Supplementary material

Wheat straw as a Bio-Sorbent for Arsenate, Chromate, Fluoride, and Nickel

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Characterization of Wheat (*Triticum aestivum*) Straw

The wheat straw used was from a local provider (Cospeito, Lugo, Spain) and was previously characterized by Coelho et al. (2016). As indicated by these authors, it was dried milled and sieved, using particles between 2.0 and 0.5 mm for analyses.

The following analyses were carried out (see Coelho et al., 2016 for more details): pH in distilled water, pH in 0.1 M KCl (pH_{water}, pH_{KCl}) (ratio solid:solution 1:5), and the point of zero charge (pH_{PZC}), using a pH-meter (model 2001, Crison Instruments, Barcelona, Spain). A CHNS Truspec elemental analyzer (Leco, St. Joseph, MI, USA) was used to quantify total C and N contents. Available P was measured using the Olsen method, quantified by UV–visible spectrophotometry (UV-1201, Shimadzu, Kyoto, Japan). Total P was measured on 1 g samples treated with nitric acid (65%) and microwave-assisted digestion, using UV–visible spectroscopy (UV-1201, Shimadzu, Kyoto, Japan). Exchangeable cations were determined by extracting with 1 M NH_4Cl and quantified by means of atomic absorption/emission spectrophotometry (AAnalyst 200, Perkin Elmer, Shelton, CT, USA). The effective cation exchange capacity (eCEC) was calculated as the sum of exchangeable Ca, Mg, Na, K, and Al. Total contents of Ca, Mg, Na, K, Al, Fe, Mn, Cu, Zn, Ni, Cd, Cr, and Co were determined using microwave digestion in a 65% nitric acid solution, quantified by ICP Mass (Varian 820-MS, Varian, Palo Alto, CA, USA). To determine soluble F, 10 g of wheat straw were added with 100 mL of distilled water, shaken for 24 h, filtered with acid-washed paper (pore size 2.5 μm), and quantified by means of an ion selective electrode (Orion Research, Jacksonville, FL, USA) after the addition of a total ionic strength adjuster and the buffer TISAB IV. Total non-crystalline Al and Fe (Al_o, Fe_o) were determined spectroscopically after the extraction on 1 g samples using ammonium oxalate solutions acidified to pH 3 with oxalic acid. All determinations were performed by triplicate.

Table S1 shows chemical characteristics of the wheat straw used.

Table S1. Results of the chemical characterization of the wheat straw used. Average values for 3 replicates, with coefficients of variation always <5%).

Parameter	Value
C (%)	43.48
N (%)	0.55
pH_{water}	7.12
pH_{KCl}	6.92
pH_{pz}	6.68
Ca_e ($cmol_c\ kg^{-1}$)	4.44
Mg_e ($cmol_c\ kg^{-1}$)	2.22
Na_e ($cmol_c\ kg^{-1}$)	1.03
K_e ($cmol_c\ kg^{-1}$)	27.51
Al_e ($cmol_c\ kg^{-1}$)	0.00
eCEC ($cmol_c\ kg^{-1}$)	35.20
P_{Olsen} ($mg\ kg^{-1}$)	314.1
P_T ($mg\ kg^{-1}$)	979.8
Ca_T ($mg\ kg^{-1}$)	2210.4
Mg_T ($mg\ kg^{-1}$)	490.2
Na_T ($mg\ kg^{-1}$)	250.1
K_T ($mg\ kg^{-1}$)	10907.0
As_T ($mg\ kg^{-1}$)	0.05
Cr_T ($mg\ kg^{-1}$)	3.47
Soluble-F ($mg\ kg^{-1}$)	0.73
Ni_T ($mg\ kg^{-1}$)	2.36
Cd_T ($mg\ kg^{-1}$)	0.08
Co_T ($mg\ kg^{-1}$)	0.25
Cu_T ($mg\ kg^{-1}$)	2.93
Pb_T ($mg\ kg^{-1}$)	0.25
Zn_T ($mg\ kg^{-1}$)	17.57
Mn_T ($mg\ kg^{-1}$)	304
Al_T ($mg\ kg^{-1}$)	147.7
Fe_T ($mg\ kg^{-1}$)	76.79
Al_o ($mg\ kg^{-1}$)	60.03
Fe_o ($mg\ kg^{-1}$)	44.01

