

Supporting Information

A bad start in life? Maternal transfer of mercury, legacy and emerging poly- and perfluoroalkyl substances in an Arctic seabird

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Internal standards used in PFAS analyses

Perfluoro-n-[2,3,4-¹³C₃]butanoic acid

Perfluoro-n-[¹³C₅]pentanoic acid

Perfluoro-n-[1,2,3,4,6-¹³C₅]hexanoic acid

Perfluoro-n-[1,2,3,4-¹³C₄]heptanoic acid

Perfluoro-n-[¹³C₈]octanoic acid

Perfluoro-n-[¹³C₉]nonanoic acid

Perfluoro-n-[1,2,3,4,5,6-¹³C₆]decanoic acid

Perfluoro-n-[1,2,3,4,5,6,7-¹³C₇]undecanoic acid

Perfluoro-n-[1,2-¹³C₂]dodecanoic acid

Perfluoro-n-[1,2-¹³C₂]tetradecanoic acid

Sodium perfluoro-1-[2,3,4-¹³C₃]butanesulfonate

Sodium perfluoro-1-[1,2,3-¹³C₃]hexanesulfonate

Sodium perfluoro-1-[¹³C₈]octanesulfonate

Perfluoro-1-[¹³C₈]octanesulfonamide

Sodium 1H,1H,2H,2H-perfluoro-1-[1,2-¹³C₂]-octane sulfonate

Sodium 1H,1H,2H,2H-perfluoro-1-[1,2-¹³C₂]-decane sulfonate

Table S1. List of targeted poly- and perfluoroalkyl substances (PFAS): their groups, abbreviations, chemical names, detection rates in females and eggs of black-legged kittiwakes, limits of detection in plasma and yolk and descriptive statistics (mean ± standard deviation *SD*; values <LOD not replaced by ½ LOD). Selected PFAS (i.e. detected in more than 70% of both samples and therefore used in analyses) are stressed in bold. PFAS considered as legacy compounds are in black, those considered as emerging are in grey.

Group	Abbreviation	Chemical name	Detection rate		Limit of detection (ng g ⁻¹ ww)	Mean ± <i>SD</i>	
			Females	Eggs		Females	Eggs
Perfluoroalkane sulfonic acids	PFBS	perfluorobutanesulfonic acid	0.0%	0.0%	0.10	na	na
	PFPS	perfluoropentanesulfonic acid	0.0%	0.0%	0.05	na	na
	PFHxS	perfluorohexanesulfonic acid	100.0%	100.0%	0.05	0.23 ± 0.09	0.24 ± 0.12
	PFHpS	perfluoroheptanesulfonic acid	0.0%	44.0%	0.08	na	0.10 ± 0.03
	brPFOS	branched perfluoroctanesulfonic acid	85.7%	100.0%	0.06	0.95 ± 0.32	2.53 ± 1.04
	linPFOS	linear perfluoroctanesulfonic acid	100.0%	100.0%	0.072	10.8 ± 4.70	25.4 ± 9.88
	PFNS	perfluorononanesulfonic acid	0.0%	0.0%	0.06	na	na
	PFDCS	perfluorodecanesulfonic acid	23.8%	84.0%	0.10	0.12 ± 0.02	0.28 ± 0.14
Perfluoroalkyl carboxylic acids	PFBA	perfluorobutanoic acid	0.0%	0.0%	0.08	na	na
	PFPA	perfluoropentanoic acid	0.0%	0.0%	0.08	na	na
	PFHxA	perfluorohexanoic acid	0.0%	4.0%	0.08	na	0.08 ± na
	PFHpA	perfluoroheptanoic acid	9.5%	24.0%	0.04	0.06 ± 0.00	0.07 ± 0.02
	PFOA	perfluoroctanoic acid	71.4%	96.0%	0.08	0.19 ± 0.13	0.23 ± 0.10
	PFNA	perfluorononanoic acid	100.0%	100.0%	0.03	1.06 ± 0.61	1.88 ± 0.95
	PFDCA	perfluorodecanoic acid	100.0%	100.0%	0.03	1.71 ± 0.89	3.39 ± 1.67
	PFUnA	perfluoroundecanoic acid	100.0%	100.0%	0.06	6.88 ± 3.21	16.2 ± 5.53
	PFDoA	perfluorododecanoic acid	95.2%	100.0%	0.03	1.81 ± 0.89	5.33 ± 1.57
	PFTriA	perfluorotridecanoic acid	100.0%	100.0%	0.07	7.80 ± 3.35	28.9 ± 7.99
	PFTeA	perfluorotetradecanoic acid	100.0%	100.0%	0.08	0.14 ± 0.60	5.80 ± 1.80
	PFHxDA	perfluorohexadecanoic acid	0.0%	84.0%	0.12	na	0.24 ± 0.08

