Supplementary Information

Interaction Rule and Mechanism of Perfluoroalkyl Sulfonates contained different carbon chain with Human Serum Albumin

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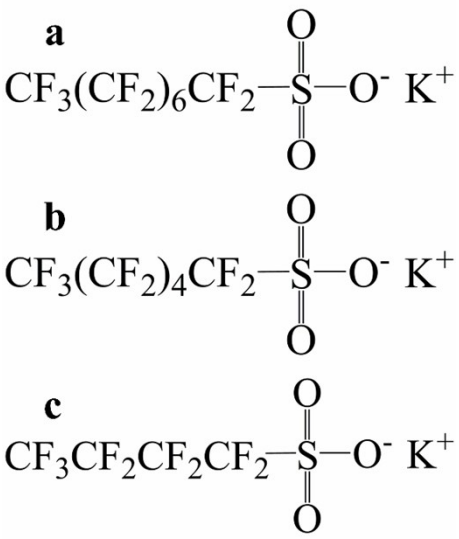
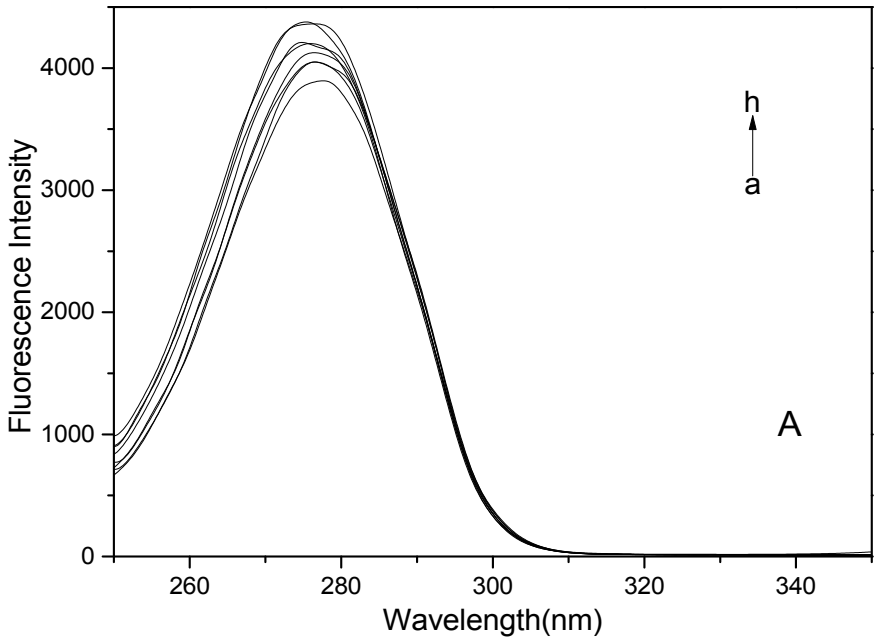


Fig. S1 Chemical structure of perfluorooctane sulfonate, perfluorohexane sulfonate and perfluorobutane sulfonate: a (potassium salt of PFOS), b (potassium salt of PFHS), c (potassium salt of PFBS).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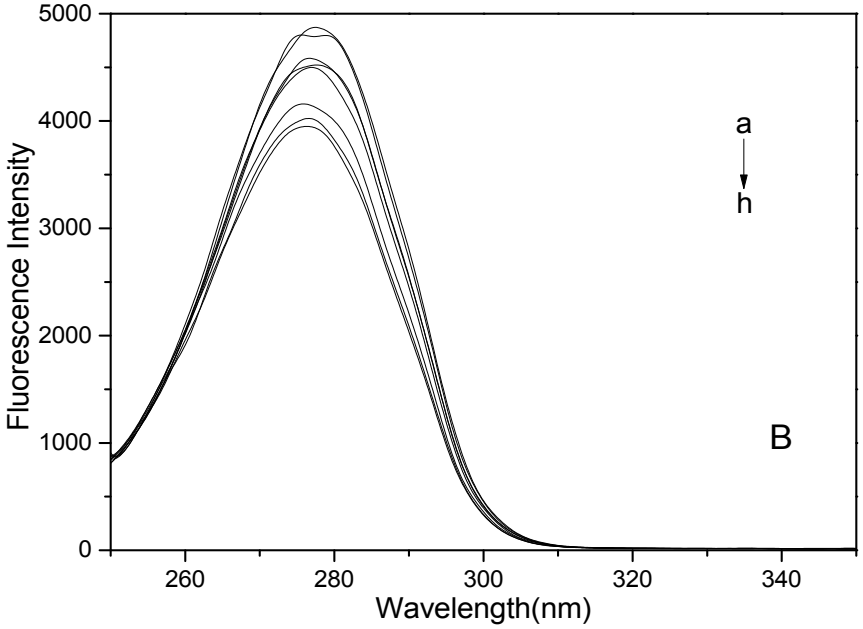
4000
260
280
300
320
340
Wavelength(nm)
h
a
A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Wavelength(nm)
a
h
B