Notes: X_e: exchangeable concentration of the element; X_T: total concentration of the element; Al_o and Fe_o: Al and Fe extracted with ammonium oxalate

Infrared spectroscopy of wheat straw

The main functional groups present in wheat straw structure were determined using infrared spectroscopy on FTIR-Bomen MB102 equipment (ABB, Zürich, Switzerland), and the results have been previously published (Coelho et al., 2016). Briefly, the spectra were obtained by transmittance using KBr pellets, carrying out determinations in the 400–4000 cm^{-1} region, with a 4 cm^{-1} resolution (Figure. S1). FTIR spectrum—in the range of 400–4000 cm^{-1} (Figure S1)—showed the presence of carboxylic, hydroxyl, and amine functional groups on the surface of wheat straw, which can be of relevance in the retention of pollutants. More detailed explanation can be found in Coelho et al. (2016).

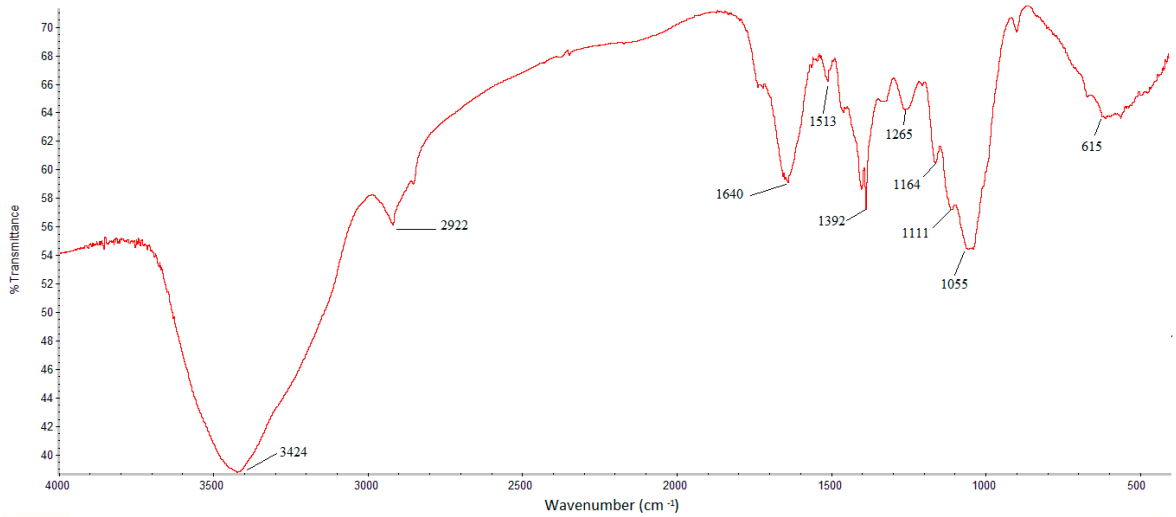

Figure S1. Infrared spectrum of wheat straw

References

Coelho, G.F.; GonÇalves, A.C., Jr.; Nóvoa-Muñoz, J.C.; Fernández-Calviño, D.; Arias-Estévez, M.; Fernández-Sanjurjo, M.J.; Álvarez-Rodríguez, E.; Núñez-Delgado, A. Competitive and non-competitive cadmium, copper and lead sorption/desorption on wheat straw affecting sustainability in vineyards. *J. Clean. Prod.* **2016**, *139*, 1496–1503, doi:10.1016/j.jclepro.2016.09.021.