Perfluoroalkane sulfonamido substances	MeFHxSA	methyl perfluorohexane sulphonamide	0.0%	0.0%	0.05	na	na
	FOSA	perfluoroctane sulfonamide	0.0%	0.0%	0.05	na	na
	MeFOSA	methylperfluoroctane sulfonamide	0.0%	0.0%	0.10	na	na
	EtFOSA	ethylperfluoroctane sulphonamide	0.0%	0.0%	0.10	na	na
	FOSAA	perfluoroctanesulfonamidoacetic acid	0.0%	0.0%	0.10	na	na
	MeFOSAA	methyl perfluoroctane sulfonamidoacetic acid	0.0%	0.0%	0.10	na	na
	EtFOSAA	ethyl perfluoroctane sulfonamidoacetic acid	0.0%	0.0%	0.10	na	na
fluorotelomer sulfonic acid	4:2 FTS	4:2 fluorotelomer sulfonic acid	0.0%	0.0%	0.05	na	na
	6:2 FTS	6:2 fluorotelomer sulfonic acid	0.0%	0.0%	0.05	na	na
	8:2 FTS	8:2 fluorotelomer sulfonic acid	0.0%	0.0%	0.10	na	na
	10:2 FTS	10:2 fluorotelomer sulfonic acid	0.0%	0.0%	1.00	na	na
fluorotelomer carboxylic acid	3:3 FTCA	3:3 fluorotelomer carboxylic acid	0.0%	0.0%	0.50	na	na
	5:3 FTCA	5:3 fluorotelomer carboxylic acid	0.0%	0.0%	0.10	na	na
	7:3 FTCA	7:3 fluorotelomer carboxylic acid	0.0%	84.0%	0.10	na	0.21 ± 0.09
Fluoro alkyl ether compo	F-53B	6:2 and 8:2 chlorinated polyfluorinated ether sulfonate	0.0%	0.0%	0.10	na	na
	ADONA	dodecafluoro-3H-4,8-dioxanonanoate	0.0%	4.0%	0.10	na	0.11 ± na
	Gen-X	hexafluoropropylene oxide dimer acid	0.0%	0.0%	1.00	na	na

Table S2. Descriptive statistics (mean \pm standard deviation SD , median and range *min-max*) for PFAS detected in more than 70% of the samples concentrations in eggs only (ng g^{-1} ww) in plasma and egg yolk and albumen of black-legged kittiwakes from Svalbard.

First laid eggs			Second laid eggs				
	Mean \pm SD	Median	Min-max		Mean \pm SD	Median	Min-max
PFDcS	0.32 ± 0.15	0.26	0.13 - 0.64		0.22 ± 0.08	0.2	0.11 - 0.37
PFHxDA	0.29 ± 0.07	0.29	0.16 - 0.38		0.19 ± 0.04	0.2	0.13 - 0.24
7:3 FTCA	0.25 ± 0.09	0.23	0.11 - 0.42		0.16 ± 0.05	0.15	0.10 - 0.25

Figure S1. Chromatograms of the sample (a), the standard (b), the blank (c) and the standard reference material (d) for the measurement of ADONA in black-legged kittiwake eggs; two ion traces are provided for ADONA and one for the internal standard (^{13}C -PFOA).

