Supplementary information

Tetracycline removal with activated carbons produced by hydrothermal carbonisation of Agave americana fibres and mimosa tannin

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The carbon yield, Y_C , was calculated according to Equation SI 1, wherein "db" means on dry basis:

$$Y_{C}(\%) = \left(\frac{CTAW(g)}{TAW(g)}\right)_{db} \times 100$$
 Equation SI 1

As the first series of materials was prepared in one single step only, the total yield of the process, $Y_{T,C}$ (%), is:

$$Y_{T,C}$$
 (%) = Y_C (%) Equation SI 2

The HTC yield, Y_H (%), was calculated according to Equation SI 3, wherein HTAW (g) is the mass of hydrochar after drying in an oven at 105°C:

$$Y_H (\%) = \left(\frac{HTAW(g)}{TAW(g)}\right)_{db} \times 100$$
 Equation SI 3

If only the HTC process is considered, we can write that the total yield of the process,

 $Y_{T,H}$ (%), is the yield of the HTC treatment:

$$Y_{T,H}(\%) = Y_H(\%)$$
Equation SI 4

The carbon yield after HTC, Y_{CH} (%), was calculated as:

$$Y_{CH} (\%) = \left(\frac{CHTAW(g)}{HTAW(g)}\right)_{db} \times 100$$
 Equation SI 5

and the total yield of the process, $Y_{T,CH}$ (%), is therefore:

$$Y_{T,CH} (\%) = \frac{Y_H (\%) \times Y_{CH} (\%)}{100} = \left(\frac{CHTAW (g)}{TAW(g)}\right)_{db} \times 100$$
 Equation SI 6



Figure SI 1: CO_2 adsorption isotherms for: (a) CTAW; (b) CHTAW; and (c) act_CHTA2/2 series.



Figure SI 2: SEM images of: (a) ac2_CHTAW2/2; and (b) ac3_CHTAW2/2.

Table SI 1: Theoretical, Y_{th} , experimental, Y_{exp} , and total, Y_T , yields (wt. %), and elemental composition (wt. %) of Tannin, Agave and T/A blends as such and after HTC, pyrolysis and activation.

				Elemental composition (wt. %)					
Sample	<i>Y_{th}</i> (wt.%)	<i>Y_{exp}</i> (wt.%)	<i>Y_T</i> (wt.%)	С	Н	Ν	0		
Agave fibres (A)	-	-		43.87	6.47	0.22	49.08		
Tannin (T)	-	-		55.29	5.04	0.23	38.86		
HTA0/4	63.4	63.4	63.3	45.58	6.39	0.14	47.61		
HTA1/3	62.1	66.8	66.8	48.66	5.89	0.24	45.19		
HTA2/2	60.8	67.3	67.3	54.2	5.41	0.21	42.14		
HTA3/1	59.5	64.3	64.3	55.08	5.27	0.18	39.69		
HTA4/0	58.2	58.2	58.2	60.39	4.40	0.23	34.81		
CTA0/4	21.4	21.4	21.4	78.78	0.95	0.43	12.89		
CTA1/3	27.8	27.9	27.9	83.12	0.77	0.61	9.42		
CTA2/2	34.1	34.5	34.5	83.52	0.73	0.41	8.56		
CTA3/1	40.44	40.38	40.4	86.33	0.77	0.46	7.64		
CTA4/0	46.77	46.77	46.8	91.04	0.64	0.71	5.78		
CHTA0/4	16.3	16.3	10.3	87.83	1.38	0.25	9.92		
CHTA1/3	24.6	24.6	16.4	92.84	1.155	0.35	7.27		
CHTA2/2	32.9	35.9	24.2	94.05	1.14	0.27	7.42		
CHTA3/1	41.2	40.1	25.7	92.86	1.23	0.23	6.06		
CHTA4/0	49.6	49.6	28.8	94.58	0.97	0.31	5.52		
ac1_CHTA2/2	-	73.3	17.7	95	0.41	0.31	3.11		
ac2_CHTA2/2	-	58.9	14.2	95.13	0.38	0.44	2.78		
ac3_CHTA2/2	-	45.0	10.9	94.93	0.35	0.42	2.42		

	N ₂						CO ₂	N ₂	$+ CO_2$
	S_{BET}	V _{DR. N2}	V_{mes}	V_{mes}	$V_{0.97}$	S_{Tot}	$V_{DR.CO2}$	S _{NLDFT}	$V_{micNLDFT}$
	(m ² /g)	(cm^3/g)	(cm^3/g)	(%)	(cm^3/g)	(m^2/g)	(cm^3/g)	(m^2/g)	(cm^3/g)
CTA0/4	321	0.12	0.03	20	0.15	68	0.21	591	0.14
CTA1/3	270	0.10	0.01	6	0.11	75	0.23	535	0.13
CTA2/2	273	0.11	0.03	22	0.14	94	0.24	539	0.13
CTA3/1	384	0.15	0.00	2	0.15	155	0.24	687	0.16
CTA4/0	546	0.21	0.01	5	0.22	255	0.27	772	0.21
CHTA0/4	406	0.15	0.05	26	0.20	41	0.27	697	0.17
CHTA1/3	666	0.25	0.10	28	0.35	109	0.28	941	0.26
CHTA2/2	654	0.25	0.05	18	0.30	158	0.29	881	0.25
CHTA3/1	657	0.25	0.04	13	0.29	169	0.29	908	0.26
CHTA4/0	683	0.26	0.02	8	0.28	197	0.31	941	0.27
ac1_CHTA2/2	621	0.24	0.07	22	0.30	110	0.36	934	0.24
ac2_CHTA2/2	1068	0.41	0.08	17	0.49	152	0.38	1292	0.40
ac3_CHTA2/2	1250	0.48	0.11	19	0.59	135	0.41	1431	0.46

