











<https://doi.org/10.17221/35/2026-SWR>

Potential of micropollutants originated from irrigation water to contaminate soil and groundwater

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Electronic Supplementary Material (ESM)

The authors are fully responsible for both the content and the formal aspects of the electronic supplementary material. No editorial adjustments were made.

Table S1. Selected compounds and their characteristics

Compound	CAS number	Use	MW (g/mol)	log Kow	pKa	H-bonds donor acceptor	Water solubility (mg/L)
1,3-Diphenylguanidine (DPG) ^a	102-06-7	Vulcanization accelerator, rubber, tires, construction materials	211.268	2.67, 3.13	9.38 (basic)	3, 3	377
Triethyl citrate (TEC) ^a	77-93-0	Plasticizer, solvent, and emulsifier, food, pharmaceuticals, cosmetics	276.285	1.17, 0.19	-4.2 (basic) 11.82 (acidic)	1, 4	10 700
Naphthalene-2-sulfonic acid (NSA) ^a	120-18-3	Dye intermediate, surfactant, dispersant	208.234	-0.38, 2.14	-1.8 (acidic)	1, 3	328
Benzo(d)thiazole-2-sulfonic acid (BTSA)	941-57-1	Dye / pigment intermediate, rubber, tires	215.3 ^b	1.5 ^b	-3.52 (acidic) ^c	1, 5 ^b	soluble
4-Acetamidoantipyrine (4-AAA) ^a	83-15-8	Metabolite of metamizole (analgesic)	245.282	1.01, 0.15	-0.76 (basic) 12.52 (acidic)	1, 3	4 430
6:2 Fluorinated telomer sulfonate (6:2 FTS)	27619-97-2	Fire-fighting foams, metal plating	428.17 ^b	3.9 ^b	-2 (acidic) ^d	1, 16 ^b	soluble

^a<https://go.drugbank.com>; ^b<https://pubchem.ncbi.nlm.nih.gov>; ^chttps://www.chemicalbook.com/ChemicalProductProperty_EN_CB41283899.htm; ^dBarzen-Hanson et al. (2017)