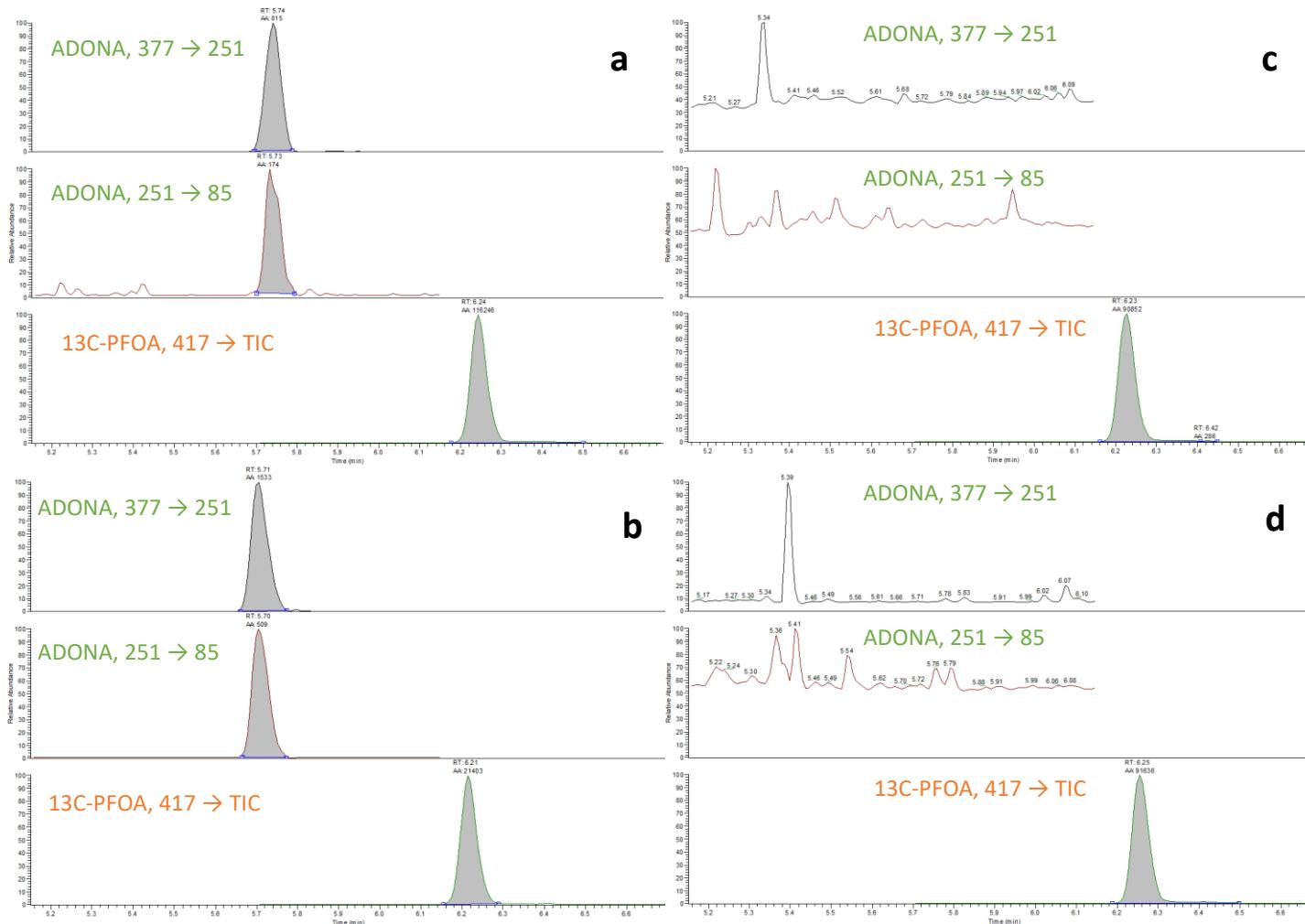


Table S3. Model selections for the relationship between PFAS and biological variables in black-legged kittiwake eggs, based on the lowest second-order Akaike's Information Criterion corrected for small sample sizes (AICc); the predicting variables were the laying date, the egg mass, the rank of the eggs in the laying order (Egg number) as well as both interactions between the laying date or the egg mass and the egg number. The most parsimonious model is given in bold. AICcwt: Akaike's weight; ΔAICc: difference between the model with the smallest AICc-value and the model of interest (*i*).

