

## Supplementary Material

# Separation of Pharmaceuticals and Nutrients in Synthetic Urine Using Biochar

Avni Solanki<sup>1,\*</sup> and Treavor H. Boyer<sup>2</sup>

<sup>1</sup>Department of Environmental Engineering Sciences  
Engineering School of Sustainable Infrastructure & Environment (ESSIE)  
University of Florida  
P.O. Box 116450  
Gainesville, Florida 32611-6450, USA

<sup>2</sup>School of Sustainable Engineering and the Built Environment  
Ira A. Fulton Schools of Engineering  
Arizona State University  
P.O. Box 873005  
Tempe, AZ 85287-3005, USA

\*Corresponding author.

Tel.: 1-321-439-4786

E-mail addresses: [avnisol@ufl.edu](mailto:avnisol@ufl.edu) (A. Solanki), [thboyer@asu.edu](mailto:thboyer@asu.edu) (T.H. Boyer).

Submitted to Environmental Science: Water Research and Technology

August 24, 2014

Revised manuscript submitted January 23, 2017

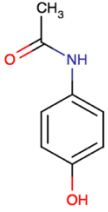
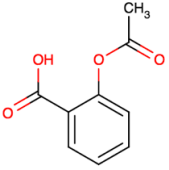
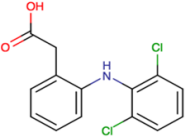
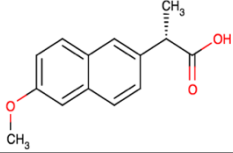
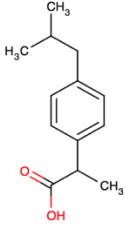
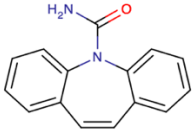
**Table S1:** Pharmaceutical loading (mg/g) on biochar at the 0.8 g/L dose.