Table S2. Soils and their properties

Code	Soil type	Texture	pH			Cox (%)	CaCO ₃ (%)	EC ($\mu\text{S}/\text{cm}$)	ρ_s (g/cm^3)	Sand	Silt (%)	Clay	CEC ($\text{mmol}^+ / 100 \text{ g}$)	HA	BCS	SCS (%)	PWI	χ_{LF}	χ_{HF}
			H ₂ O	KCl	CaCl ₂														
B	HCa-B	sandy loam	6.40	5.11	5.45	1.30	0.0	31.4	2.51	62.3	24.3	13.4	9.7	1.9	7.8	80.1	0.024	20.7	19.5
C	GP	silty clay	7.90	6.43	7.29	1.07	0.0	58.4	2.50	42.0	41.4	16.6	17.4	0.8	16.6	95.5	0.017	46.4	44.2
D	HCh	silty clay loam	7.84	6.94	6.78	1.44	2.5	100.4	2.51	8.8	55.4	35.8	10.1	0.7	9.4	92.7	0.019	88.4	83.5
E	AR-A	loamy sand	5.40	4.42	4.86	0.58	0.0	78.6	2.51	82.3	7.9	9.8	5.0	2.6	2.4	47.6	0.014	11.1	11.7
F	GF	loam	7.80	7.02	6.97	1.27	0.0	150.2	2.48	32.5	46.9	20.7	13.5	2.4	11.1	81.9	0.029	14.8	15.7
G	HF-A	loam	6.95	6.07	6.41	1.11	0.0	24.5	2.51	29.5	47.6	22.9	15.8	1.7	14.1	89.5	0.024	8.6	9.9
H	HCa-A	loam	5.32	4.19	4.74	1.39	0.0	301.3	2.46	32.2	42.2	25.6	14.0	7.4	6.6	47.1	0.028	45.5	45.3
K	ACh-A	loam	5.30	4.23	4.67	0.98	0.0	48.6	2.54	49.5	29.4	21.1	9.6	5.7	3.9	40.2	0.012	81.1	73.6
N	AR-B	sandy loam	5.97	4.23	5.03	1.80	0.0	25.5	2.45	65.4	18.8	15.8	8.9	2.5	6.4	72.3	0.023	37.8	36.9
R	HF-B	sandy loam	5.72	4.30	4.83	2.28	0.0	62.3	2.50	73.8	13.0	13.2	22.7	4.5	18.2	80.2	0.031	20.7	21.3
S	HL	silty loam	6.59	5.99	6.13	0.71	0.1	100.2	2.49	7.0	68.4	24.6	14.3	2.6	11.7	81.7	0.016	34.8	34.5
V	ACh-C	loam	7.96	7.27	7.41	1.78	1.2	54.4	2.47	42.1	22.2	35.7	23.2	0.7	22.5	97.0	0.023	11.3	11.9
W	DCa	silty loam	5.65	4.66	5.16	2.28	0.0	29.0	2.47	16.8	62.9	20.4	18.5	8.2	10.3	55.9	0.044	46.2	46.6
X	SChS	clay loam	7.97	7.48	7.61	3.14	21.8	51.8	2.41	26.2	34.1	39.8	29.2	0.7	28.5	97.6	0.058	15.4	16.3
Y	HF-C	silty clay loam	6.86	5.83	6.66	1.43	0.0	56.1	2.44	12.1	48.5	39.4	26.0	2.3	23.7	91.2	0.011	14.8	14.5
Z	ACh-B	sandy loam	7.65	6.63	6.86	1.71	0.1	87.5	2.52	62.2	21.3	16.5	13.2	1.1	12.1	92.0	0.023	48.9	43.4
	Avg.		6.70	5.68	6.05	1.52		78.8	2.49	40.3	36.5	23.2	15.7	2.9	12.8	77.7	0.025	34.2	33.0
	St.Dev.		1.04	1.22	1.07	0.65		68.1	0.03	23.8	17.9	9.7	6.8	2.4	7.4	19.4	0.012	24.5	22.3
	Max.		7.97	7.48	7.61	3.14		301.3	2.54	82.3	68.4	39.8	29.2	8.2	28.5	97.6	0.058	88.4	83.5
	Min.		5.30	4.19	4.67	0.58		24.5	2.41	7.0	7.9	9.8	5.0	0.7	2.4	40.2	0.011	8.6	9.9
	Range		2.66	3.28	2.95	2.56		276.8	0.14	75.3	60.5	29.9	24.2	7.5	26.1	57.5	0.047	79.8	73.6

SChS – Stagnic Chernozem Siltic on marlite; HCh – Haplic Chernozem on loess; ACh-A and ACh-B – two Arenic Chernozems on sand and gravel; ACh-C – Arenic Chernozem on sandy marlstone; GP – Greyic Phaeozem on loess; HL – Haplic Luvisol on loess; HCa-A and HCa-B – two Haplic Cambisol on paragneiss; DCa – Dystric Cambisol on orthogneiss; HF-A, HF-B, HF-C, and GF – three Haplic Fluvisols and Gleyic Fluvisol on fluvial sediments; AR-A and AR-B – two Arenic Regolols on sand or sand and gravel; pH_{H2O}, pH_{KCl}, and pH_{CaCl2} – active and potential soil reactions; Cox – organic carbon content; EC – soil salinity (electrical conductivity), ρ_s – particle density; CEC – cation exchange capacity; HA – hydrolytic acidity; BCS – base cation saturation; SCS – sorption complex saturation; PWI – potential wettability index; χ_{HF} and χ_{LF} – mass magnetic susceptibility at high and low frequency, respectively

Table S3. Correlation coefficients describing relationship between soil properties

	pH _{H₂O}	pH _{CaCl₂}	pH _{KCl}	ln(EC)	CEC	ln(HA)				
pH _{CaCl₂}	0.975***									
pH _{KCl}	0.969***	0.974***								
ln(EC)	0.055	0.049	0.119							
CEC	0.387	0.502*	0.420	-0.098						
ln(HA)	-0.883***	-0.848***	-0.832***	0.096	-0.230					
BCS	0.609*	0.700**	0.620*	-0.133	0.948***	-0.511*				
SCS	0.883***	0.859***	0.818***	-0.145	0.524*	-0.826***				
Cox	0.207	0.212	0.200	-0.224	0.672**	-0.131				
ρ _s	-0.220	-0.321	-0.248	-0.025	-0.676**	0.125				
Sand	-0.349	-0.432	-0.450	-0.167	-0.375	0.087				
Silt	0.198	0.260	0.281	0.149	0.164	0.096				
Clay	0.493	0.582*	0.585*	0.135	0.618*	-0.391				
χ _{LF}	-0.110	-0.190	-0.144	0.176	-0.391	0.110				
χ _{HF}	-0.122	-0.200	-0.153	0.185	-0.381	0.130				
ln(PWI)	0.156	0.133	0.183	-0.077	0.403	-0.012				