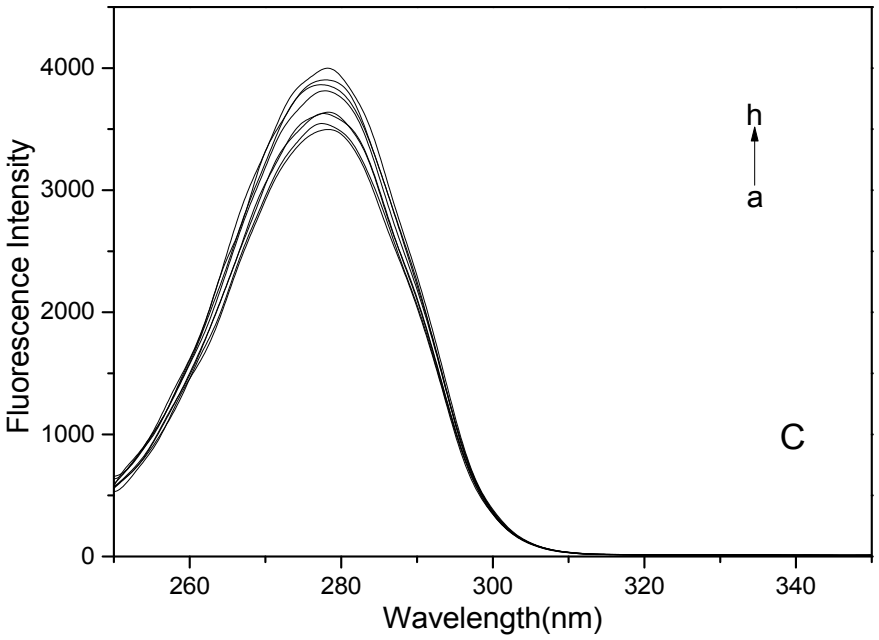
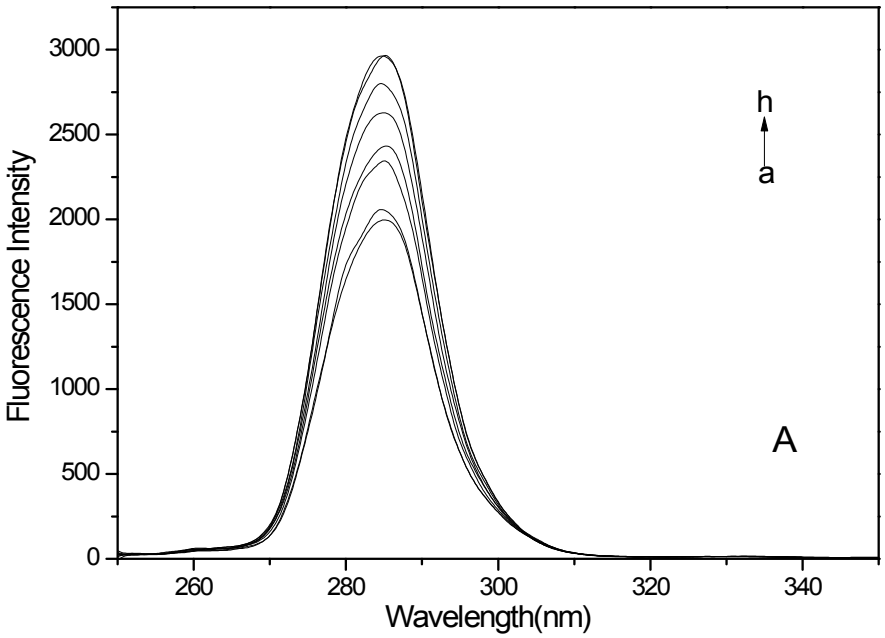


Fig. S2 Synchronous fluorescence spectra of HSA with different concentrations of PFASs. Conditions: HSA: 1×10^{-6} mol/L; A (PFOS), B (PFHS) and C (PFBS) (a-h): 0, 2×10^{-6}, 6×10^{-6}, 1×10^{-5}, 3×10^{-5}, 5×10^{-5}, 7×10^{-5}, 1×10^{-4} mol/L; pH=7.4; T=298 K; $\Delta\lambda$=60 nm.


