Electronic Supplementary Material (ESI) for Environmental Science: Processes & Impacts.


# Supporting Information for:

## Feedstock nitrogen content mediates maximum possible Pb sorption capacity of biochars

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This Supporting Information file contains text and references describing the assignment of FTIR peaks to functional groups, 4 Tables and 5 Figures:

**Assignment of FTIR (Fourier-transform infrared) spectroscopy peaks to functional groups**

The peaks observed at 3380 $cm^{-1}$ were attributed to O-H stretching which may belong to the hydroxyl, alcohol, carboxylic acid, and water groups (Figueredo et el., 2018; Keiluweit et al., 2010). The peaks around 2940 $cm^{-1}$ were attributed to vibrations of asymmetric and symmetric aliphatic C-H stretching (Keiluweit et al., 2010; Li et al., 2020; Zhao et al., 2017). The peaks at 2158 $cm^{-1}$ could be linked to overtones of aromatic ring bonds C≡C (Korus et al., 2019). The stretching vibration at 1590 $cm^{-1}$ could be attributed to aromatic compounds C=C and carbonyl groups C=O (Figueredo et al., 2017; Li et al., 2020). The peaks at 1416 $cm^{-1}$ could be ascribed to asymmetric deformation vibration of $CH_3$ aliphatic group as seen in a study by Li et al., (2020). The peaks which appeared at 1351 $cm^{-1}$ signify the phenolic stretching vibrations of O-H (Zhao et al., 2017). The stretching at 1160 $cm^{-1}$ could arise from C-O-C oxygen containing functional group, while the stretching at 876 $cm^{-1}$ were attributed to the out of plane deformation of aromatic C-H groups (Zhao et al., 2017).

**References**


Figueiredo, C., Lopes, H., Coser, T., Vale, A., Busato, J., Aguiar, N., Novotny, E., Canellas, L., 2018. Influence of pyrolysis temperature on chemical and physical properties of biochar from sewage sludge. Arch. Agron. Soil Sci. 64, 881–889. https://doi.org/10.1080/03650340.2017.1407870

Keiluweit, M., Nico, P.S., Johnson, M.G., Kleber, M., 2010. Dynamic Molecular Structure of Plant Biomass-Derived Black Carbon (Biochar). Environ. Sci. Technol. 44, 1247–1253. https://doi.org/10.1021/es9031419

Li, B., Liu, D., Lin, D., Xie, X., Wang, S., Xu, H., Wang, J., Huang, Y., Zhang, S., Hu, X., 2020. Changes in Biochar Functional Groups and Its Reactivity after Volatile-Char Interactions during Biomass Pyrolysis. Energy and Fuels 34, 14291–14299. https://doi.org/10.1021/acs.energyfuels.0c03243

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Korus, A., Szlęk, A., Samson, A., 2019. Physicochemical properties of biochars prepared from raw and acetone-extracted pine wood. Fuel Process. Technol. 185, 106–116. https://doi.org/10.1016/j.fuproc.2018.12.004

**Table S-1. Functional groups observed in the Fourier-transform infrared (FTIR) spectra of biochars produced at different pyrolysis temperatures**

| FTIR Peak ($cm^{-1}$) | Functional groups assigned |
|---|---|
| 3380 | O–H stretching (water, hydrogen-bonded hydroxyl) |
| 2940 | C–H stretching (aliphatic CHx; 2935-asymmetric), C-H stretching aliphatic CHx |
| 2158 | C≡C Overtones of aromatic rings |
| 1590 | Aromatic C=C and C=O stretching of conjugated ketones and quinones, aromatic components and C]O of conjugated ketones and quinones |
| 1416 | Asymmetric deformation vibration of CH3, CH2 added to carboxymethyl cellulose |
| 1351 | in plane bending of phenolic -OH |
| 1160 | C-O-C ester groups in cellulose and hemicellulose |
| 876 | C–H bending (aromatic C–H out-of-plane deformation), C=C polycyclic aromatic structures |