	BCS	SCS	Cox	ρ _s	Sand	Silt	Clay	χ _{LF}	χ _{HF}
SCS	0.738**								
Cox	0.601*	0.298							
ρ _s	-0.631**	-0.288	-0.622*						
Sand	-0.332	-0.274	-0.062	0.352					
Silt	0.093	0.130	-0.106	-0.158	-0.930***				
Clay	0.643**	0.434	0.348	-0.573**	-0.733**	0.432			
χ _{LF}	-0.437	-0.278	-0.122	0.435	-0.202	0.254	0.026		
χ _{HF}	-0.437	-0.287	-0.108	0.407	-0.229	0.285	0.035	0.998***	
ln(PWI)	0.319	0.158	0.800***	-0.485	-0.062	0.039	0.080	-0.226	-0.196

***, **, *P < 0.001, 0.01, 0.05

pH_{H₂O}, pH_{KCl}, and pH_{CaCl₂} – active and potential soil reactions; EC – soil salinity (electrical conductivity), CEC – cation exchange capacity; HA – hydrolytic acidity; BCS – base cation saturation; SCS – sorption complex saturation; Cox – organic carbon content; ρ_s – particle density; χ_{HF} and χ_{LF} – mass magnetic susceptibility at high and low frequency, respectively; PWI – potential wettability index

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Table S4. LC gradient for target analyte separation on QqQ Altis and QExactive-HF using Arion Plus C18 Column (30 × 2.1 mm, 5 μm)

Time (min)	Water	ACN	Flow (μL/min)	Time (min)	Water	ACN	Flow (μL/min)
	+ 0.1% FA	+ 0.1% FA			+ 0.1% FA	+ 0.1% FA	
	(%)				(%)		
QqQ Altis				Q Exactive-HF			
0.00	95	5	350	0.00	95	5	350
0.50	95	5	350	0.50	95	5	350
3.00	0	100	400	3.00	0	100	400
4.00	0	100	400	5.00	0	100	400
4.01	95	5	350	5.01	95	5	350
6.00	95	5	350	7.00	95	5	350

FA – formic acid; ACN – acetonitrile

Table S5. MS conditions for target analysis on QqQ Altis and QExactive-HF with direct injection (10 μL on QqQ Altis, 5 μL on QExactive-HF)

MS conditions	QqQ Altis	Q Exactive-HF
Ion source type	H-ESI	H-ESI
Positive ionization spray volatage (V)	3 500	3 500
Negative ionization spray volatage (V)	2 800	2 800
Sheath gas (N ₂) au	42	40
Auxiliary gas (Ar) au	12	10
Vaporizer temp. (°C)	338	275
Ion transfer tube temp. (°C)	338	325

9 Table S6. Compounds – MS transitions, retention time (RT), and limits of quantification (LOQ)

Analyte	Used IS	Producer	Ionization mode	Precursor	Quan	Qual	RT (min)	LOQ min	LOQ max	Equipment
				(m/z)				(µg/mL)		
1,3-Diphenylguanidine	Trimethoprim_IS	HPC	positive	212	195.1	119.1	1.9	0.026	0.026	Altis
4-Acetamidoantipyrine	Atrazine_IS	TFS	positive	246	228.3	204.1	1.9	0.036	0.045	Altis
Benzo(d)thiazole-2-sulfonic acid	Atrazine_IS	FCh	positive	216	198.0	134.0	2.4	0.0042	0.0095	Altis
Naphtalen-2-sulfonic acid	2,4-D_IS	TFS	negative	207	143.1	80.0	2.8	0.018	0.025	Altis
Triethyl Citrate	Atrazine_IS	TCI	positive	227	203.1	157.1	2.6	0.020	0.020	Altis
2,4-D_IS		HPC	negative	225	167.1		2.8			Altis
Atrazine_IS		Chiron	positive	221	179.1		2.7			Altis
Trimethoprim_IS		TRC	positive	294	231.1		1.8			Altis
6:2 FTS	2,4-D IS	SQL	negative	427	387.0		3.0	0.0051	0.025	QExactive-HF
2,4-D_IS		HPC	negative	225	167.1		2.8			QExactive-HF