Fluorescence Intensity
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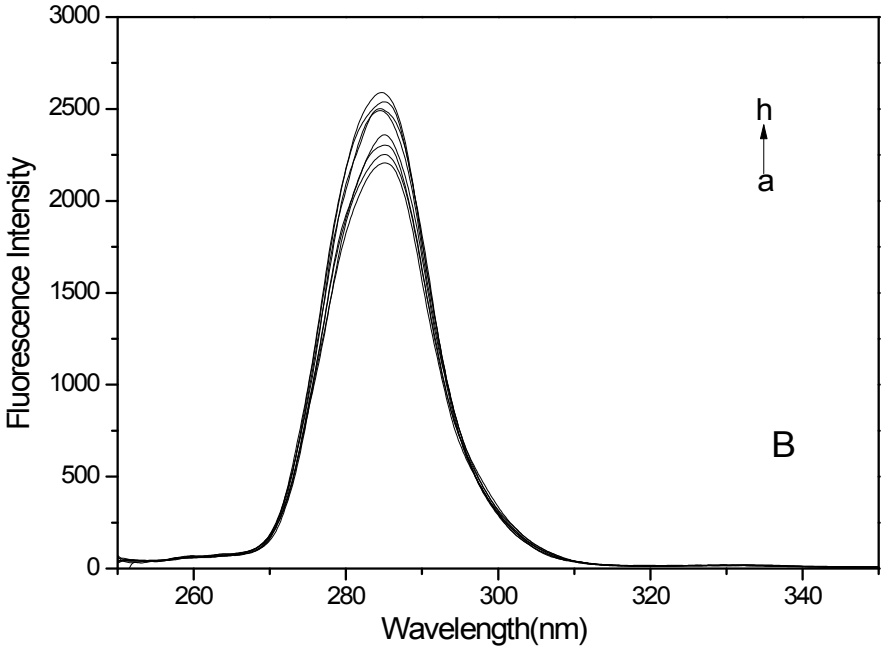
1500
1000
500
0
260
280
300
320
340
Wavelength(nm)
h
a
A


Fluorescence Intensity
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2000
1500
1000
500
0
260
280
300
320
340
Wavelength(nm)
h
a
B