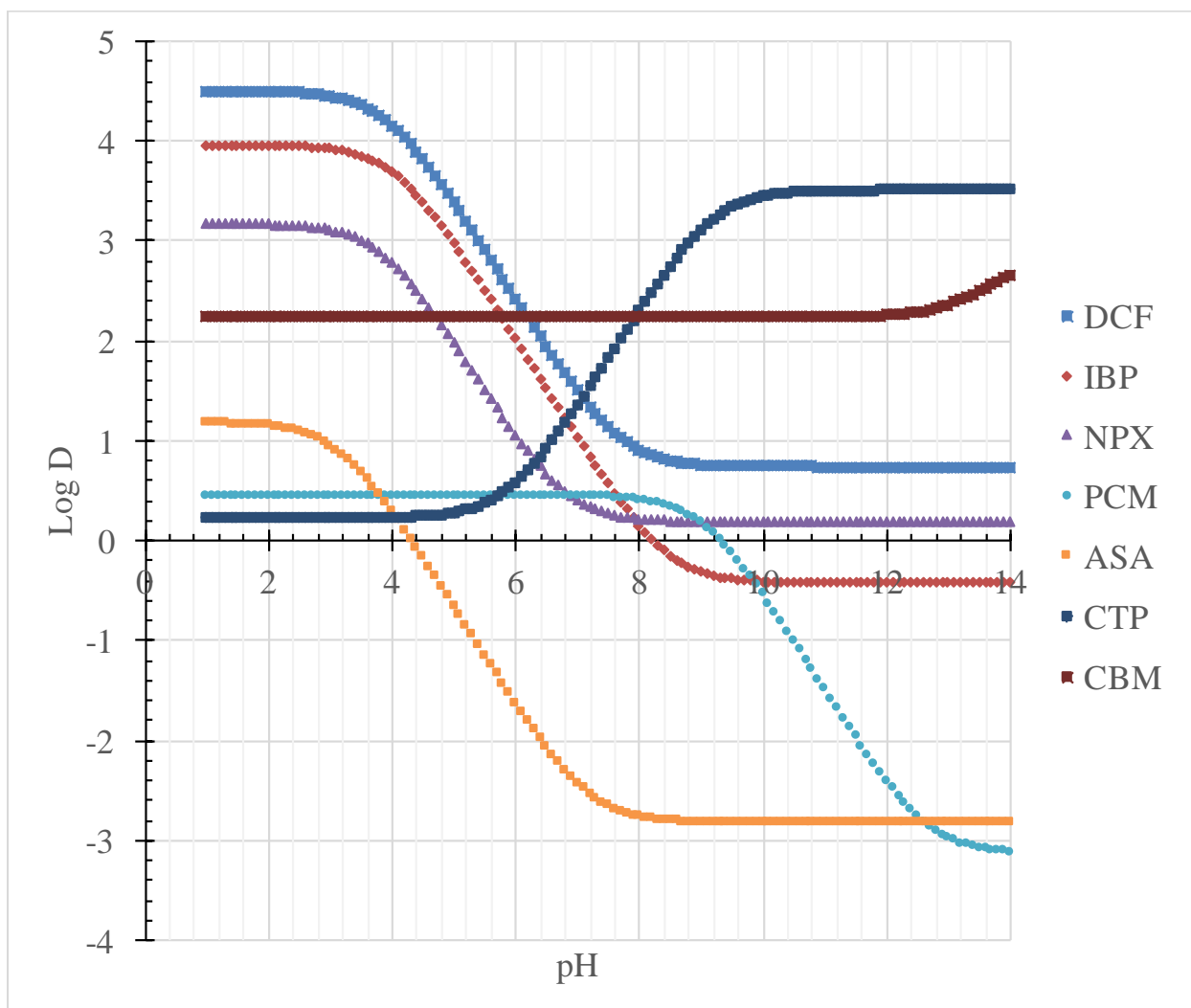
<b>Pharmaceutical</b>	<b>Bamboo</b>	<b>Activated Coconut</b>	<b>Southern Yellow Pine</b>	<b>Coconut Shell</b>	<b>Northern Hardwood</b>
<b>ASA</b>	3.13	38.9	7.94	1.13	0.28
<b>CBM</b>	8.09	55.7	14.3	1.03	1.30
<b>CTP</b>	9.71	62.7	20.5	4.29	1.55
<b>DCF</b>	9.72	73.4	16.2	0.53	2.39
<b>IBP</b>	6.43	44.8	10.2	1.67	1.66
<b>NPX</b>	8.83	56.6	21.3	8.55	2.16
<b>PCM</b>	11.1	37.2	18.0	1.13	1.83

**Table S2:** Pharmaceutical loading (mg/g) on biochar at the 40 g/L dose.

<b>Pharmaceutical</b>	<b>Bamboo</b>	<b>Activated Coconut</b>	<b>Southern Yellow Pine</b>	<b>Coconut Shell</b>	<b>Northern Hardwood</b>
<b>ASA</b>	0.27	0.78	0.67	0.00	0.41
<b>CBM</b>	1.00	1.12	1.11	0.43	0.73
<b>CTP</b>	1.31	1.81	1.78	0.88	0.78
<b>DCF</b>	1.44	1.52	1.51	0.12	0.71
<b>IBP</b>	0.76	0.94	0.92	0.08	0.57
<b>NPX</b>	1.02	1.16	1.13	0.43	0.78
<b>PCM</b>	0.61	0.76	0.74	0.35	0.74

**Table S3:** Hydrogen bonding inclination for each pharmaceutical.<sup>1</sup>

Pharmaceutical	Chemical Structure	H-bonding acceptor count	H-Bonding donor count
Paracetamol CAS 103-90-2		2	2
Acetylsalicylic Acid CAS 50-78-2		3	1
Diclofenac CAS 15307-79-6		3	2
Naproxen CAS 26159-54-2		3	1
Ibuprofen CAS 31121-9304		2	1
Carbamazepine CAS 298-46-4		1	1



**Figure S1:** Octanol-water partition coefficient (log D) versus pH for seven pharmaceuticals tested following methods by Jafvert et al.<sup>2</sup>