HPC – HPC Standards GmbH (Germany); TFC – Thermo Fisher Scientific (USA); SQL – SynQuest Laboratories, Inc. (USA); FCh – Fluorochem Limited (UK); TCI – TOKYO CHEMICAL INDUSTRY CO., LTD. (Japan); Chiron – Chiron AS (Norway); TRC – Toronto Research Chemicals (Canada)

Table S7. The Freundlich sorption coefficients for studied compounds and soils compounds

Code	Soil type	DPG			TEC			4-AAA			NSA			BTSA			6:2 FTS		
		K_F	n	R^2	K_F	n	R^2	K_F	n	R^2	K_F	n	R^2	K_F	n	R^2	K_F	n	R^2
B	HCa-B	10.1	1.27	0.978	1.82	1.70	0.933	1.78	1.66	0.927	0.14	1.13	0.920	0.28	1.15	0.484	1.05	1.37	0.708
C	GP	11.3	1.50	0.990	6.26	2.39	0.951	1.58	1.19	0.998	0.26	1.30	0.809	0.94	1.56	0.851	0.84	0.84	0.910
D	HCh	16.6	1.46	0.990	5.24	1.95	0.903	1.37	1.15	0.959	0.52	1.16	0.849	1.14	1.60	0.931	1.45	1.80	0.514
E	AR-A	3.6	1.27	0.823	0.34	1.45	0.497	1.14	1.41	0.781	NC	NC	NC	0.60	2.07	0.621	0.58	0.91	0.392
F	GF	8.6	1.30	0.946	1.92	1.52	0.890	1.37	1.25	0.957	0.11	0.96	0.779	1.33	1.70	0.899	0.79	1.04	0.549
G	HF-A	10.7	1.33	0.976	7.31	2.34	0.989	1.00	1.28	0.888	0.14	1.08	0.838	0.79	1.57	0.859	1.19	1.18	0.748
H	HCa-A	9.6	1.45	0.961	1.43	2.14	0.842	1.54	1.20	0.991	0.31	1.27	0.875	1.17	1.88	0.861	1.82	1.41	0.805
K	ACh-A	3.4	1.46	0.857	0.21	1.68	0.036	1.26	1.36	0.881	NC	NC	NC	0.91	1.69	0.900	0.87	1.31	0.731
N	AR-B	9.8	1.44	0.989	1.32	1.86	0.904	1.23	1.40	0.978	0.23	1.17	0.719	1.01	1.52	0.846	0.84	1.21	0.764
R	HF-B	9.5	1.29	0.965	0.46	1.77	0.637	1.28	1.28	0.940	0.18	1.42	0.758	0.99	1.33	0.882	1.21	1.33	0.899
S	HL	13.7	1.28	0.996	1.67	1.47	0.816	1.49	1.18	0.995	0.18	1.80	0.873	0.97	1.92	0.889	0.91	1.22	0.835
V	ACh-C	16.2	1.27	0.995	7.03	1.81	0.946	1.51	1.31	0.809	0.26	1.27	0.881	1.09	1.66	0.914	0.89	1.05	0.806
W	DCa	14.4	1.30	0.994	2.04	2.51	0.905	1.45	1.32	0.838	0.54	1.13	0.898	1.96	1.99	0.972	1.96	1.13	0.948
X	SChS	18.5	1.45	0.993	23.31	1.67	0.959	1.42	1.41	0.694	0.70	1.37	0.903	1.79	2.04	0.916	2.03	1.32	0.917
Y	HF-C	21.9	1.43	0.995	8.46	2.08	0.904	1.37	1.22	0.905	0.25	1.13	0.765	0.88	1.42	0.840	1.41	1.51	0.951
Z	ACh-B	10.0	1.43	0.969	5.87	1.97	0.905	1.30	1.29	0.933	0.21	1.31	0.296	1.01	1.76	0.725	1.42	1.88	0.739