PFHxS

	Laying date	Egg mass	Egg number	Laying date : Egg number	Egg mass : Egg number	K	AICc	AICcwt	ΔAICc
mod13						3	-37.53	0.26	0.00
mod10	X					4	-37.24	0.22	0.29
mod5	X		X	X		6	-37.12	0.21	0.41
mod12			X			4	-35.22	0.08	2.31
mod11		X				4	-34.82	0.07	2.71
mod8	X		X			5	-34.23	0.05	3.30
mod7	X	X				5	-34.09	0.05	3.44
mod2	X	X	X	X		7	-33.53	0.03	4.00
mod9		X	X			5	-32.07	0.02	5.46
mod4	X	X	X			6	-30.74	0.01	6.79
mod1	X	X	X	X	X	8	-29.54	0.00	7.99
mod6		X	X		X	6	-28.56	0.00	8.97
mod3	X	X	X		X	7	-26.81	0.00	10.71

brPFOS

	Laying date	Egg mass	Egg number	Laying date : Egg number	Egg mass : Egg number	K	AICc	AICcw _t	ΔAICc
mod12			X			4	62.22	0.59	0.00
mod8	X		X			5	64.79	0.16	2.57
mod9		X	X			5	65.05	0.14	2.83
mod5	X		X	X		6	67.60	0.04	5.37
mod4	X	X	X			6	68.18	0.03	5.96
mod6		X	X		X	6	68.55	0.02	6.32
mod2	X	X	X	X		7	71.25	0.01	9.03
mod3	X	X	X		X	7	72.09	0.00	9.87
mod1	X	X	X	X	X	8	75.57	0.00	13.35
mod7	X	X				5	76.97	0.00	14.75
mod13						3	78.49	0.00	16.27
mod11			X			4	80.52	0.00	18.30
mod10	X					4	80.64	0.00	18.42

linPFOS

	Laying date	Egg mass	Egg number	Laying date : Egg number	Egg mass : Egg number	K	AICc	AICcw _t	ΔAICc
mod12			X			4	170.51	0.54	0.00
mod8	X		X			5	172.15	0.24	1.64
mod9		X	X			5	173.67	0.11	3.16
mod4	X	X	X			6	175.64	0.04	5.13
mod5	X		X	X		6	175.65	0.04	5.14
mod6		X	X		X	6	177.17	0.02	6.66
mod3	X	X	X		X	7	179.56	0.01	9.04
mod2	X	X	X	X		7	179.56	0.01	9.05
mod1	X	X	X	X	X	8	183.96	0.00	13.45
mod13						3	188.70	0.00	18.19
mod7	X	X				5	189.17	0.00	18.65
mod11			X			4	189.45	0.00	18.94
mod10	X					4	190.43	0.00	19.92

PFOA

	Laying date	Egg mass	Egg number	Laying date : Egg number	Egg mass : Egg number	K	AICc	AICcwt	ΔAICc
mod13						3	-46.46	0.23	0.00
mod4	X	X	X			6	-46.39	0.22	0.06
mod12				X		4	-45.16	0.12	1.30
mod8	X			X		5	-44.78	0.10	1.68
mod9		X	X			5	-44.65	0.09	1.81
mod11		X				4	-43.92	0.06	2.54
mod10	X					4	-43.66	0.06	2.80
mod2	X	X	X	X		7	-42.53	0.03	3.93
mod3	X	X	X		X	7	-42.47	0.03	3.98
mod5	X		X	X		6	-41.28	0.02	5.18
mod6		X	X		X	6	-41.17	0.02	5.29
mod7	X	X				5	-40.82	0.01	5.64
mod1	X	X	X	X	X	8	-38.13	0.00	8.33

PFNA

	Laying date	Egg mass	Egg number	Laying date : Egg number	Egg mass : Egg number	K	AICc	AICcwt	ΔAICc
mod12			X			4	60.17	0.41	0.00
mod13						3	62.66	0.12	2.49
mod8	X		X			5	62.85	0.11	2.68
mod9		X	X			5	63.30	0.09	3.14
mod11		X				4	63.48	0.08	3.31
mod10	X					4	63.81	0.07	3.65
mod5	X		X	X		6	64.39	0.05	4.22
mod7	X	X				5	65.35	0.03	5.18
mod4	X	X	X			6	66.33	0.02	6.17
mod6		X	X		X	6	66.54	0.02	6.37
mod2	X	X	X	X		7	68.30	0.01	8.14
mod3	X	X	X		X	7	70.04	0.00	9.87
mod1	X	X	X	X	X	8	71.96	0.00	11.79