### Log D Calculation Method and Results:

The logD calculations were completed as prescribed in previous research<sup>3</sup> with values obtained from ChemAxon in Marvin Suite v6.3.0.<sup>1</sup> Figure S1 shows that DCF, IBP, NPX, PCM and ASA have decreasing log D values as pH increases. DCF and NPX have two aromatic rings which account for the higher hydrophobicity in comparison to IBP and NPX. In addition, DCF contains two chlorine groups that enhance the hydrophobicity of this compound due to the larger size of chlorine atoms. CBM displays consistent hydrophobic behavior due to the high pK<sub>a</sub> value, presence of 2 aromatic rings and a heterocyclic feature. CTP is the only positively charged pharmaceutical studied, as a result, CTP exhibits an opposite trend of increasing hydrophobicity as pH increases. The presence of one aromatic ring, heterocyclic feature, and halogen functional group generate the increased hydrophobicity. The logD results demonstrate that the refractive

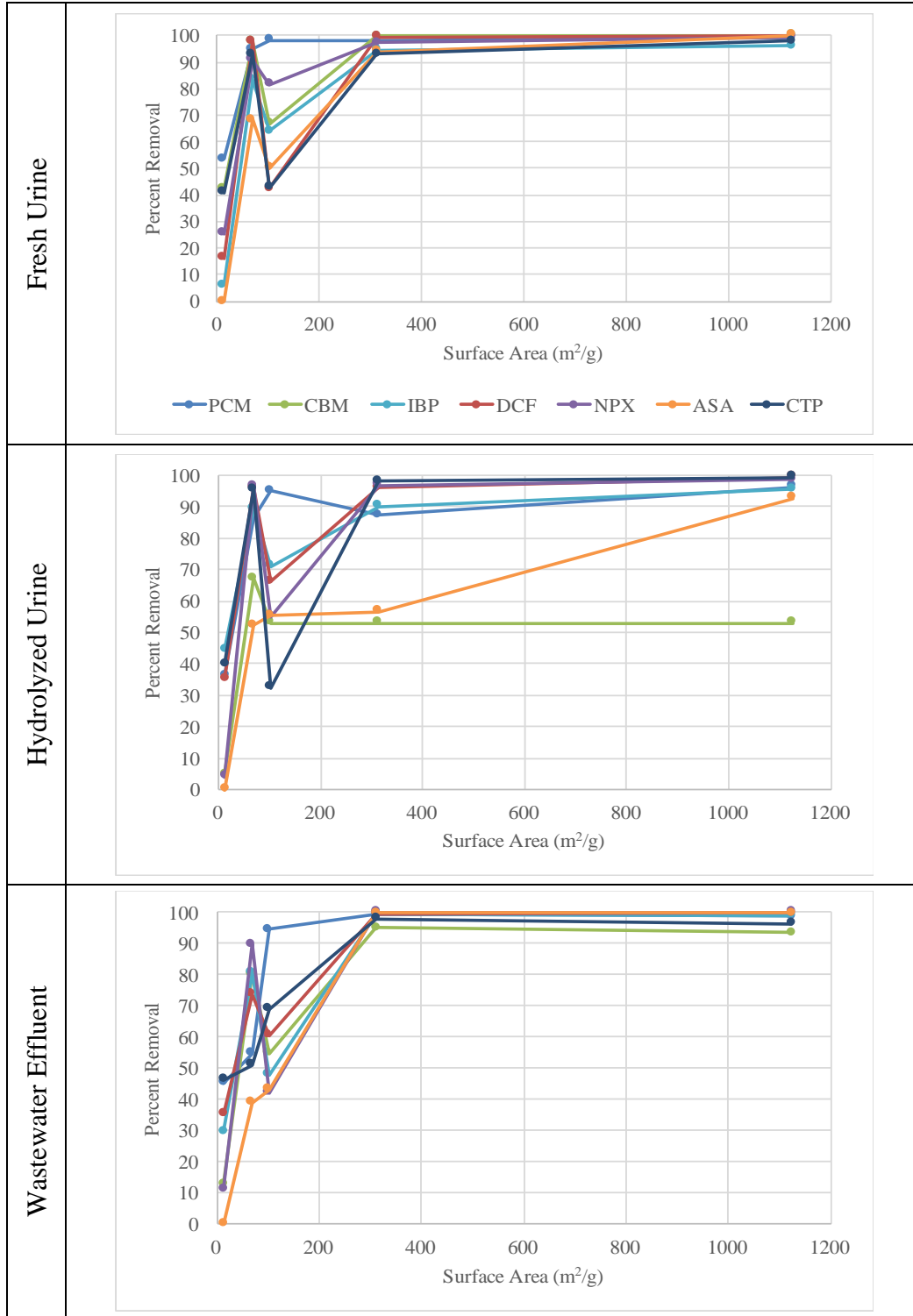
index and logK<sub>ow</sub> values alone are not suitable indicators of the hydrophobicity of a compound that has ionizable fractions.

