

Supplementary Information

Selective Sorption of PAHs from TX100 Solution by Resin

SP850: Effects of TX100 Concentrations and PAHs Solubility

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Figure S2 Calculated K_f values ($\log K_{fcal}$) using equation 6 versus experimental K_f values ($\log K_{fexp}$). Solid lines is the reference line, $y = x$, indicating that the $\log K_{fcal}$ values equal to the $\log K_{fexp}$ values. Dashed lines indicate the SD values from the reference lines.

Figure S3 $1/n$ values of 6 PAHs by SP850 from TX100 solution with their sequence number (Table S1). Solid line is the reference line of average $1/n$ value ($1/n = 0.775$) of 6 PAHs by SP850 from TX100 solution. Dashed lines indicate the SD value from the reference line.

Figure S4 Correlations between the modified selectivity parameters (S^*) of phenanthrene by SP850 with various doses and TX100 equilibrium concentrations ($C_{e, TX100}$). Solid lines are fitted by the Parabolic equation.

Table S1 Freundlich model fitted isotherm parameters of PAHs by SP850 in the presence of TX100^a

Sequence number	PAHs	$C_{0, TX100}$ (mg/L)	K_f	1/n	F	P	R ²	N
1	Naphthalene	1500	12.5±0.4	0.849±0.017	7455	<0.001	0.998	16
2		2000	6.85±0.33	0.823±0.018	5836	<0.001	0.997	16
3		3000	4.58±0.22	0.846±0.016	7921	<0.001	0.998	16
4		5000	2.22±0.05	0.874±0.007	49517	<0.001	0.999	17
5		8000	1.38±0.04	0.883±0.008	42974	<0.001	0.999	16
6		10000	0.814±0.027	0.853±0.008	32362	<0.001	0.999	16
7	Acenaphthene	1500	15.5±0.4	0.780±0.014	10170	<0.001	0.998	14
8		2000	11.0±0.4	0.758±0.014	9311	<0.001	0.998	14
9		3000	7.41±0.31	0.740±0.015	8049	<0.001	0.997	14
10		5000	4.34±0.19	0.774±0.014	9789	<0.001	0.998	15
11		8000	2.41±0.04	0.804±0.005	82914	<0.001	0.999	14
12		10000	1.80±0.05	0.805±0.008	32740	<0.001	0.999	14
13	Phenanthrene	1500	32.8±0.5	0.743±0.014	8891	<0.001	0.998	16
14		2000	17.3±0.2	0.749±0.007	36458	<0.001	0.999	16
15		3000	9.65±0.36	0.773±0.016	7507	<0.001	0.997	16
16		5000	4.89±0.09	0.803±0.006	48599	<0.001	0.999	17
17		8000	2.98±0.11	0.808±0.011	18186	<0.001	0.999	16
18		10000	2.03±0.07	0.817±0.010	20060	<0.001	0.999	17
19	Pyrene	1500	24.2±0.3	0.745±0.019	4001	<0.001	0.996	18
20		2000	13.4±0.2	0.784±0.014	8787	<0.001	0.998	19
21		3000	9.10±0.32	0.801±0.022	3787	<0.001	0.995	19
22		5000	6.26±0.20	0.798±0.019	5536	<0.001	0.996	16
23		8000	2.94±0.11	0.863±0.015	10233	<0.001	0.998	19
24		10000	2.22±0.14	0.874±0.024	4107	<0.001	0.996	19

Sequence number	PAHs	$C_{0,TX100}$ (mg/L)	K_f	1/n	F	P	R ²	N
25	Anthracene	1500	34.9±0.6	0.714±0.011	10817	<0.001	0.998	19
26		2000	24.3±0.2	0.776±0.010	18985	<0.001	0.999	19
27		3000	13.9±0.1	0.753±0.009	22058	<0.001	0.999	18
28		4000	9.51±0.08	0.742±0.012	10974	<0.001	0.998	19
29		5000	7.08±0.07	0.71±0.01	11767	<0.001	0.998	19
30		8000	5.26±0.06	0.777±0.011	15197	<0.001	0.999	19
31		10000	3.51±0.05	0.779±0.009	20332	<0.001	0.999	19
32	Benzanthracene	1500	38.5±0.7	0.701±0.012	9377	<0.001	0.998	19
33		2000	25.6±0.3	0.699±0.012	9259	<0.001	0.998	19
34		3000	14.4±0.1	0.742±0.008	27872	<0.001	0.999	18
35		4000	9.70±0.04	0.695±0.006	43623	<0.001	0.999	19
36		5000	7.43±0.05	0.702±0.008	24906	<0.001	0.999	19
37		8000	5.84±0.06	0.715±0.009	18970	<0.001	0.999	19
38		10000	4.22±0.05	0.685±0.008	19098	<0.001	0.999	19

