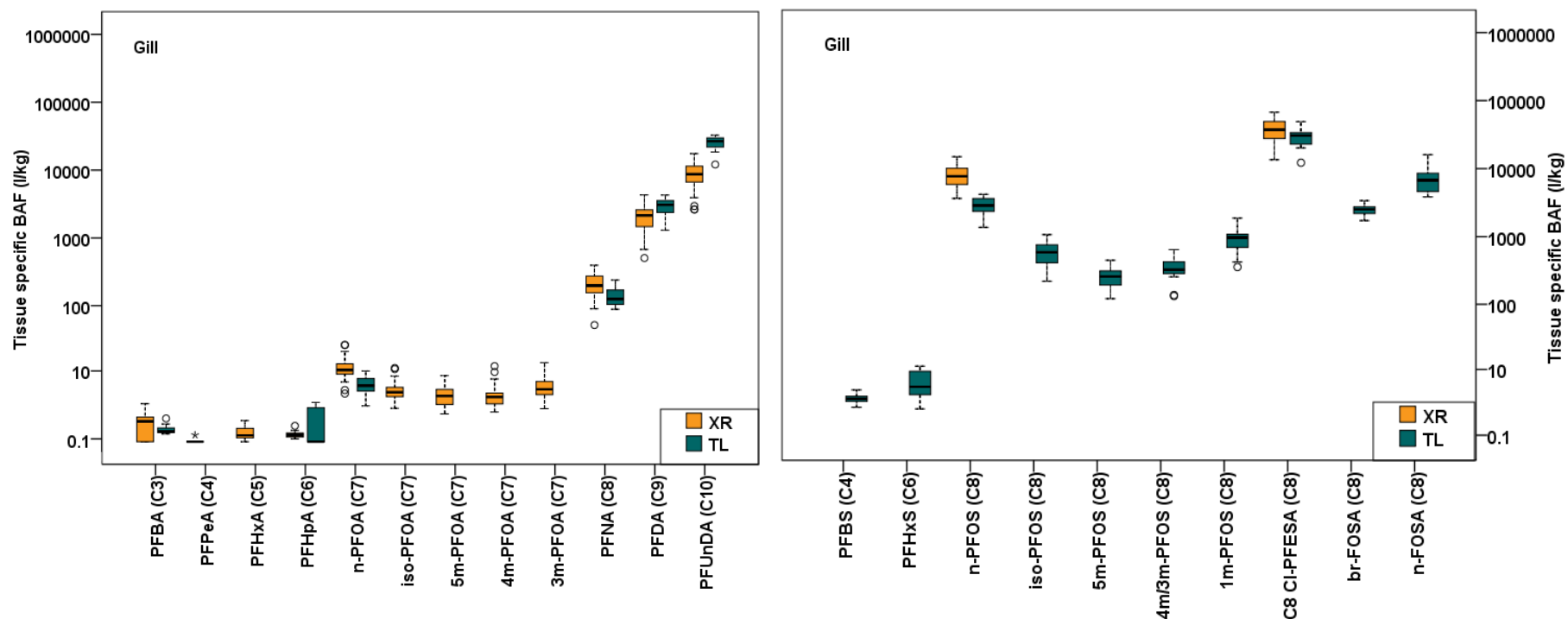


Figure S12. Tissue-specific BAF for gill with varying chain-length, isomeric structures and functional groups for XR (orange) and TL (blue). Data with <80% detected concentrations in all tissues were excluded. Boxes indicate 25th, 50th and 75th percentiles and whiskers indicate 5th and 95th percentiles. Extreme values in the data sets are indicated as circles.

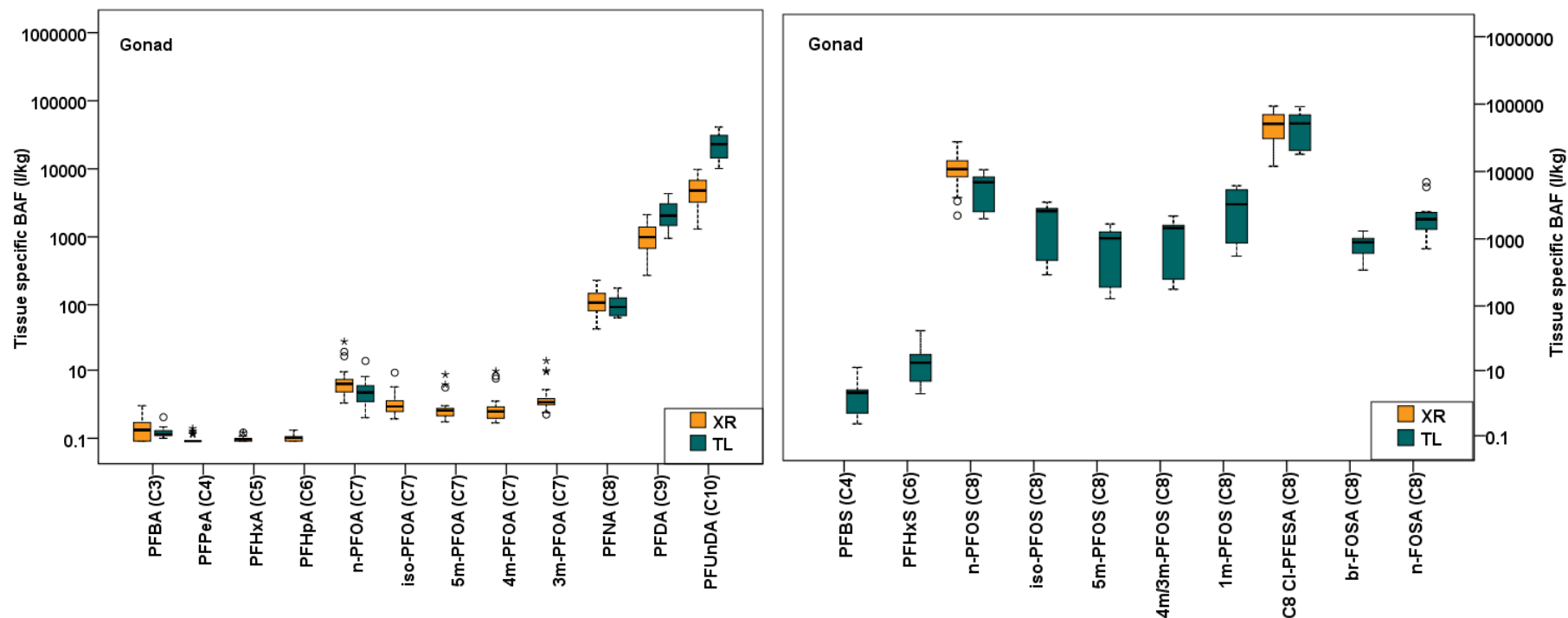


Figure S13. Tissue-specific BAF for gonads with varying chain-length, isomeric structures and functional groups for XR (orange) and TL (blue). Data with <80% detected concentrations in all tissues were excluded. Boxes indicate 25th, 50th and 75th percentiles and whiskers indicate 5th and 95th percentiles. Extreme values in the data sets are indicated as circles.