**Table S4:** Two factor ANOVA statistical analysis ( $\alpha = 0.05$ )

<b>Pharmaceutical</b>	<b>Biochar dose (g/L)</b>	<b>p-value factor i.<sup>a</sup></b>	<b>p-value factor ii.<sup>b</sup></b>
<b>ASA</b>	0.8	5.13E-31	4.02E-10
<b>ASA</b>	40	1.88E-25	5.66E-10
<b>CBM</b>	0.8	1.46E-41	1.70E-12
<b>CBM</b>	40	1.24E-30	3.71E-10
<b>CTP</b>	0.8	7.77E-36	7.80E-10
<b>CTP</b>	40	7.37E-20	9.72E-02
<b>DCF</b>	0.8	4.10E-27	8.52E-03
<b>DCF</b>	40	6.47E-38	3.38E-05
<b>IBP</b>	0.8	5.20E-33	2.02E-07
<b>IBP</b>	40	8.86E-37	1.21E-02
<b>NPX</b>	0.8	3.82E-31	5.84E-13
<b>NPX</b>	40	1.67E-33	1.35E-18
<b>PCM</b>	0.8	1.17E-42	3.18E-04
<b>PCM</b>	40	2.78E-22	7.82E-07

<sup>a</sup>Factor i. conducted for statistical significance for pharmaceutical removal between biochars.

<sup>b</sup>Factor ii. conducted for statistical significance for waste water compositions



**Figure S2:** Surface area versus percent removal in fresh urine, hydrolyzed urine and wastewater effluent.

**Table S5:** Biopolymer make-up for each biochar <sup>4-6</sup>

<b>Biochar</b>	<b>Source Material</b>	<b>Lignin (%)</b>	<b>Hemicellulose (%)</b>	<b>Cellulose (%)</b>
<b>BB</b>	Bamboo	23	25	47
<b>AC</b>	Coconut	28	27	42
<b>SW</b>	Softwood	22	32	41
<b>CS</b>	Coconut Shell	50	35	15
<b>HW</b>	Hardwood	30	68	19

**Table S6:** Phosphate loading (mg/g) on biochar in fresh urine

	<b>ASA</b>	<b>CBM</b>	<b>CTP</b>	<b>DCF</b>	<b>IBP</b>	<b>NPX</b>	<b>PCM</b>
<b>Bamboo</b>	-0.20	0.14	0.89	6.36	1.28	7.67	1.93
<b>Activated Coconut</b>	7.23	4.59	7.57	16.2	6.24	14.7	8.18
<b>Southern Yellow Pine</b>	3.52	2.68	3.38	7.32	4.00	11.4	3.35
<b>Coconut Shell</b>	-0.61	0.14	-0.48	2.75	0.27	5.23	0.15
<b>Northern Hardwood</b>	5.51	3.96	7.33	6.52	6.35	11.2	7.90

**Table S7:** Phosphate loading (mg/g) on biochar in hydrolyzed urine.

	<b>ASA</b>	<b>CBM</b>	<b>CTP</b>	<b>DCF</b>	<b>IBP</b>	<b>NPX</b>	<b>PCM</b>
<b>Bamboo</b>	-0.12	-0.41	-0.15	1.33	-1.47	-0.95	-0.60
<b>Activated Coconut</b>	1.80	1.29	1.91	1.90	1.37	2.21	1.49
<b>Southern Yellow Pine</b>	3.05	1.74	2.78	-1.65	1.71	0.99	2.57