Table SI 2: Textural parameters of ACs synthetised, obtained by adsorption-desorption of N_2 at -196°C and CO₂ at 0°C and applying BET, DR and NLDFT methods.

Table SI 3: Porosity data of act_CHTA2/2 derived from mercury porosimetry.

	ac1_CHTA2/2	Ac2_CHTA2/2	Ac3_CHTA2/2
Total intrusion volume ($cm^3 g^{-1}$)	3.69	5.11	5.55
Median pore diameter (Area) (µm)	0.68	1.28	1.39
Average pore diameter (4V/A) (μ m)	5.51	9.43	10.13
Apparent density $(g \text{ cm}^{-3})$	0.90	0.84	0.89
Available porosity (%)	76.88	81.11	83.12

Table SI 4: Kinetic parameters for TC adsorption calculated from the fits of kinetic models at 25° C, pH 4.5 and $C_0 = 100$ mg/L.

		PFO				PSO kinetics					
Sample	$q_{e,exp}$	<i>a</i> .	k.			h_1	<i>a</i> .	k_2			h_2
Sumple	(mg/g)	$q_{e,I}$	(\min^{-1})	R^2	χ^2	(mg/(g	$q_{e,2}$	(g/(mg.	g/(mg. R^2	χ^2	(mg/(g
		(1115/5)	(11111)			.min))	(1115/5)	min))			.min))
ac2_CHTA2/2	51.35	45.24	0.0385	0.919	17.94	1.741	49.79	0.0010	<u>0.975</u>	<u>5.53</u>	2.479
F300	28.58	28.73	0.0065	0.986	1.20	0.187	38.14	0.0001	<u>0.993</u>	<u>0.57</u>	0.145

Table SI 5: Constants of adsorption kinetics of TC onto ac2_CHTA2/2 sample at 25°C and pH 7 for different initial concentrations.

TC adsorption			Initia	l concent	ration of	TC (mg/	′L)	
TC ausorption	0.5	10	20	30	50	70	100	400
$q_{e,exp}$ (mg/g)	9.33	15.93	27.61	31.80	41.61	46.11	58.83	239.41
PFO kinetics								
$q_{e.1}(\mathrm{mg/g})$	8.70	13.74	25.13	27.99	35.68	39.85	54.53	216.84
$k_1 (\min^{-1})$	0.050	0.038	0.039	0.049	0.036	0.044	0.039	0.022
R^2	0.966	0.873	0.947	0.923	0.859	0.884	0.962	0.953
χ^2	0.258	2.646	3.541	6.327	19.931	19.914	12.146	260.085
h_1 (mg/(g.min))	0.437	0.519	0.969	1.379	1.293	1.744	2.146	4.749
PSO kinetics								
$q_{e.2}(\mathrm{mg/g})$	9.351	15.198	27.499	30.377	39.585	43.757	59.599	245.632
k_2 (g/(mg.min))	0.008	0.003	0.002	0.002	0.001	0.001	0.001	0.0001
R^2	<u>0.996</u>	<u>0.948</u>	<u>0.990</u>	<u>0.975</u>	<u>0.939</u>	<u>0.954</u>	<u>0.994</u>	<u>0.989</u>
χ^2	<u>0.031</u>	<u>1.076</u>	<u>0.668</u>	<u>2.029</u>	<u>8.522</u>	<u>7.925</u>	<u>1.854</u>	<u>63.554</u>
h_2 (mg/(g.min))	0.719	0.765	1.512	2.122	1.896	2.566	3.339	7.240

Table SI 6: Effect of pH and temperature on Langmuir and Freundlich isotherm constants for the adsorption of TC onto ac2_CHTA2/2.

Temperature		a		Langr	nuir		Freundlich				
(°C)	pН	(ma/a)	q_{max}	K_L	v^2	\mathbf{P}^2	K_F	11	χ^2	\mathbf{P}^2	
(C)		(IIIg/g)	(mg/g)	(L/mg)	ng) X	Λ	$(mg'g)(L/mg)^{1/n}$	п	λ	n	
	4	51.35	52.29	0.46	2.83	0.990	20.59	4.25	44.97	0.842	
25	7	58.83	62.23	0.33	2.22	0.995	22.05	3.91	53.28	0.872	
	10	59.23	65.56	0.14	5.18	0.988	15.38	2.97	23.74	0.943	
35	7	58.91	58.99	0.57	4.74	0.987	24.28	4.36	44.57	0.882	
50	7	81.21	87.21	0.42	28.07	0.968	31.26	3.82	197.17	0.775	