Relationship Between Perfluoroalkyl Acids in Human Serum and Sjogren's Syndrome: A Case–Control Study of Populations in Hangzhou, China

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Table S1. Detailed liquid and mass spectrometry conditions

Mobile phase	Milli-Q water (containing 2 mM ammonium acetate) (A) and methanol (B)			
Gradient	Time (min)	Flow rate (mL/min)	A (%)	B (%)
	0.0		5	95
	1.0		25	75
	5.0		75	25
	9.0	0.3	90	10
	10.0		90	10
	10.1		5	95
	12.0		5	95
Injection volume	2 μL			
Analyzed substances	Parent ion	Daughter ion	Cone voltage (V)	Collision energy (V)
PFHpA	363	319	30	10
PFOA	413	369	30	10
PFNA	463	419	30	10
PFDA	513	469	12	10
PFUDA	563	519	30	10
PFDoA	613	569	18	10
PFTrDA	663	619	20	12
PFTeDA	713	669	20	12
PFBS	299	80	40	30
PFHxS	399	80	45	33
PFOS	499	99	30	38

Table S2. The results of the normal distribution test for the concentrations of perfluoroalkyl acids

Target compounds	K-S test p-value[a]			S-W test p-value[b]		
	Total	Case	Control	Total	Case	Control
PFOA	<0.001	<0.001	<0.001	<0.001	<0.001	<0.001
PFNA	<0.001	<0.001	<0.001	<0.001	<0.001	<0.001
PFDA	<0.001	<0.001	<0.001	<0.001	<0.001	<0.001
PFUDA	<0.001	<0.001	<0.001	<0.001	<0.001	<0.001
PFDoA	<0.001	<0.001	<0.001	<0.001	<0.001	<0.001
PFTrDA	<0.001	<0.001	<0.001	<0.001	<0.001	<0.001
PFHxS	<0.001	<0.001	<0.001	<0.001	<0.001	<0.001
PFOS	<0.001	<0.001	<0.001	<0.001	<0.001	<0.001

Note: The normal distribution tests for the concentrations of perfluoroalkyl acids in serum were performed separately using Kolmogorov-Smirnov test and Shapiro—Wilk test.
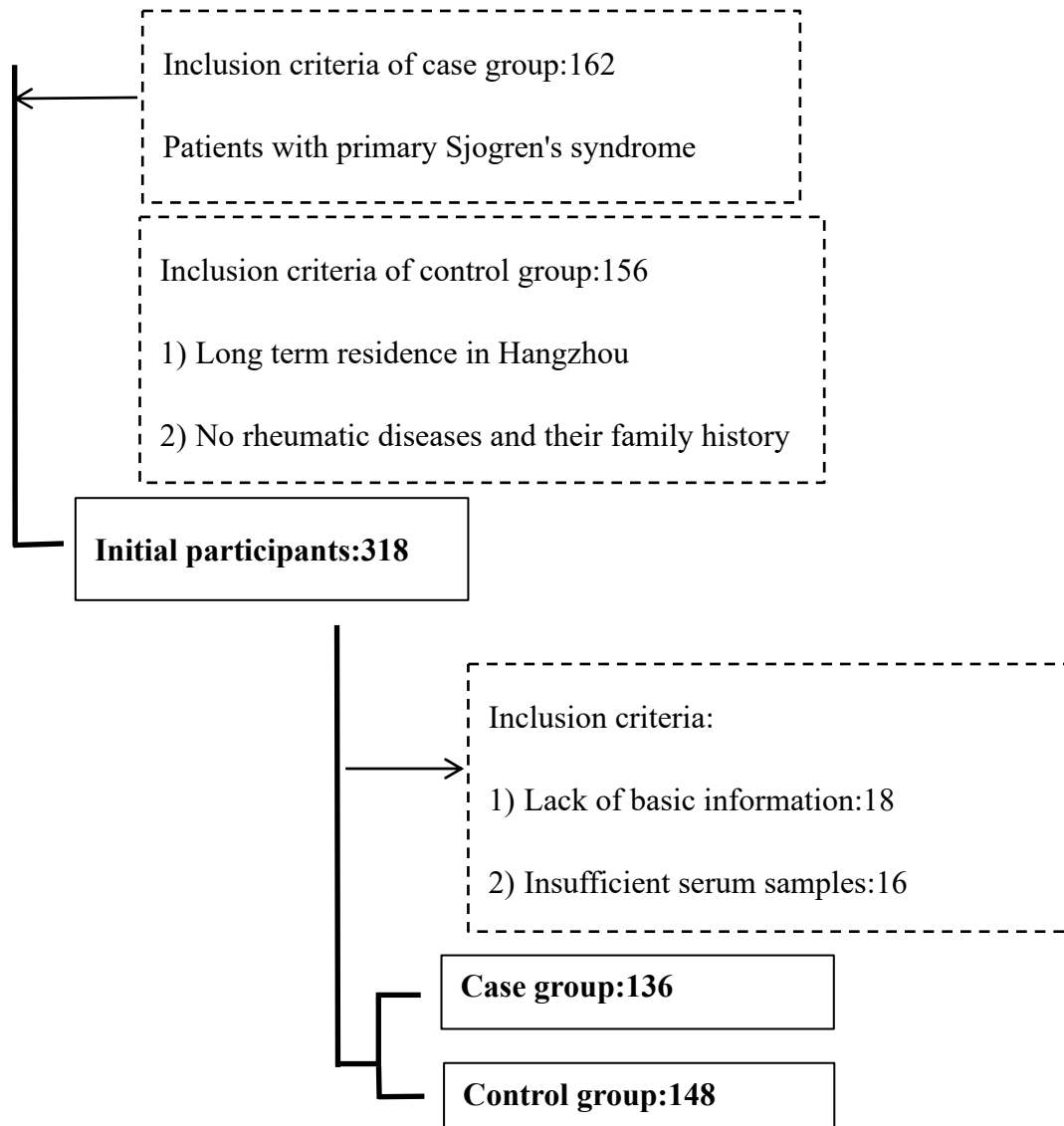
Table S3. The concentration of PFAAs in serum