<b>Coconut Shell</b>	1.22	-0.04	1.28	-1.83	-0.07	-0.81	0.13
<b>Northern Hardwood</b>	0.88	1.14	0.05	0.32	0.17	0.27	0.06

**Table S8:** Phosphate loading (mg/g) on biochar in wastewater effluent.

	<b>ASA</b>	<b>CBM</b>	<b>CTP</b>	<b>DCF</b>	<b>IBP</b>	<b>NPX</b>	<b>PCM</b>
<b>Bamboo</b>	-0.51	-0.63	-0.51	-0.43	-0.37	-0.41	-0.51
<b>Activated Coconut</b>	0.04	0.04	0.03	0.03	0.04	0.03	0.04
<b>Southern Yellow Pine</b>	-0.06	-0.06	-0.06	-0.09	-0.07	-0.04	-0.06
<b>Coconut Shell</b>	-0.16	-0.13	-0.10	-0.12	-0.13	-0.09	-0.11
<b>Northern Hardwood</b>	0.02	0.01	0.02	0.01	0.01	0.01	0.01

**Table S9:** Nitrogen loading (mg/g) on biochar in fresh urine and hydrolyzed urine for representative batch

	<b>Fresh</b>	<b>Hydrolyzed</b>
<b>Bamboo</b>	18.9	20.4
<b>Activated Coconut</b>	17.34	27.5
<b>Southern Yellow Pine</b>	6.89	35.9
<b>Coconut Shell</b>	-1.82	28.3



<b>Northern Hardwood</b>	-6.83	24.7
--------------------------	-------	------

**Table S10:** pH and conductivity values for ASA

<b>Fresh Urine</b>				
<b>Biochar</b>	<b><u>0.8 g/L dose</u></b>		<b><u>40 g/L dose</u></b>	
	<b>pH</b>	<b>Conductivity (mS/cm)</b>	<b>pH</b>	<b>Conductivity (mS/cm)</b>
Bamboo	6.03	17.2	7.29	19.1
Activated Coconut	5.89	17.5	7.40	17.3
Southern Yellow Pine	5.94	17.4	6.31	17.2
Coconut Shell	6.01	17.7	6.17	17.6
Northern Hardwoods	5.99	17.5	6.99	17.7
Control	6.05	17.7	6.05	17.7
<b>Hydrolyzed Urine</b>				
<b>Biochar</b>	<b><u>0.8 g/L dose</u></b>		<b><u>40 g/L dose</u></b>	
	<b>pH</b>	<b>Conductivity (mS/cm)</b>	<b>pH</b>	<b>Conductivity (mS/cm)</b>
Bamboo	9.25	39.2	9.25	38.1
Activated Coconut	9.24	37.6	9.23	37.7
Southern Yellow Pine	9.23	39.0	9.20	38.4
Coconut Shell	9.24	38.5	9.20	37.1
Northern Hardwoods	9.23	39.0	9.23	38.7
Control	9.23	39.0	9.23	39.0
<b>Wastewater Effluent</b>				
<b>Biochar</b>	<b><u>0.8 g/L dose</u></b>		<b><u>40 g/L dose</u></b>	
	<b>pH</b>	<b>Conductivity (<math>\mu</math>S/cm)</b>	<b>pH</b>	<b>Conductivity (<math>\mu</math>S/cm)</b>
Bamboo	7.22	162	10.2	1690
Activated Coconut	7.60	119	8.75	317
Southern Yellow Pine	7.50	117	8.15	292
Coconut Shell	7.32	102	7.74	271
Northern Hardwoods	7.42	116	8.11	232
Control	7.25	100	7.25	100