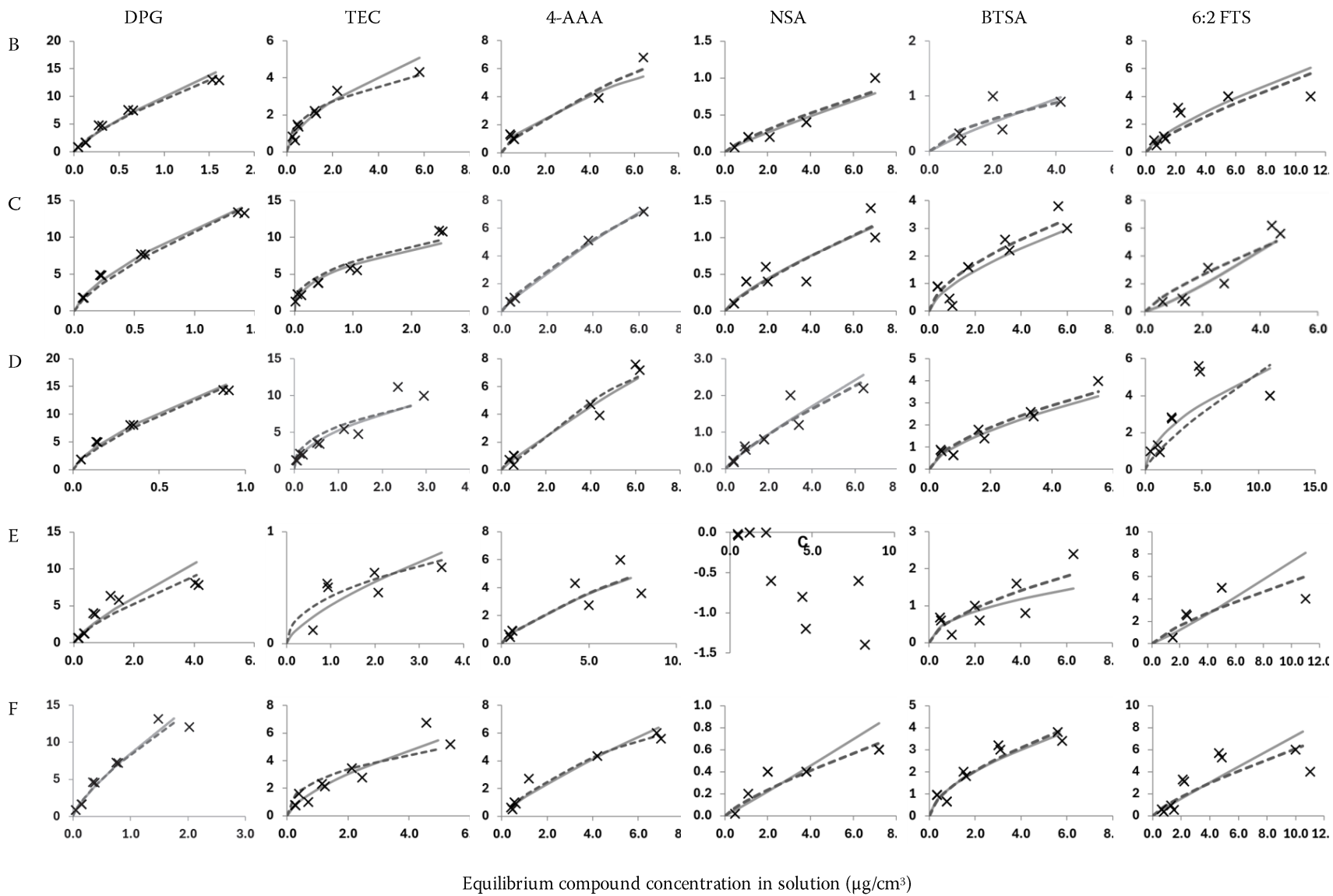
K_F ($\text{cm}^{3/n} \mu\text{g}^{1-1/n} / \text{g}$) – Freundlich sorption coefficients, n (–) – Freundlich exponent, and R^2 – coefficients of determination; SChS – Stagnic Chernozem Siltic on marlite; HCh – Haplic Chernozem on loess; ACh-A and ACh-B – two Arenic Chernozems on sand and gravel; ACh-C – Arenic Chernozem on sandy marlstone; GP – Greyic Phaeozem on loess; HL – Haplic Luvisol on loess; HCa-A and HCa-B – two Haplic Cambisol on paragneiss; DCa – Dystric Cambisol on orthogneiss; HF-A, HF-B, HF-C, and GF – three Haplic Fluvisols and Gleyic Fluvisol on fluvial sediments; AR-A and AR-B – two Arenic Regolols on sand or sand and gravel; DPG – 1,3-diphenylguanidine; TEC – triethyl citrate; 4-AAA – 4-acetamidoantipyrine; NSA – naphthalene-2-sulfonic acid; BTSA – benzo(d)thiazole-2-sulfonic acid; 6:2 FTS – 6:2 fluorinated telomer sulfonate; NC – not calculated