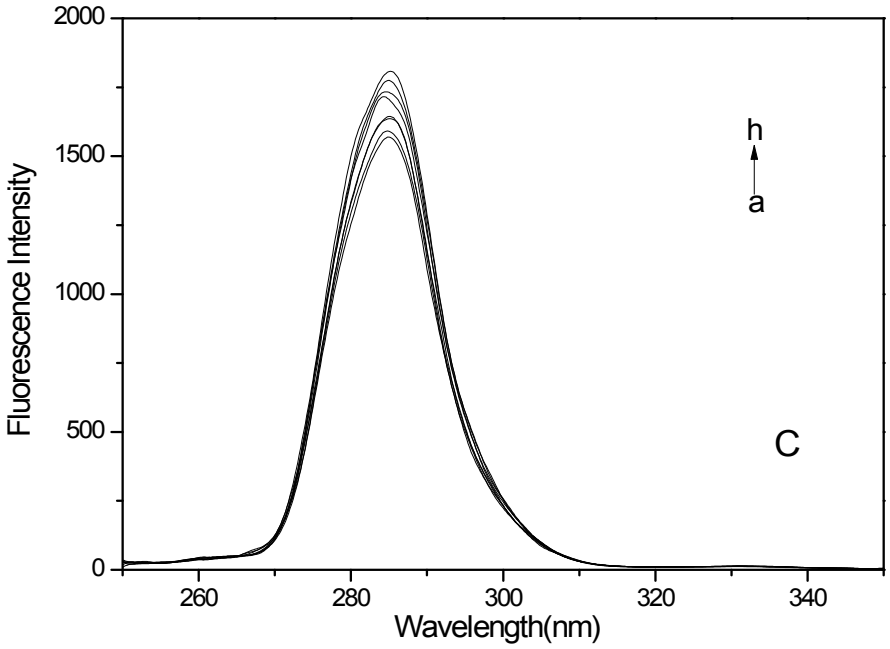
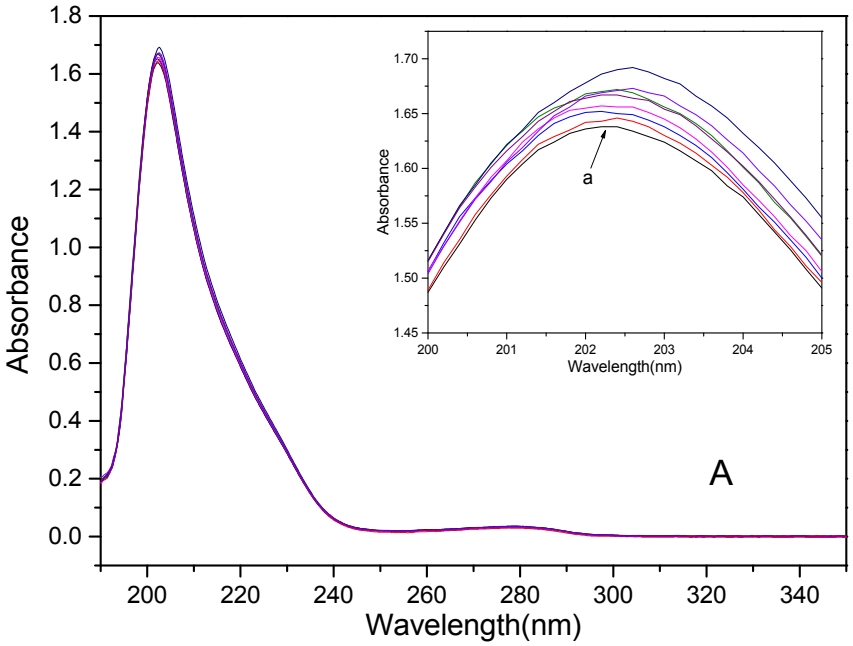
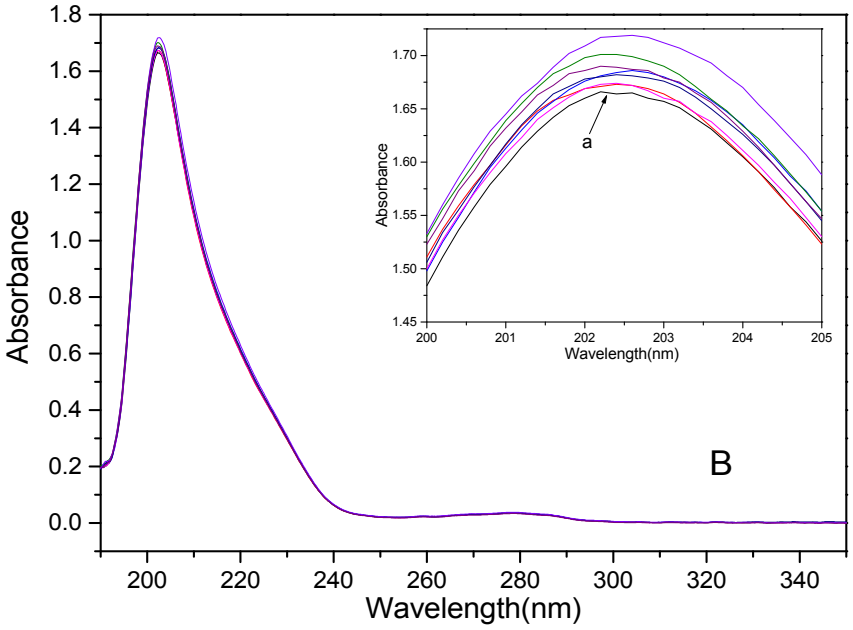


Fig. S3 Synchronous fluorescence spectra of HSA with different concentrations of PFASs. Conditions: HSA: 1×10^{-6} mol/L; A (PFOS), B (PFHS) and C (PFBS) (a-h): 0, 2×10^{-6}, 6×10^{-6}, 1×10^{-5}, 3×10^{-5}, 5×10^{-5}, 7×10^{-5}, 1×10^{-4} mol/L; pH=7.4; T=298 K; $\Delta\lambda$=15 nm.