**Table S11:** pH and conductivity values for CBM

<b>Fresh Urine</b>				
<b>Biochar</b>	<b><u>0.8 g/L dose</u></b>		<b><u>40 g/L dose</u></b>	
	<b>pH</b>	<b>Conductivity (mS/cm)</b>	<b>pH</b>	<b>Conductivity (mS/cm)</b>
Bamboo	6.01	17.8	7.13	19.2

Activated Coconut	5.96	17.8	7.72	17.8
Southern Yellow Pine	6.01	17.8	6.33	17.5
Coconut Shell	5.93	17.7	6.20	18.1
Northern Hardwoods	5.94	17.8	6.72	17.9
Control	5.91	18.1	5.91	18.1

### Hydrolyzed Urine

Biochar	<u>0.8 g/L dose</u>		<u>40 g/L dose</u>	
	pH	Conductivity (mS/cm)	pH	Conductivity (mS/cm)
Bamboo	9.49	47.0	9.49	47.4
Activated Coconut	9.50	46.7	9.49	46.9
Southern Yellow Pine	9.50	46.7	9.45	46.3
Coconut Shell	9.50	46.8	9.47	46.6
Northern Hardwoods	9.49	46.7	9.49	46.4
Control	9.49	46.2	9.49	46.2

### Wastewater Effluent

Biochar	<u>0.8 g/L dose</u>		<u>40 g/L dose</u>	
	pH	Conductivity ( $\mu$ S/cm)	pH	Conductivity ( $\mu$ S/cm)
Bamboo	6.11	144	10.3	1630
Activated Coconut	6.20	124	10.4	359
Southern Yellow Pine	5.82	123	6.46	295
Coconut Shell	6.03	108	6.09	263
Northern Hardwoods	5.74	114	7.90	263
Control	7.78	225	7.78	225

**Table S12:** pH and conductivity values for CTP

### Fresh Urine

Biochar	<u>0.8 g/L dose</u>		<u>40 g/L dose</u>	
	pH	Conductivity (mS/cm)	pH	Conductivity (mS/cm)
Bamboo	6.02	17.7	7.23	19.1
Activated Coconut	5.99	17.6	7.52	17.8
Southern Yellow Pine	6.00	17.4	6.30	17.5
Coconut Shell	6.14	17.4	6.10	17.4
Northern Hardwoods	5.96	17.1	6.70	17.6
Control	6.02	17.6	6.05	17.6

### Hydrolyzed Urine

	<u>0.8 g/L dose</u>	<u>40 g/L dose</u>
--	---------------------	--------------------

<b>Biochar</b>	<b>pH</b>	<b>Conductivity (mS/cm)</b>	<b>pH</b>	<b>Conductivity (mS/cm)</b>
Bamboo	9.22	41.3	9.25	42.5
Activated Coconut	9.21	40.2	9.23	39.9
Southern Yellow Pine	9.23	39.9	9.20	41.4
Coconut Shell	9.23	40.1	9.20	38.1
Northern Hardwoods	9.25	41.1	9.23	41.2
Control	9.23	40.8	9.23	40.8

### **Wastewater Effluent**

<b>Biochar</b>	<b><u>0.8 g/L dose</u></b>		<b><u>40 g/L dose</u></b>	
	<b>pH</b>	<b>Conductivity (<math>\mu</math>S/cm)</b>	<b>pH</b>	<b>Conductivity (<math>\mu</math>S/cm)</b>
Bamboo	7.32	172	10.2	1616
Activated Coconut	7.81	166	8.75	380
Southern Yellow Pine	7.45	144	8.15	315
Coconut Shell	7.22	128	7.74	285
Northern Hardwoods	7.45	142	8.11	301
Control	7.28	127	7.28	127

**Table S13:** pH and conductivity values for DCF

### **Fresh Urine**

<b>Biochar</b>	<b><u>0.8 g/L dose</u></b>		<b><u>40 g/L dose</u></b>	
	<b>pH</b>	<b>Conductivity (mS/cm)</b>	<b>pH</b>	<b>Conductivity (mS/cm)</b>
Bamboo	6.08	14.4	6.91	15.1
Activated Coconut	5.95	14.3	7.58	14.4
Southern Yellow Pine	5.98	14.2	6.41	14.1
Coconut Shell	5.92	14.2	6.14	14.5
Northern Hardwoods	5.98	14.3	6.58	14.3
Control	6.07	14.3	6.07	14.4