Table S8. Correlation coefficients describing relationships between the Freundlich sorption coefficients and soil properties

	Freundlich sorption coefficients K_F					
	DPG (16 soils)	ln(TEC) (16 soils)	4-AAA (16 soils)	BTSA (16 soils)	ln(6:2 FTS) (16 soils)	ln(NSA) (14 soils)
DPG						
ln(TEC)	0.776***					
4-AAA	0.434	0.534*				
BTSA	0.462	0.332	0.083			
ln(6:2 FTS)	0.371	0.347	0.425	0.641**		
ln(NSA)	0.549*	0.323	-0.104	0.649*	0.574*	
pH _{H₂O}	0.517*	0.839***	0.370	0.261	0.046	0.079
pH _{CaCl₂}	0.599*	0.887***	0.478	0.298	0.155	0.123
pH _{KCl}	0.542*	0.831***	0.394	0.285	0.085	0.126
ln(EC)	-0.111	-0.075	0.163	0.032	-0.101	-0.038
CEC	0.731**	0.589*	0.512*	0.588*	0.591*	0.337
ln(HA)	-0.403	-0.741**	-0.206	0.011	0.108	-0.093
BCS	0.762***	0.736**	0.496	0.467	0.435	0.239
SCS	0.637**	0.838***	0.366	0.177	0.046	-0.089
Cox	0.460	0.363	-0.031	0.705**	0.521*	0.614*
ρ_s	-0.662**	-0.516*	-0.323	-0.547*	-0.571*	-0.421
Sand	-0.702**	-0.535*	-0.477	-0.460	-0.383	-0.409
Silt	0.480	0.351	0.424	0.369	0.378	0.239
Clay	0.835***	0.665**	0.387	0.446	0.241	0.518
χ_{LF}	-0.125	-0.224	-0.216	0.120	-0.221	0.457
χ_{HF}	-0.111	-0.223	-0.211	0.151	-0.179	0.477
ln(PWI)	0.158	0.268	0.026	0.596*	0.635**	0.417

***, **, * $P < 0.001, 0.01, 0.05$

DPG – 1,3-diphenylguanidine; TEC – triethyl citrate; 4-AAA – 4-acetamidoantipyrine; NSA – naphthalene-2-sulfonic acid; BTSA – benzo(d)thiazole-2-sulfonic acid; 6:2 FTS – 6:2 fluorinated telomer sulfonate; pH_{H₂O}, pH_{KCl}, and pH_{CaCl₂}, – active and potential soil reactions; EC – soil salinity (electrical conductivity), CEC – cation exchange capacity; HA – hydrolytic acidity; BCS – base cation saturation; SCS – sorption complex saturation; Cox – organic carbon content; ρ_s – particle density; χ_{HF} and χ_{LF} – mass magnetic susceptibility at high and low frequency, respectively; PWI – potential wettability index



Equilibrium concentration of compound sorbed on solid (g/g)

Equilibrium compound concentration in solution (µg/cm³)