PFDcA

	Laying date	Egg mass	Egg number	Laying date : Egg number	Egg mass : Egg number	K	AICc	AICc _{wt}	ΔAICc
mod12			X			4	82.43	0.54	0.00
mod9		X	X			5	85.26	0.13	2.84
mod8	X		X			5	85.32	0.13	2.89
mod5	X		X	X		6	86.51	0.07	4.09
mod10	X					4	88.61	0.02	6.18
mod4	X	X	X			6	88.62	0.02	6.19
mod6		X	X		X	6	88.72	0.02	6.30
mod7	X	X				5	89.03	0.02	6.60
mod11		X				4	89.93	0.01	7.50
mod2	X	X	X	X		7	90.23	0.01	7.80
mod13						3	92.19	0.00	9.76
mod3	X	X	X		X	7	92.49	0.00	10.07
mod1	X	X	X	X	X	8	94.27	0.00	11.85

PFUnA

	Laying date	Egg mass	Egg number	Laying date : Egg number	Egg mass : Egg number	K	AICc	AICc _{wt}	ΔAICc
mod12			X			4	138.50	0.43	0.00
mod8	X		X			5	139.42	0.27	0.92
mod9		X	X			5	140.80	0.14	2.30
mod4	X	X	X			6	142.39	0.06	3.89
mod5	X		X	X		6	142.84	0.05	4.34
mod6		X	X		X	6	144.31	0.02	5.81
mod2	X	X	X	X		7	146.17	0.01	7.67
mod3	X	X	X		X	7	146.30	0.01	7.80
mod1	X	X	X	X	X	8	150.55	0.00	12.05
mod7	X	X				5	156.77	0.00	18.27
mod11		X				4	158.30	0.00	19.80
mod13						3	159.50	0.00	21.00
mod10	X					4	160.91	0.00	22.41

PFDa

	Laying date	Egg mass	Egg number	Laying date : Egg number	Egg mass : Egg number	K	AICc	AICcwt	ΔAICc
mod8	X		X			5	78.49	0.51	0.00
mod12			X			4	80.36	0.20	1.86
mod5	X		X	X		6	81.47	0.11	2.97
mod4	X	X	X			6	81.99	0.09	3.49
mod9		X	X			5	83.45	0.04	4.96
mod3	X	X	X		X	7	84.97	0.02	6.47
mod2	X	X	X	X		7	85.38	0.02	6.89
mod6		X	X		X	6	86.03	0.01	7.53
mod1	X	X	X	X	X	8	88.38	0.00	9.88
mod13						3	99.39	0.00	20.89
mod11		X				4	101.16	0.00	22.66
mod10	X					4	102.08	0.00	23.58
mod7	X	X				5	104.21	0.00	25.71

PFTriA

	Laying date	Egg mass	Egg number	Laying date : Egg number	Egg mass : Egg number	K	AICc	AICcwt	ΔAICc
mod8	X		X			5	161.79	0.37	0.00
mod12			X			4	162.14	0.31	0.35
mod5	X		X	X		6	164.45	0.10	2.65
mod9		X	X			5	164.73	0.09	2.94
mod4	X	X	X			6	165.12	0.07	3.33
mod6		X	X		X	6	167.57	0.02	5.78
mod2	X	X	X	X		7	168.12	0.02	6.32
mod3	X	X	X		X	7	168.39	0.01	6.60
mod1	X	X	X	X	X	8	171.35	0.00	9.56
mod13						3	180.97	0.00	19.18
mod11		X				4	182.00	0.00	20.21
mod10	X					4	183.82	0.00	22.03
mod7	X	X				5	184.66	0.00	22.87

PFTeA

	Laying date	Egg mass	Egg number	Laying date : Egg number	Egg mass : Egg number	K	AICc	AICcwt	ΔAICc
mod12			X			4	89.20	0.44	0.00
mod8	X		X			5	90.17	0.27	0.97
mod9		X	X			5	92.15	0.10	2.95
mod5	X		X	X		6	92.52	0.08	3.32
mod4	X	X	X			6	93.64	0.05	4.44
mod6		X	X		X	6	94.83	0.03	5.63
mod2	X	X	X	X		7	96.37	0.01	7.17
mod3	X	X	X		X	7	96.73	0.01	7.54
mod1	X	X	X	X	X	8	99.18	0.00	9.98
mod13						3	106.09	0.00	16.89
mod11			X			4	106.72	0.00	17.52
mod10	X					4	108.61	0.00	19.41
mod7	X	X				5	108.64	0.00	19.44

Table S4. Model selections for maternal transfer ratios of PFAS in black-legged kittiwakes, based on the lowest second-order Akaike's Information Criterion corrected for small sample sizes (AICc); the predicting variables were the carbon chain length of PFCAs compounds, the rank of the eggs in the laying order (Egg number) as well as the interaction between these variables; see Table S3 for additional information.