### **Hydrolyzed Urine**

<b>Biochar</b>	<b><u>0.8 g/L dose</u></b>		<b><u>40 g/L dose</u></b>	
	<b>pH</b>	<b>Conductivity (mS/cm)</b>	<b>pH</b>	<b>Conductivity (mS/cm)</b>
Bamboo	9.28	36.1	9.28	36.6
Activated Coconut	9.33	36.4	9.33	36.5
Southern Yellow Pine	9.33	36.7	9.31	36.2
Coconut Shell	9.33	36.9	9.29	36.9
Northern Hardwoods	9.32	36.9	9.31	36.9
Control	9.32	36.9	9.32	36.9

<b>Wastewater Effluent</b>				
<b>Biochar</b>	<b>0.8 g/L dose</b>		<b>40 g/L dose</b>	
	<b>pH</b>	<b>Conductivity (<math>\mu\text{S/cm}</math>)</b>	<b>pH</b>	<b>Conductivity (<math>\mu\text{S/cm}</math>)</b>
Bamboo	7.50	145	10.2	1700
Activated Coconut	7.98	148	10.6	368
Southern Yellow Pine	7.92	153	8.04	313
Coconut Shell	7.76	130	7.96	281
Northern Hardwoods	7.19	142	10.2	298
Control	7.73	125	7.73	125

**Table S14:** pH and conductivity values for IBP

<b>Fresh Urine</b>				
<b>Biochar</b>	<b>0.8 g/L dose</b>		<b>40 g/L dose</b>	
	<b>pH</b>	<b>Conductivity (mS/cm)</b>	<b>pH</b>	<b>Conductivity (mS/cm)</b>
Bamboo	6.01	17.8	7.13	19.2
Activated Coconut	5.96	17.8	7.72	17.7
Southern Yellow Pine	6.01	17.8	6.33	17.5
Coconut Shell	5.93	17.7	6.20	18.1
Northern Hardwoods	5.94	17.8	6.72	17.9
Control	5.91	18.1	5.91	18.1

<b>Hydrolyzed Urine</b>				
<b>Biochar</b>	<b>0.8 g/L dose</b>		<b>40 g/L dose</b>	
	<b>pH</b>	<b>Conductivity (mS/cm)</b>	<b>pH</b>	<b>Conductivity (mS/cm)</b>
Bamboo	9.31	41.4	9.49	42.1
Activated Coconut	9.30	39.2	9.49	40.3
Southern Yellow Pine	9.25	40.4	9.45	41.0
Coconut Shell	9.35	38.9	9.47	39.4
Northern Hardwoods	9.37	40.3	9.49	40.2
Control	9.34	40.1	9.34	40.1

<b>Wastewater Effluent</b>				
<b>Biochar</b>	<b>0.8 g/L dose</b>		<b>40 g/L dose</b>	
	<b>pH</b>	<b>Conductivity (<math>\mu\text{S/cm}</math>)</b>	<b>pH</b>	<b>Conductivity (<math>\mu\text{S/cm}</math>)</b>
Bamboo	7.55	186	9.93	1210
Activated Coconut	8.02	199	10.1	382
Southern Yellow Pine	8.11	165	7.91	331
Coconut Shell	7.85	152	7.77	301
Northern Hardwoods	7.45	171	9.35	299