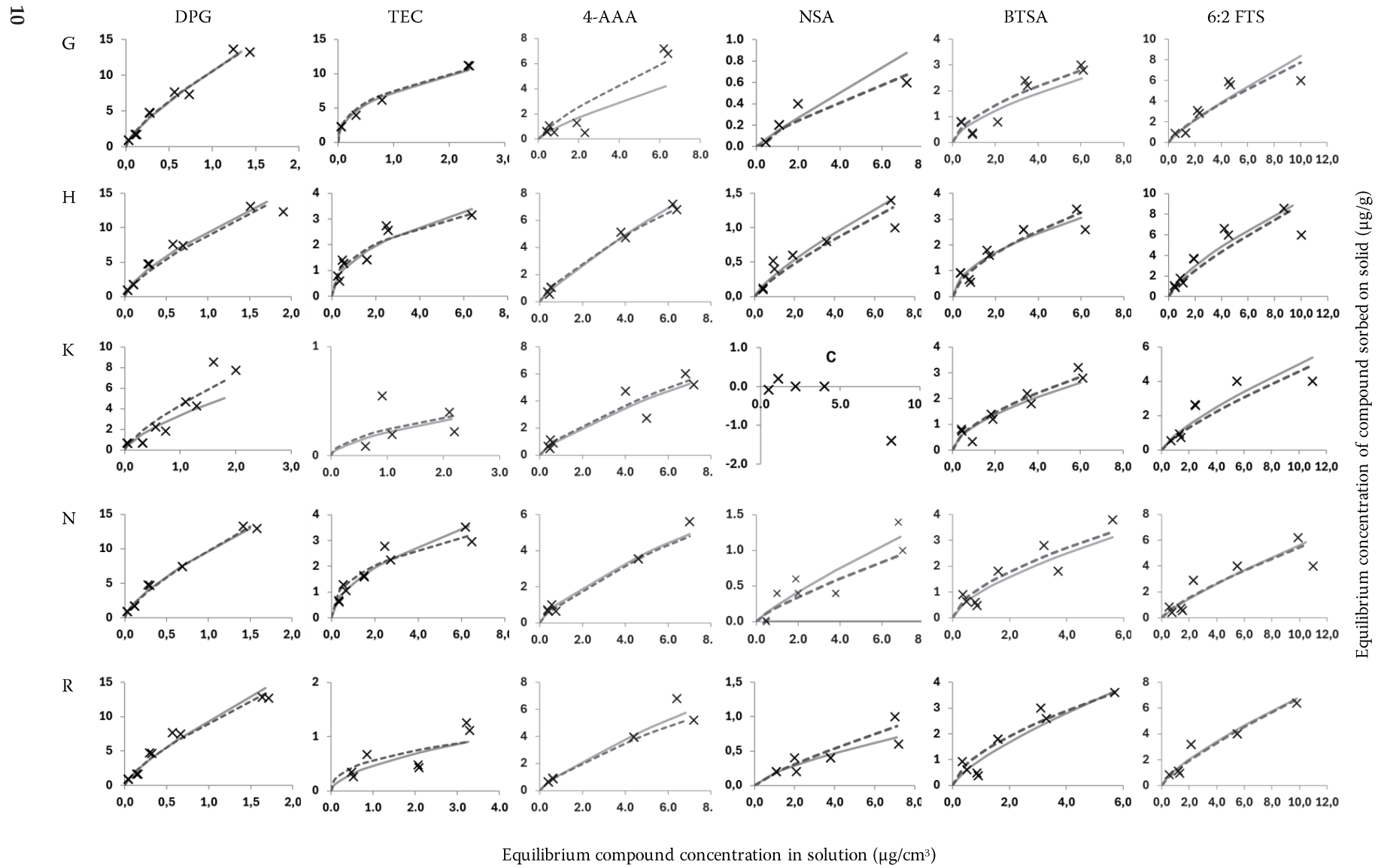
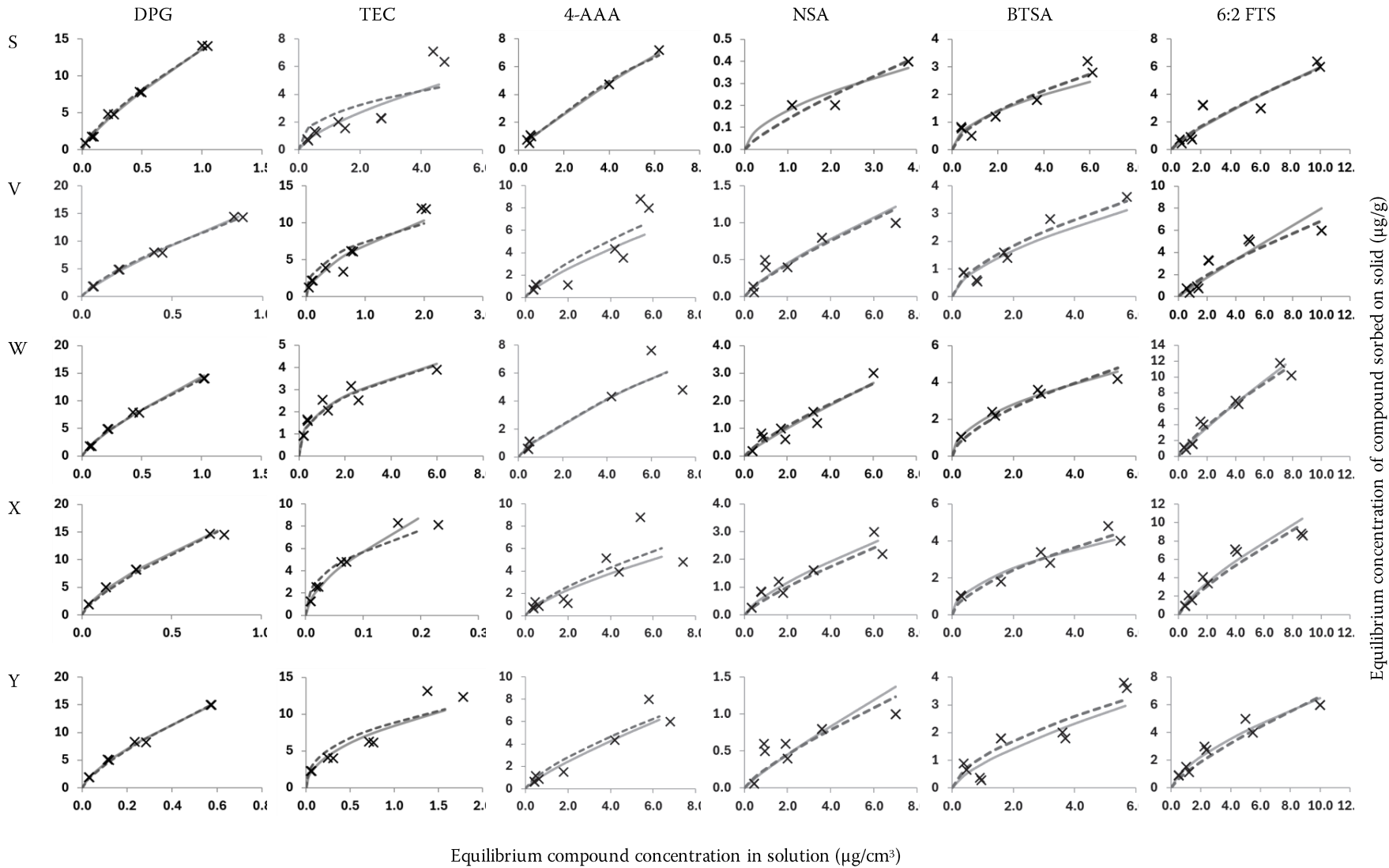