Target PFAAs	Case					Control				
	mean ±SD	25	50	75	Range	mean ±SD	25	50	75	Range
PFOA	35.19 ±38.62	10.75	20.12	38.96	0.07~ 189.62	37.85 ±30.02	16.10	27.30	51.89	<LOD~ 128.09
PFNA	2.75 ±2.60	1.35	1.92	3.37	0.33~ 23.90	3.14 ±2.58	1.44	2.67	4.05	<LOD~ 20.80
PFDA	2.44 ±2.49	1.00	1.68	2.98	0.16~ 18.15	2.66 ±2.55	1.20	1.88	3.12	0.16~ 15.40
PFUDA	1.63 ±1.34	0.78	1.28	2.02	<LOD~ 9.24	1.99 ±1.68	0.88	1.47	2.37	0.07~ 9.69
PFDoA	0.23 ±0.22	0.10	0.17	0.26	<LOD~ 1.44	0.21 ±0.18	0.10	0.15	0.28	<LOD~ 0.91
PFTrDA	0.28 ±0.22	0.13	0.22	0.35	<LOD~ 1.47	0.36 ±0.26	0.18	0.30	0.49	<LOD~ 1.66
PFHxS	3.14 ±3.37	0.96	1.90	3.91	0.10~ 19.18	3.50 ±5.15	1.26	2.51	4.30	0.11~ 57.23
PFOS	14.36 ±15.73	3.80	8.80	20.02	<LOD~ 75.04	15.26 ±13.64	5.92	11.63	19.26	<LOD~ 66.28

Note: Concentration unit: ng/mL. <LOD: The concentration is lower than the detection limit, 0.05 ng/mL.

Table S4. Multiple regression analysis of concentrations of perfluoroalkyl acids and immune and inflammatory markers in the case group

	PFOA (95% CI)	PFTrDA (95% CI)
CRP	-4.05 (-5.56,-2.54)*	0.44(-1.75,2.63)
ESR	-7.83(-12.36,-3.30)	-2.79(-9.34,3.76)
IgG	-0.43(-1.24,0.38)	-0.85(-2.02,0.32)
IgA	8.76(3.89,13.63)	0.98(-6.06,8.02)
IgM	0.00(-0.13,0.13)	0.26(0.07,0.45)
ANA	13.77(-0.93,28.47)	19.1(-2.16,40.36)
Anti-**Ro52**	-2.89(-6.8,1.02)	-4.01(-9.66,1.64)
Anti-**SSA**	5.51(-0.01,11.03)	-8.33(-16.32,-0.34)
Anti-**SSB**	6.23(2.84,9.62)	-2.73(-7.63,2.17)

Note: CI, confidence interval. Adjusted by age, BMI, smoking and drinking habits, education level, occupation, income, parity and dietary habits. All concentrations of perfluoroalkyl acids (ng/mL) and immune and inflammatory markers concentrations were log-transformed. *p-value < 0.05, **p-value ≤ 0.01.

Inclusion criteria of case group:162

Patients with primary Sjogren's syndrome

Inclusion criteria of control group:156

1) Long term residence in Hangzhou

2) No rheumatic diseases and their family history

Initial participants:318

Inclusion criteria:

1) Lack of basic information:18

2) Insufficient serum samples:16

Case group:136

Control group:148

Figure S1. The specific inclusion and exclusion criteria for the case and control groups