**Table SI-2. Final pH of solutions after sorption**

| Biochar Feedstock | Pyrolysis temp (°C) | 100 mg Pb $L^{-1}$ | 200 mg Pb $L^{-1}$ | 500 mg Pb $L^{-1}$ | 1000 mg Pb $L^{-1}$ | 5000 mg Pb $L^{-1}$ |
|---|---|---|---|---|---|---|
| Coco Coir | 300 | 6.31 | 5.43 | 4.81 | 4.35 | 3.82 |
| Coco Coir | 350 | 8.59 | 8.34 | 7.74 | 7.15 | 5.27 |
| Coco Coir | 400 | 9.56 | 9.34 | 8.66 | 7.15 | 5.27 |
| Coco Coir | 450 | 10.37 | 10.27 | 9.95 | 8.99 | 6.09 |
| Coco Coir | 500 | 10.57 | 10.41 | 10.13 | 9.59 | 5.63 |
| Coco Coir | 550 | 10.83 | 10.73 | 10.45 | 10.13 | 5.60 |
| Coco Coir | 600 | 10.8 | 10.67 | 10.48 | 10.23 | 5.34 |
| Coco Coir | 650 | 10.69 | 10.63 | 10.48 | 10.36 | 5.30 |
| Coco Coir | 700 | 11.03 | 10.96 | 10.8 | 10.62 | 5.28 |
| Coco Coir | 750 | 11.00 | 11.00 | 10.83 | 10.66 | 5.49 |
| Hay | 300 | 6.23 | 6.33 | 5.66 | 5.47 | 4.36 |
| Hay | 350 | 7.19 | 7.23 | 5.75 | 5.89 | 4.95 |
| Hay | 400 | 8.23 | 7.34 | 7.99 | 7.41 | 5.10 |
| Hay | 450 | 9.21 | 9.12 | 8.88 | 8.22 | 5.11 |
| Hay | 500 | 9.74 | 9.60 | 9.27 | 8.82 | 5.11 |
| Hay | 550 | 10.33 | 10.30 | 10.04 | 9.63 | 5.30 |
| Hay | 600 | 10.46 | 10.38 | 10.16 | 9.74 | 5.28 |
| Hay | 650 | 10.83 | 10.78 | 10.56 | 10.14 | 5.42 |
| Hay | 700 | 11.04 | 10.98 | 10.83 | 10.66 | 6.06 |
| Hay | 750 | 11.26 | 11.17 | 11.09 | 10.87 | 6.55 |
| Wheat straw | 300 | 6.27 | 6.13 | 4.84 | 4.63 | 4.03 |
| Wheat straw | 350 | 7.01 | 7.41 | 6.80 | 6.47 | 4.89 |
| Wheat straw | 400 | 8.80 | 8.63 | 8.21 | 7.40 | 5.19 |
| Wheat straw | 450 | 9.68 | 9.50 | 9.18 | 8.52 | 5.29 |
| Wheat straw | 500 | 10.44 | 10.37 | 10.18 | 9.68 | 5.32 |
| Wheat straw | 550 | 10.40 | 10.32 | 10.15 | 9.69 | 5.23 |
| Wheat straw | 600 | 10.38 | 10.31 | 10.19 | 9.85 | 5.32 |
| Wheat straw | 650 | 10.47 | 10.40 | 10.30 | 9.96 | 5.55 |
| Wheat straw | 700 | 10.30 | 10.24 | 10.17 | 9.93 | 5.53 |
| Wheat straw | 750 | 10.45 | 10.38 | 10.35 | 10.4 | 6.50 |
| Pine bark | 300 | 4.26 | 4.02 | 3.32 | 3.31 | 3.04 |
| Pine bark | 350 | 4.45 | 4.30 | 3.88 | 3.81 | 3.66 |
| Pine bark | 400 | 4.71 | 4.50 | 4.19 | 4.11 | 4.02 |
| Pine bark | 450 | 5.42 | 5.14 | 4.23 | 4.64 | 4.60 |
| Pine bark | 500 | 6.03 | 5.56 | 5.01 | 4.89 | 4.74 |
| Pine bark | 550 | 6.54 | 6.01 | 5.16 | 5.03 | 4.88 |
| Pine bark | 600 | 7.21 | 6.72 | 5.36 | 5.16 | 5.13 |
| Pine bark | 650 | 7.77 | 7.26 | 6.15 | 5.30 | 5.21 |
| Pine bark | 700 | 8.85 | 8.41 | 7.21 | 5.72 | 5.80 |
| Pine bark | 750 | 9.67 | 9.36 | 7.63 | 6.61 | 5.93 |

**Table S-3. Biochar feedstock properties**

| Feedstock | N (%) | C (%) | C/N ratio | Ca (mg/kg) | K (mg/kg) | Mg (mg/kg) | P (mg/kg) | S (mg/kg) | Na (mg/kg) | Al (mg/kg) | Fe (mg/kg) | Cu (mg/kg) | Pb (mg/kg) | Mn (mg/kg) | Zn (mg/kg) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Hay | 1.11 | 41.4 | 37.3 | 4490 | 16032 | 1303 | 2008 | 1308 | 996 | 53.3 | 87.3 | 3.40 | 1.14 | 27.2 | 19.7 |
| Wheat straw | 0.73 | 44.1 | 60.7 | 5361 | 8794 | 328 | 695 | 733 | 343 | 98.0 | 397 | 2.50 | 1.64 | 29.2 | 9.9 |
| Pine bark | 0.09 | 45.9 | 534 | 1356 | 776 | 262 | 101 | 441 | 12 | 80.3 | 141 | 1.94 | 1.89 | 35.6 | 10.4 |
| Coco coir | 0.44 | 44.2 | 101 | 2307 | 12584 | 1763 | 364 | 765 | 4046 | 660 | 1774 | 1.49 | 1.39 | 68.6 | 16.7 |