Figure S1 to be continued



11 Figure S1 to be continued

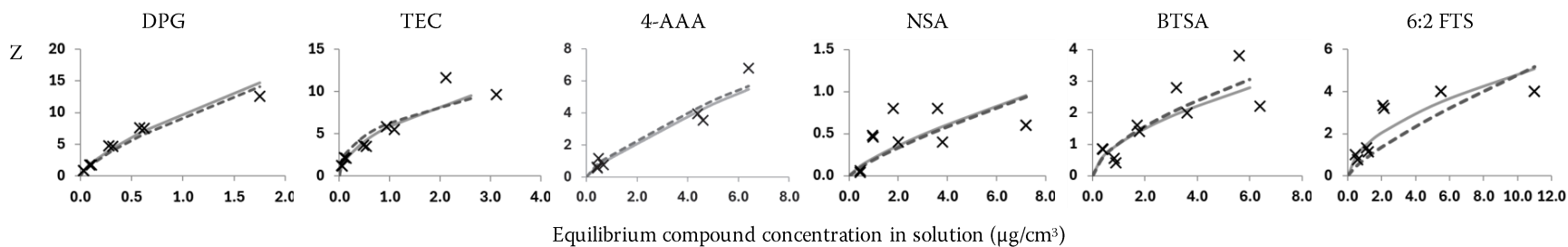


Figure S1. Freundlich sorption isotherms for particular compounds (columns) and soils (rows); experimental data (data-points), initially fitted with variable n value (solid line), and fitted with the average n value for each compound (dashed line)

DPG – 1,3-diphenylguanidine; TEC – triethyl citrate; 4-AAA – 4-acetamidoantipyrine; NSA – naphthalene-2-sulfonic acid; BTSA – benzo(d)thiazole-2-sulfonic acid; 6:2 FTS – 6:2 fluorinated telomer sulfonate

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