^a All estimated parameter values and their standard errors were determined by a commercial software (SPSS 20.0) with nonlinear regression; N is the number of experimental data.

Table S2 Correlations of PAHs sorption coefficient ($\log K_f$) with TX100 equilibrium concentrations ($\log C_{e,TX100}$)^a

PAHs	Equations	F	P	R ²	N
Naphthalene	$\log K_f = -0.935(\pm 0.038)\log C_{e,TX100} + 3.75(\pm 0.13)$	608	<0.001	0.995	5
Acenaphthene	$\log K_f = -0.831(\pm 0.049)\log C_{e,TX100} + 3.60(\pm 0.17)$	291	<0.001	0.986	6
Phenanthrene	$\log K_f = -1.05(\pm 0.02)\log C_{e,TX100} + 4.49(\pm 0.08)$	1993	<0.001	0.998	6
Pyrene	$\log K_f = -0.882(\pm 0.063)\log C_{e,TX100} + 3.89(\pm 0.22)$	196	<0.001	0.980	6
Anthracene	$\log K_f = -0.883(\pm 0.034)\log C_{e,TX100} + 4.08(\pm 0.12)$	658	<0.001	0.992	7
Benzanthracene	$\log K_f = -0.857(\pm 0.036)\log C_{e,TX100} + 4.02(\pm 0.12)$	575	<0.001	0.991	7

^a All estimated parameter values and their standard errors were determined by a commercial software (SPSS 20.0) with linear regression; N is the number of experimental data.

Table S3 Results of linear regressions between $\log K_f$ and $\log S_w$ of PAHs^a

$C_{0, TX100}$ (mg/L)	α	β	F	P	R ²	N
1500	-0.136(±0.039)	1.34(±0.05)	12.4	0.024	0.756	6
2000	-0.154(±0.035)	1.12(±0.04)	19.4	0.012	0.829	6
3000	-0.135(±0.024)	0.918(±0.029)	32.0	0.005	0.889	6
5000	-0.143(±0.025)	0.652(±0.030)	33.6	0.004	0.894	6
8000	-0.170(±0.026)	0.436(±0.032)	41.7	0.003	0.912	6
10000	-0.186(±0.028)	0.270(±0.035)	43.6	0.003	0.916	6

^a All estimated parameter values and standard errors were determined by a commercial software (SPSS 20.0) with linear regression; N is the number of experimental data.

Table S4 Parabolic equation fitted S^* values of PAHs by SP850 from TX100 solution^a

PAHs	A/($\times 10^{-8}$) ^b	B/($\times 10^{-4}$) ^b	F	P	R ²	N	B/(-2A) ^c
Naphthalene	-12.6(±1.11)	10.5(±0.89)	70.8	0.00109	0.928	6	4167
Acenaphthene	-7.16(±0.61)	10.2(±0.72)	136	<0.001	0.862	8	7121
Phenanthrene	-7.03(±0.61)	11.1(±0.7)	205	<0.001	0.695	8	7895
Pyrene	-4.88(±0.56)	9.79(±0.89)	79.0	<0.001	0.757	8	10021
Anthracene	-2.77(±0.19)	9.85(±0.56)	201	<0.001	0.877	11	17772
Benanthracene	-2.65(±0.19)	10.3(±0.5)	290	<0.001	0.905	11	19457

^a All estimated parameter values and standard errors were determined by a commercial software (SPSS 20.0) with nonlinear regression; N is the number of experimental data;

^b A and B are the coefficients of the quadratic and primary terms of the parabolic equation, respectively;

^c $C_{e, TX100} = -B/(2A)$ are the optimal TX100 concentrations ($C_{op, TX100}$) in soil washing solution.

