

Sorption to soil, biochar and compost: is prediction to multicomponent mixtures possible based on single sorbent measurements?

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Table S1. Main properties of the two soils studied

	Sand (%)	Silt (%)	Clay (%)	OC (%)	pH (0.01M CaCl ₂)
Clay Loam^a	45	28	27	1.7	6.2
Sandy Loam	64	21	15	1.0	4.2

^a Following the USDA textural classes

Table S2. Main properties of the four biochars studied

						N ₂ (NLDFT ^b)		CO ₂ (GCMC ^c)	
	C (%)	H/C	O/C	Ash (%)	pH ^a	Surface Area (m ² /g)	Pore volume (cc/g)	Surface Area (m ² /g)	Pore volume (cc/g)
MSP550	75.41	0.38	0.09	12.15	9.77	16	0.024	320	0.092
MSP700	79.18	0.19	0.07	11.55	9.72	38	0.029	369	0.103
SWP550	85.52	0.39	0.09	1.25	7.91	31	0.029	375	0.118
SWP700	90.21	0.24	0.05	1.89	8.44	173	0.119	449	0.132

^a measured in 0.01M CaCl₂

^b Nonlocal Density Functional Theory

^c Grand Canonical Monte Carlo analysis

Table S3. Calculated organic carbon content (OC%) of the mixtures.

	Clay Loam + B	Clay Loam + C	Clay Loam + B + C	B + C	Sandy Loam + B	Sandy Loam + C	Sandy Loam + B + C
OC%	5.4	2.7	6.4	32.6	4.7	2.0	5.7

Table S4. Freundlich isotherm parameters K_f (sorption affinity) and n (linearity parameter) for pyrene sorption measured by batch to the series of four biochars derived from miscanthus (MS) and soft wood (SW) at 550 and 700 °C.

s.e. is the standard error associated with nonlinear fit, and N is the number of data point considered.

	$K_f (\mu\text{g/kg})/(\mu\text{g/L})^n$	<i>s.e.</i>	<i>n</i>	<i>Std.</i>	r^2	N
MS550	231472	11530	0.67	0.05	0.95	18
MS700	180889	9677	0.55	0.05	0.92	18
SW550	47216	2789	0.48	0.03	0.97	18
SW700	74397	3618	0.45	0.03	0.96	18

Table S5. Freundlich isotherm parameters K_f (sorption affinity, $(\mu\text{g/kg})/(\mu\text{g/L})^n$) and n (linearity parameter) for pyrene sorption to the series of sorbents and their mixtures measured by a combination of batch and passive sampling methods (biochar was only measured by batch). K_d and K_{oc} values were calculated at 0.02 and 2 $\mu\text{g/L}$ to allow direct comparisons.

s.e. is the standard error associated with nonlinear fit, and N is the number of data point considered. CL and SL refer to Clay Loam and Sandy Loam, respectively.

	K_f	<i>s.e.</i>	<i>n</i>	<i>s.e.</i>	r^2	N	$K_d0.02$	K_d2	$K_{oc0.02}$	K_{oc2}
Biochar (B) ^a	231472	11530	0.67	0.05	0.95	18	8.32E+05	1.85E+05	1.11E+06	2.46E+05
Compost (C)	30780	410	0.89	0.01	1.00	29	4.75E+04	2.85E+04	7.57E+04	7.80E+03
B + C	44513	770	0.73	0.02	0.99	27	1.26E+05	3.70E+04	3.87E+05	1.14E+05
Clay Loam	2322	74	0.75	0.02	1.00	25	6.18E+03	1.95E+03	3.55E+05	1.12E+05
CL + B	6482	74	0.69	0.01	0.99	29	2.19E+04	5.23E+03	4.05E+05	9.67E+04
CL + C	5050	79	0.90	0.02	0.99	28	7.41E+03	4.72E+03	2.74E+05	1.74E+05
CL + B + C	9978	213	0.89	0.03	0.98	31	1.53E+04	9.25E+03	2.41E+05	1.45E+05
Sandy Loam	1699	107	0.73	0.03	0.99	24	4.87E+03	1.41E+03	4.87E+05	1.41E+05
SL + B	4168	110	0.69	0.03	0.98	29	1.38E+04	3.37E+03	2.93E+05	7.18E+04
SL + C	4926	89	0.88	0.03	0.99	29	7.84E+03	4.54E+03	3.84E+05	2.22E+05
SL + B + C	6990	169	0.81	0.03	0.97	30	1.46E+04	6.13E+03	2.55E+05	1.07E+05

^a Sorption to the biochar (MS550) was only measured by batch.