Absorbance
Wavelength(nm)
A
a
Absorbance
Wavelength(nm)


Absorbance
Wavelength(nm)
B
a
Absorbance
Wavelength(nm)

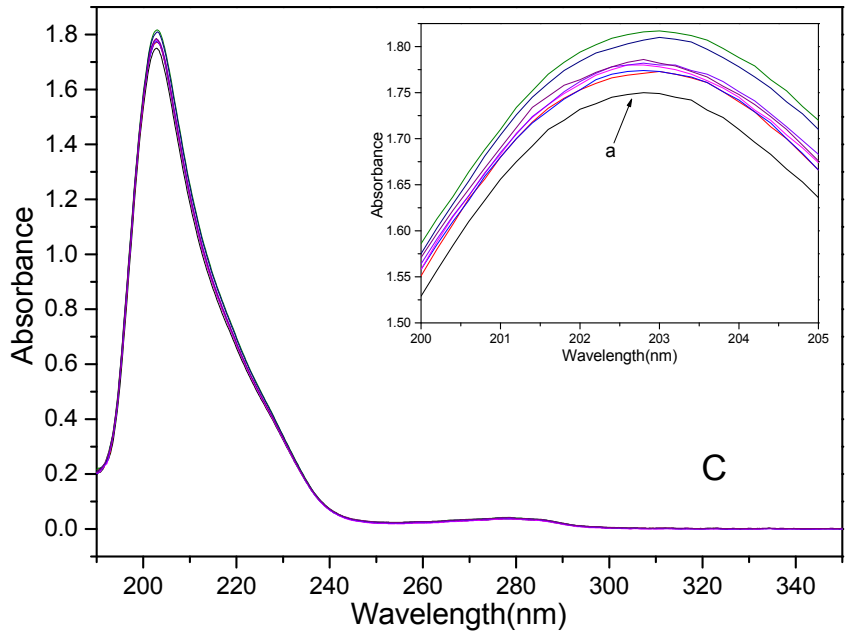
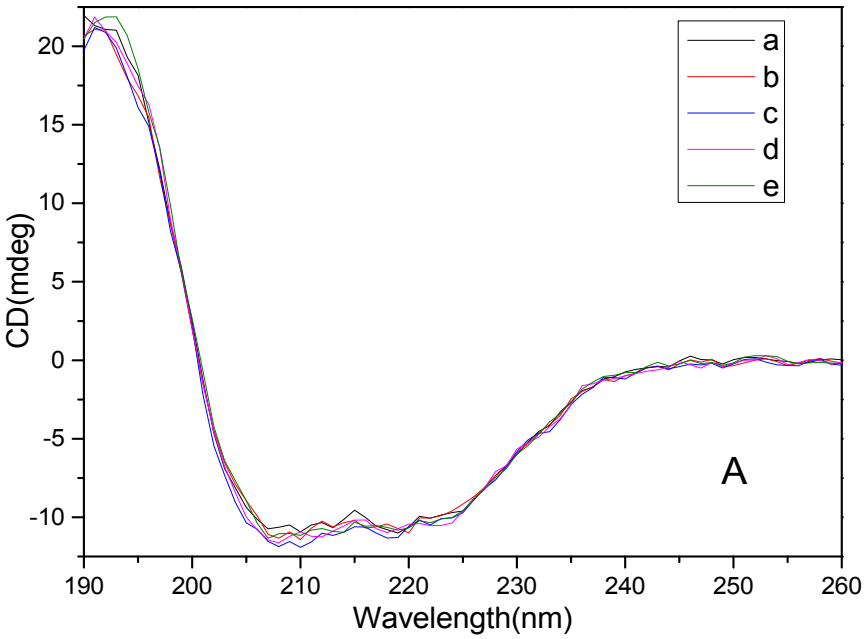


Fig. S4 UV-visible absorption spectra of HSA with different concentrations of PFASs. Conditions: HSA: 1×10^{-6} mol/L;A (PFOS), B (PFHS) and C (PFBS): 0, 2×10^{-6}, 6×10^{-6}, 1×10^{-5}, 3×10^{-5}, 5×10^{-5}, 7×10^{-5}, 1×10^{-4} mol/L; pH=7.4; T=298 K;