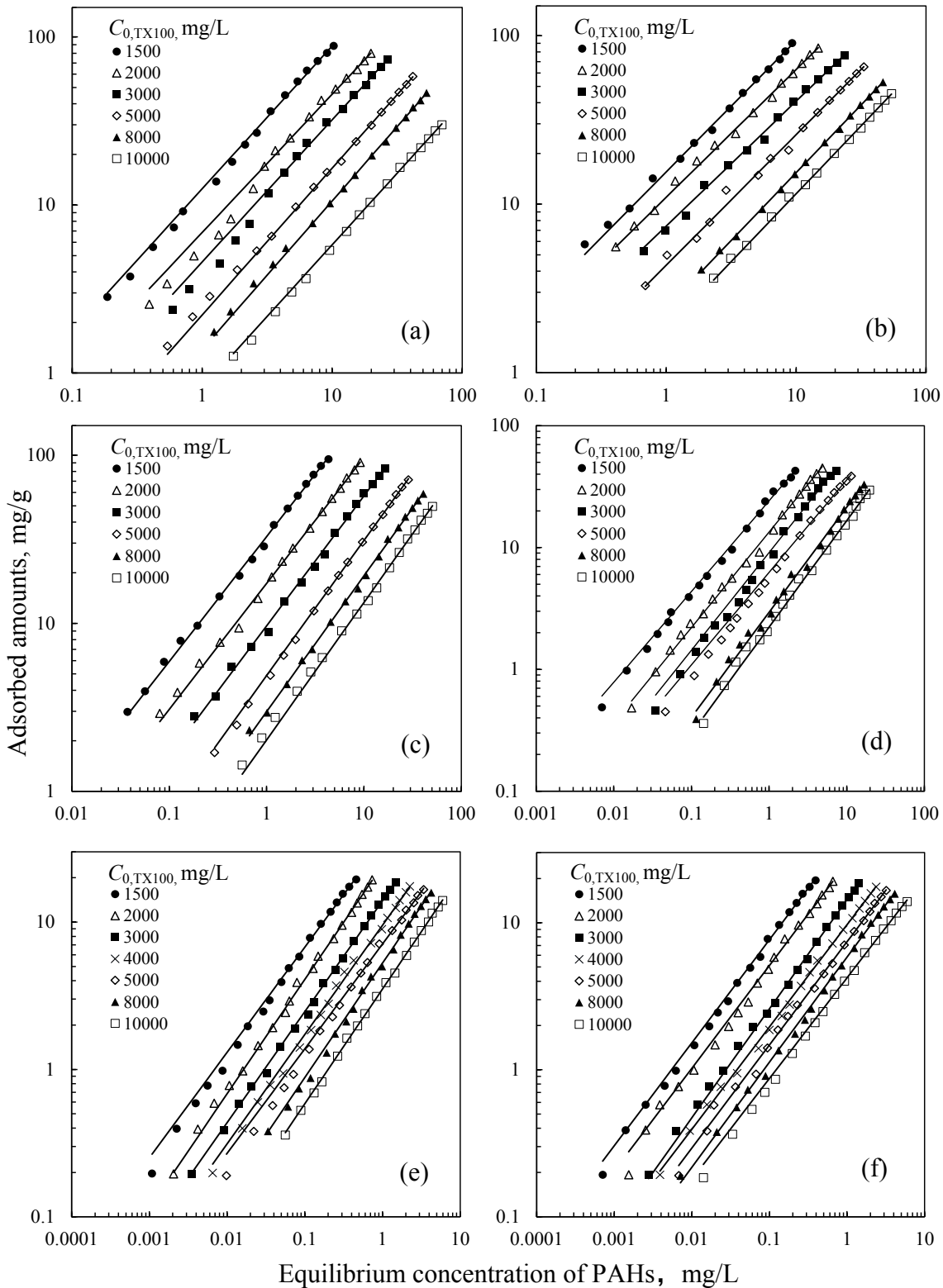


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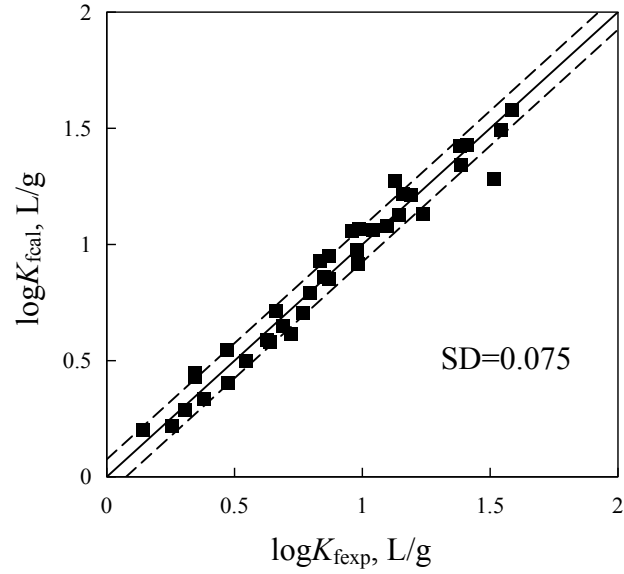


Figure S2 Calculated K_f values ($\log K_{fcal}$) using equation 6 versus experimental K_f values ($\log K_{fexp}$). Solid lines is the reference line, $y = x$, indicating that the $\log K_{fcal}$ values equal to the $\log K_{fexp}$ values. Dashed lines indicate the SD values from the reference lines.