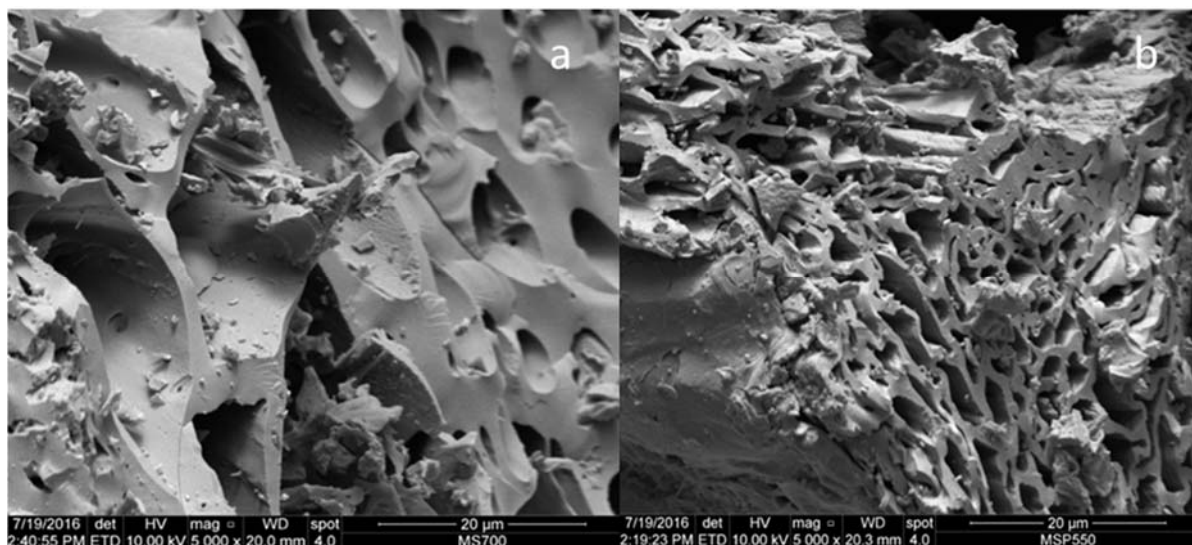


Figure S1. Scanning electron microscope images of the biochars produced from miscanthus straw at (a) 700°C and (b) 550°C

