

-Supporting Information-

Chemodiversity and Molecular Mechanism Between Per-/Polyfluoroalkyl Substance Complexation Behavior of Humic Substances in Landfill Leachate

Jia Li ^{1,†}, Haoqun Sha ^{2,†}, Rongchuan Ye ³, Peipei Zhang ⁴, Shuhe Chen ²,

Ganghui Zhu ^{1,*} and Wenbing Tan ^{2,*}

¹ Technical Centre for Soil, Agriculture and Rural Ecology and Environment,
Ministry of Ecology and Environment, Beijing 100012, China

² State Environmental Protection Key Laboratory of Simulation and Control of
Groundwater Pollution, Chinese Research Academy of Environmental Sciences,
Beijing 100012, China

³ School of Chemical and Environmental Engineering, China University of Mining
and Technology (Beijing), Beijing 100083, China

⁴ College of Biological Science and Biotechnology, Beijing Forestry University,
Beijing 100083, China

* Correspondence: zhuganghui@tcare-mee.cn (G.Z.); wenbingtan@126.com (W.T.)

† The authors contributed equally to this work.

Table S1. Information of 16 landfill sites in the studied area

No.	Sample ID of the landfill sites	Age (years)	Operation Status	Volume (ton/year)	Aera (m ²)	Anti-seepage function
1	BDY	2	In operation	10,000	35,700	yes
2	BZ	5	Closed	452,000	14,000	yes
3	BJD	5	Closed	27,375	59,557	yes
4	WAJ	8	Closing	73,000	150,498	yes
5	DCh	9	Closing	71,175	53,000	yes
6	WAR	10	Closing	112,130	96,587	yes
7	BJH	11	Closed	541,910	94,000	yes
8	XH	13	Closed	200,000	85,564	yes
9	LS	13	Closed	157,273	158,010	yes
10	XX	13	Closed	73,819	48,000	yes
11	TJQ	13	Closed	73,000	85,867	yes
12	LX	13	Closed	60,225	76,402	yes
13	ZZ	14	Closing	432,000	85,000	yes
14	SH	14	Closed	241,400	65,152	yes
15	DCh	14	Closing	73,000	54,543	yes
16	BDW	22	Closed	20,000	196,821	yes

Table S2. Fluorescence-quenching titration experiment between humic substances and PFAS

Group	Test No.	HA (mg/L)	FA (mg/L)	PFBS ($\mu\text{mol/L}$)	PFBA ($\mu\text{mol/L}$)
Blank 1	1	10	0	0	0
	2	10	0	10	0
	3	10	0	30	0
D1PS	4	10	0	50	0
	5	10	0	75	0
	6	10	0	100	0
	7	10	0	0	10
	8	10	0	0	30
D1PA	9	10	0	0	50
	10	10	0	0	75
	11	10	0	0	100
Blank 2	12	0	10	0	0
	13	0	10	10	0
	14	0	10	30	0
D2PS	15	0	10	50	0
	16	0	10	75	0
	17	0	10	100	0
	18	0	10	0	10
	19	0	10	0	30
D2PA	20	0	10	0	50
	21	0	10	0	75
	22	0	10	0	100

Note: Blank 1 refers to only HA without PFAS test group, D1PS refers to HA and PFBS test group, D1PA refers to HA and PFBA test group, blank 2 refers to only FA without PFAS test group, D2PS refers to FA and PFBS test group, and D2PA refers to FA and PFBA test group.

Table S3. Table of parameters for the complexation models

Group	modified Stern-Volmer model			site-specific complexation model		
	$\log K_{sv}$	f	R^2	$\log K_b$	n	R^2
D1PS	1.112	0.036	0.999	0.435	0.693	0.858
D1PA	1.684	0.044	0.793	1.380	0.157	0.703
D2PS	1.066	0.189	0.763	2.380	0.506	0.993
D2PA	1.547	0.061	0.806	1.354	0.520	0.944