	Carbon chain length	Egg number	Carbon chain length : Egg number	K	AICc	AICc_{wt}	ΔAICc
mod1	X	X	X	6	130.12	0.98	0.00
mod2	X	X		5	138.39	0.02	8.27
mod3	X			4	165.48	0.00	35.36
mod4		X		4	254.96	0.00	124.84
mod5				3	267.96	0.00	137.85

Table S5. Model selections for maternal transfer of PFAS in black-legged kittiwakes, based on the lowest second-order Akaike's Information Criterion corrected for small sample sizes (AICc); the predicting variables were the female contamination and the number of the eggs in the laying order (Egg number); see Table S3 for additional information.

PFHxS

	Females contamination	Egg number	K	AICc	AICcwt	ΔAICc
mod2	X		4	-44.55	0.77	0.00
mod1	X	X	5	-45.12	0.23	2.43
mod4			3	-37.53	0.01	10.03
mod3		X	4	-35.22	0.00	12.33

brPFOS

	Females contamination	Egg number	K	AICc	AICcwt	ΔAICc
mod1	X	X	5	56.07	0.96	0.00
mod3		X	4	62.22	0.04	6.15
mod2	X		4	71.59	0.00	15.52
mod4			3	78.49	0.00	22.42

linPFOS

	Females contamination	Egg number	K	AICc	AICcwt	ΔAICc
mod1	X	X	5	162.91	0.98	0.00
mod3		X	4	170.51	0.02	7.60
mod2	X		4	182.11	0.00	19.20
mod4			3	188.70	0.00	25.79

PFOA

	Females contamination	Egg number	K	AICc	AICcwt	Δ AICc
mod4			3	-46.46	0.35	0.00
mod2	X		4	-46.34	0.33	0.12
mod3		X	4	-45.16	0.18	1.30
mod1	X	X	5	-44.76	0.15	1.70

PFNA

	Females contamination	Egg number	K	AICc	AICcwt	Δ AICc
mod1	X	X	5	52.93	0.78	0.00
mod2	X		4	55.76	0.19	2.84
mod3		X	4	60.17	0.02	7.24
mod4	X	X	3	62.66	0.01	9.73

PFDeA

	Females contamination	Egg number	K	AICc	AICcwt	Δ AICc
mod1	X	X	5	73.19	0.99	0.00
mod3		X	4	82.43	0.01	9.23
mod2	X		4	83.05	0.00	10.76
mod4			3	92.19	0.00	19.00

PFUnA

	Females contamination	Egg number	K	AICc	AICcwt	Δ AICc
mod1	X	X	5	136.09	0.77	0.00
mod3		X	4	138.50	0.23	2.41
mod2	X		4	158.19	0.00	22.10
mod4			3	159.50	0.00	23.41

PFDoA

	Females contamination	Egg number	K	AICc	AICcwt	ΔAICc
mod1	X	X	5	80.30	0.51	0.00
mod3		X	4	80.36	0.49	0.06
mod4			3	99.39	0.00	19.09
mod2	X		4	99.77	0.00	19.48

PFTriA

	Females contamination	Egg number	K	AICc	AICcwt	ΔAICc
mod1	X	X	5	157.85	0.90	0.00
mod3		X	4	162.14	0.10	4.29
mod2	X		4	179.73	0.00	21.88
mod4			3	180.97	0.00	23.12

PFTeA

	Females contamination	Egg number	K	AICc	AICcwt	ΔAICc
mod1	X	X	5	86.33	0.81	0.00
mod3		X	4	89.20	0.19	2.87
mod2	X		4	104.74	0.00	18.41
mod4			3	106.09	0.00	19.77