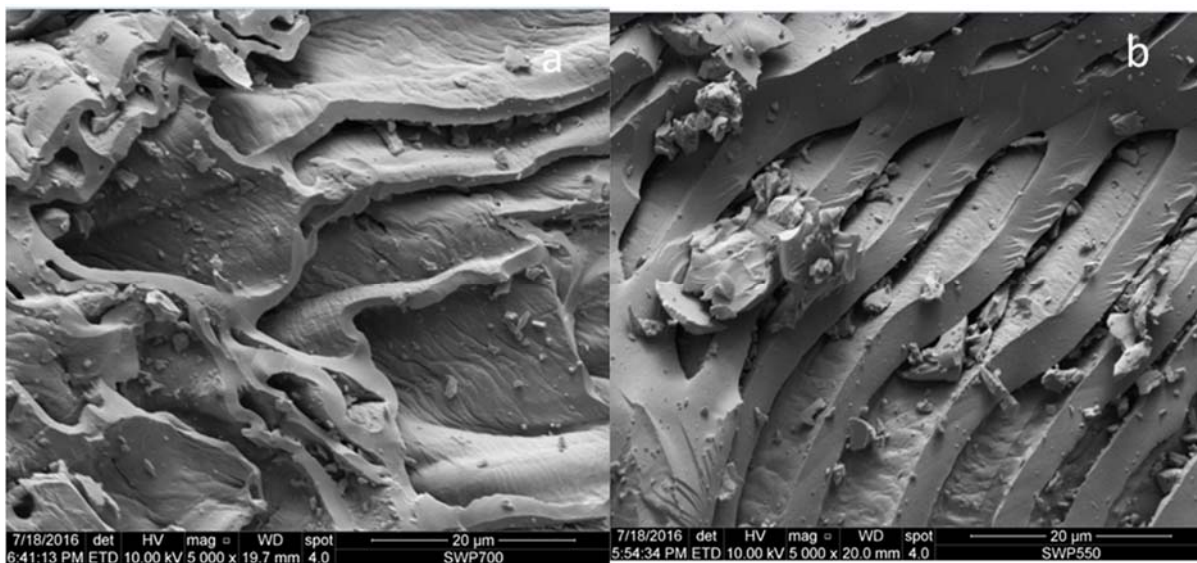


Figure S2. Scanning electron microscope images of the biochars produced from soft wood at (a) 700°C and (b) 550°C

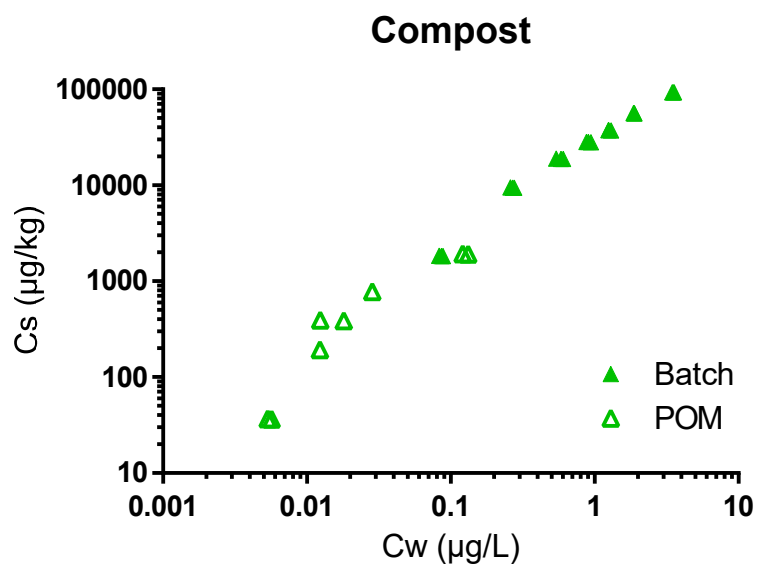


Figure S3. Sorption isotherm of pyrene to compost measured by batch (full symbols) and the POM method (open symbols).

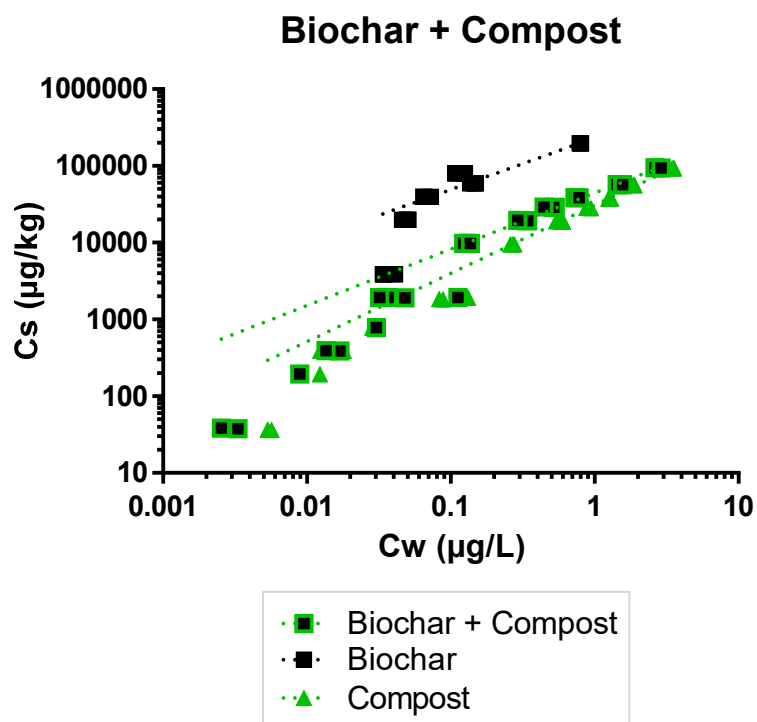


Figure S4. Sorption isotherms of pyrene to the biochar (black squares), compost (green triangles), and their mixture (1:2, green and black squares) represented in a logarithmic scale.