a
b
c
d
e
A
CD(mdeg)
Wavelength(nm)
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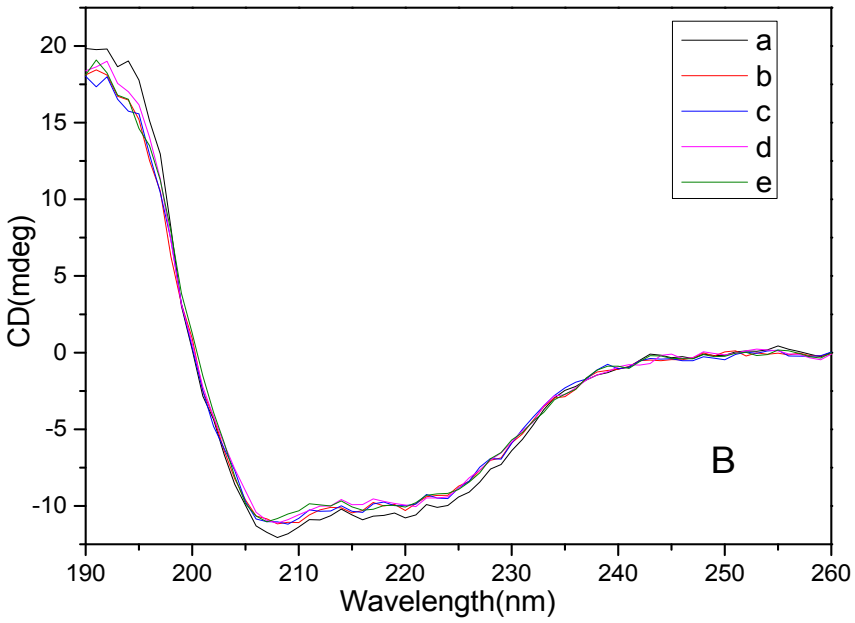
15
10
5
0
-5
-10
190
200
210
220
230
240
250
260


a
b
c
d
e
B
CD(mdeg)
Wavelength(nm)
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15
10
5
0
-5
-10
190
200
210
220
230
240
250
260

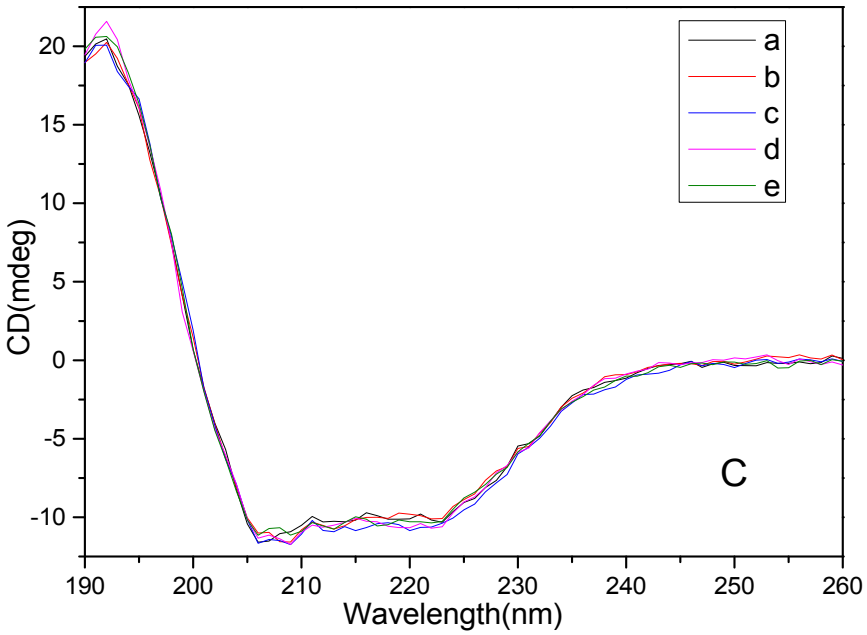

Fig. S5 CD Spectra of HSA with different concentrations of PFASs. Conditions: HSA: 1×10^{-6} mol/L; A (PFOS), B (PFHS) and C (PFBS) (a-e) : 0, 5×10^{-6}, 1×10^{-5}, 5×10^{-5}, 1×10^{-4} mol/L; pH=7.4; T=298K.

Table S1 The interaction data between PFOS and HSA

Ligand	Receptor	Residue	Type	Distance
H 8881	OD 5973	Asn 391	H-don	1.39
O 8880	NH 6284	Arg 410	H-acc	2.65
O 8878	OH 6306	Tyr 411	H-acc	2.48

Table S2 The interaction data between PFHS and HSA

Ligand	Receptor	Residue	Type	Distance
H 8880	OD 5973	Asn 391	H-don	1.28
O 8879	NH 6284	Arg 410	H-acc	2.50
O 8877	OH 6306	Tyr 411	H-acc	2.53

Table S3 The interaction data between PFBS and HSA

Ligand	Receptor	Residue	Type	Distance
H 8887	OD 5973	Asn 391	H-don	1.32
O 8886	NH 6284	Arg 410	H-acc	2.60
O 8877	OH 6306	Tyr 411	H-acc	2.49