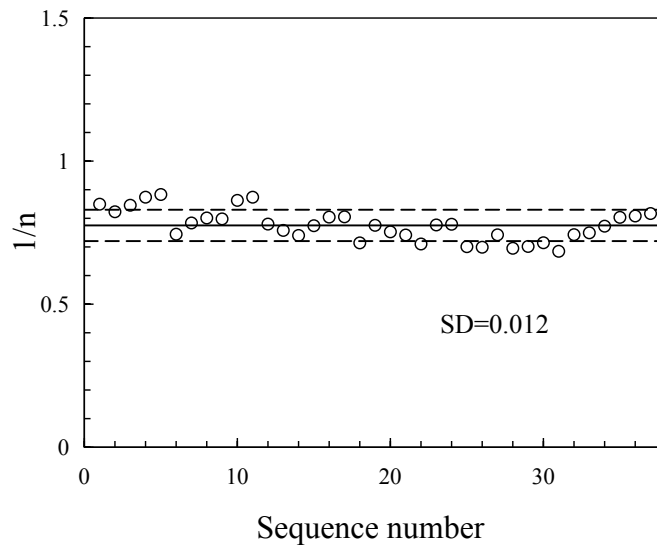


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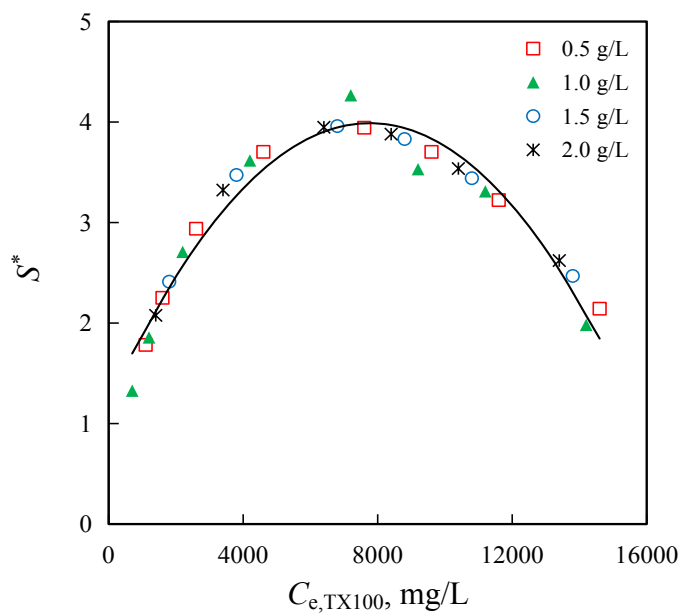


Figure S4 Correlations between the modified selectivity parameters (S^*) of phenanthrene by SP850 with various doses and TX100 equilibrium concentrations ($C_{e, TX100}$). Solid lines are fitted by the Parabolic equation.