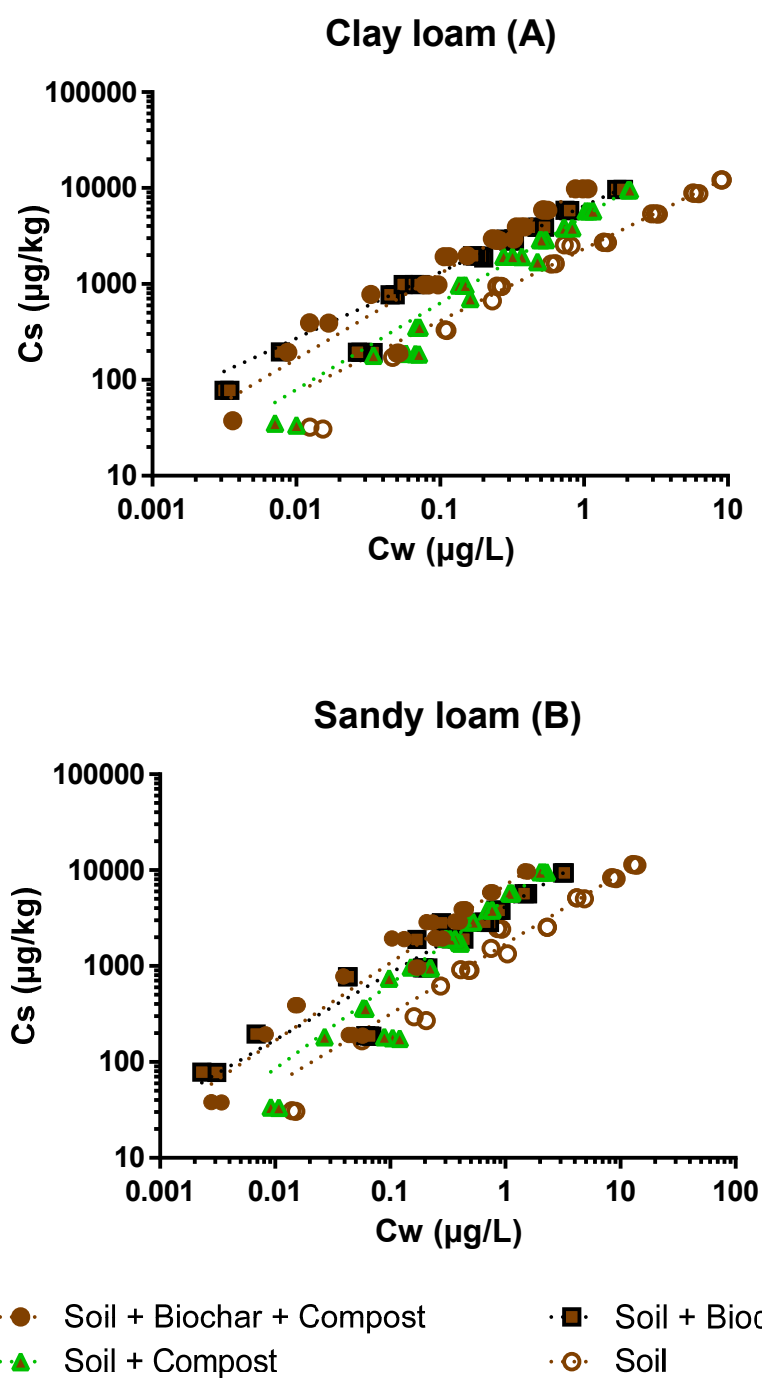


Figure S5. Sorption isotherms of pyrene to the clay loam (A) and sandy loam (B) before (open brown circles) and after addition of 5% biochar (black squares), 10% compost (green triangles) or both (full brown circles).