Control	8.18	154	8.18	154
---------	------	-----	------	-----

**Table S15:** pH and conductivity values for NPX

<b>Fresh Urine</b>				
<b>Biochar</b>	<b>0.8 g/L dose</b>		<b>40 g/L dose</b>	
	<b>pH</b>	<b>Conductivity (mS/cm)</b>	<b>pH</b>	<b>Conductivity (mS/cm)</b>
Bamboo	5.06	13.7	6.87	15.1
Activated Coconut	5.27	13.8	7.32	13.6
Southern Yellow Pine	5.12	13.8	6.14	13.6
Coconut Shell	4.78	13.8	5.81	14.0
Northern Hardwoods	5.01	13.9	6.27	13.8
Control	5.04	13.8	5.04	13.7
<b>Hydrolyzed Urine</b>				
<b>Biochar</b>	<b>0.8 g/L dose</b>		<b>40 g/L dose</b>	
	<b>pH</b>	<b>Conductivity (mS/cm)</b>	<b>pH</b>	<b>Conductivity (mS/cm)</b>
Bamboo	9.25	38.3	9.26	39.3
Activated Coconut	9.26	38.3	9.25	37.8
Southern Yellow Pine	9.26	38.2	9.21	37.7
Coconut Shell	9.24	38.2	9.20	38.3
Northern Hardwoods	9.26	38.3	9.24	38.3
Control	9.26	38.6	9.26	38.6
<b>Wastewater Effluent</b>				
<b>Biochar</b>	<b>0.8 g/L dose</b>		<b>40 g/L dose</b>	
	<b>pH</b>	<b>Conductivity (<math>\mu</math>S/cm)</b>	<b>pH</b>	<b>Conductivity (<math>\mu</math>S/cm)</b>
Bamboo	7.01	170	10.19	1710
Activated Coconut	7.32	121	9.42	389
Southern Yellow Pine	6.99	147	7.40	312
Coconut Shell	7.12	167	7.39	287
Northern Hardwoods	7.09	155	8.10	230
Control	7.25	167	7.25	167

**Table S16:** pH and conductivity values for PCM

<b>Fresh Urine</b>				
<b>Biochar</b>	<b>0.8 g/L dose</b>		<b>40 g/L dose</b>	
	<b>pH</b>	<b>Conductivity (mS/cm)</b>	<b>pH</b>	<b>Conductivity (mS/cm)</b>
Bamboo	6.01	17.8	7.13	19.2
Activated Coconut	5.96	17.8	7.72	17.7
Southern Yellow Pine	6.01	17.8	6.33	17.5

Coconut Shell	5.93	17.7	6.20	18.1
Northern Hardwoods	5.94	17.8	6.72	17.9
Control	5.91	18.1	5.91	18.1

### Hydrolyzed Urine

Biochar	<u>0.8 g/L dose</u>		<u>40 g/L dose</u>	
	pH	Conductivity (mS/cm)	pH	Conductivity (mS/cm)
Bamboo	9.49	47.0	9.49	47.3
Activated Coconut	9.50	46.6	9.49	46.9
Southern Yellow Pine	9.50	46.6	9.45	46.2
Coconut Shell	9.50	46.8	9.47	46.6
Northern Hardwoods	9.49	46.6	9.49	46.4
Control	9.49	46.1	9.49	46.1

### Wastewater Effluent

Biochar	<u>0.8 g/L dose</u>		<u>40 g/L dose</u>	
	pH	Conductivity ( $\mu$ S/cm)	pH	Conductivity ( $\mu$ S/cm)
Bamboo	5.91	143	10.32	1670
Activated Coconut	6.21	124	10.31	356
Southern Yellow Pine	5.78	117	6.48	298
Coconut Shell	5.99	108	6.26	267
Northern Hardwoods	5.94	121	9.23	260
Control	6.58	106	6.58	106

1. ChemAxon, *Journal*, 2014, **v6.3.0**.
2. C. T. Jafvert, J. C. Westall, E. Grieder and R. P. Schwarzenbach, *Environmental Science & Technology*, 1990, **24**, 1795-1803.
3. C. T. Jafvert, J. C. Westall, E. Grieder and R. P. Schwarzenbach, *Environmental Science & Technology*, 1990, **24**, 1795-1803.
4. B. Cagnon, X. Py, A. Guillot, F. Stoeckli and G. Chambat, *Bioresource Technology*, 2009, **100**, 292-298.
5. W. M. Daud and W. S. Ali, *Bioresour Technol*, 2004, **93**, 63-69.
6. R. C. Pettersen, *Advances in Chemistry Series*, 1984, **207**, 57-126.