**Table S-4. The relationship between biochar feedstock properties and maximum possible Pb sorption capacity at optimum pyrolysis temperature**

| Feedstock property | $R^2$ | p-value |
|---|---|---|
| N | 0.954 | 0.023 |
| C | 0.813 | 0.099 |
| C/N ratio | 0.863 | 0.071 |
| Ca | 0.782 | 0.116 |
| K | 0.759 | 0.129 |
| Mg | 0.135 | 0.633 |
| P | 0.706 | 0.160 |
| S | 0.763 | 0.127 |
| Na | 0.007 | 0.914 |
| Cu | 0.525 | 0.276 |
| Pb | 0.656 | 0.190 |
| Mn | 0.086 | 0.708 |
| Zn | 0.302 | 0.451 |
| Al | 0.016 | 0.872 |
| Fe | 0.006 | 0.920 |

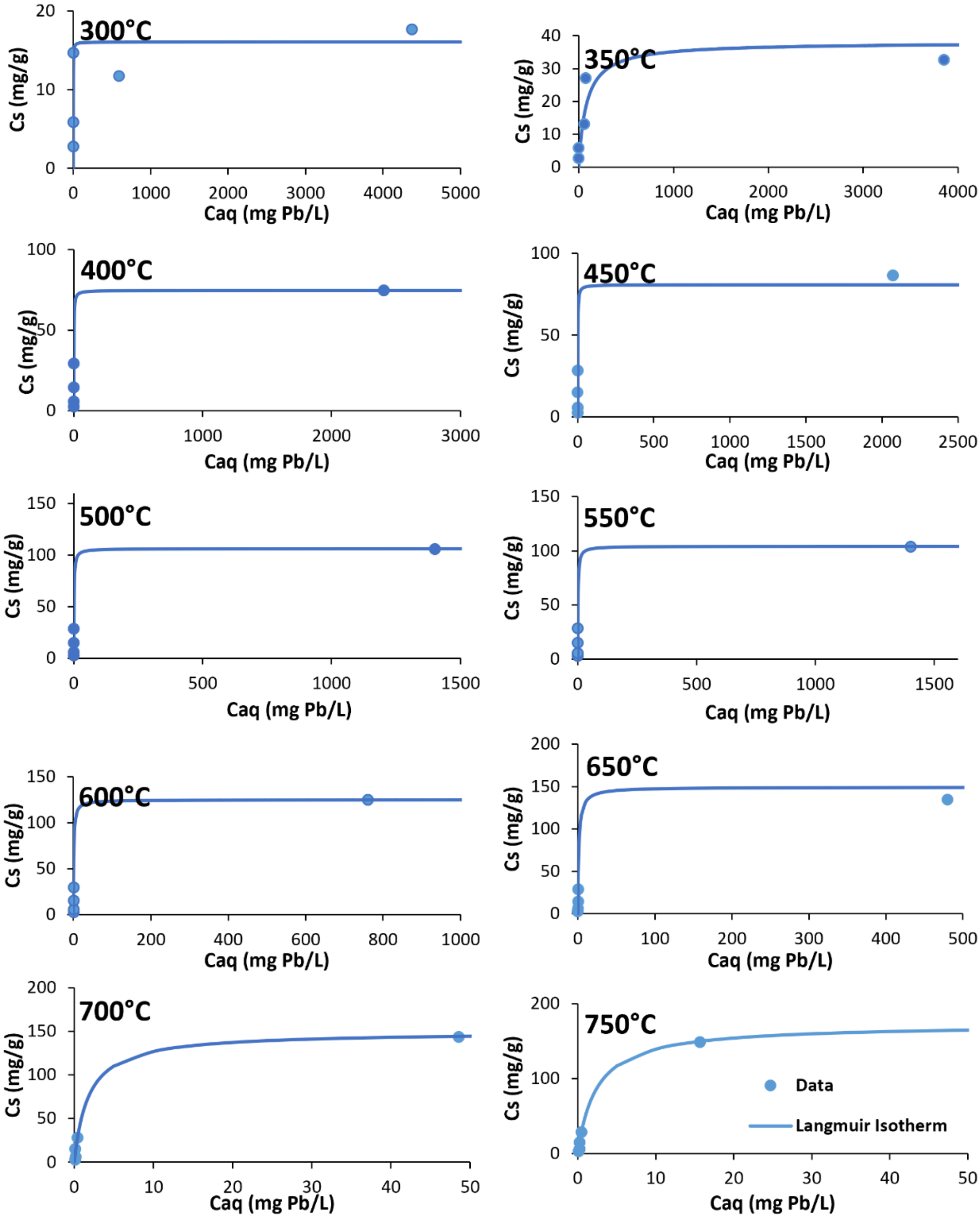


**Figure S-1; Sorption isotherm for hay biochars pyrolyzed at 300 °C, 350 °C, 400 °C, 450 °C, 500 °C, 550 °C, 600 °C, 650 °C, 700 °C, and 750 °C shaken with 100, 200, 500, 1000, and 5000 mg/L of Pb and fitted to a Langmuir sorption isotherm model**

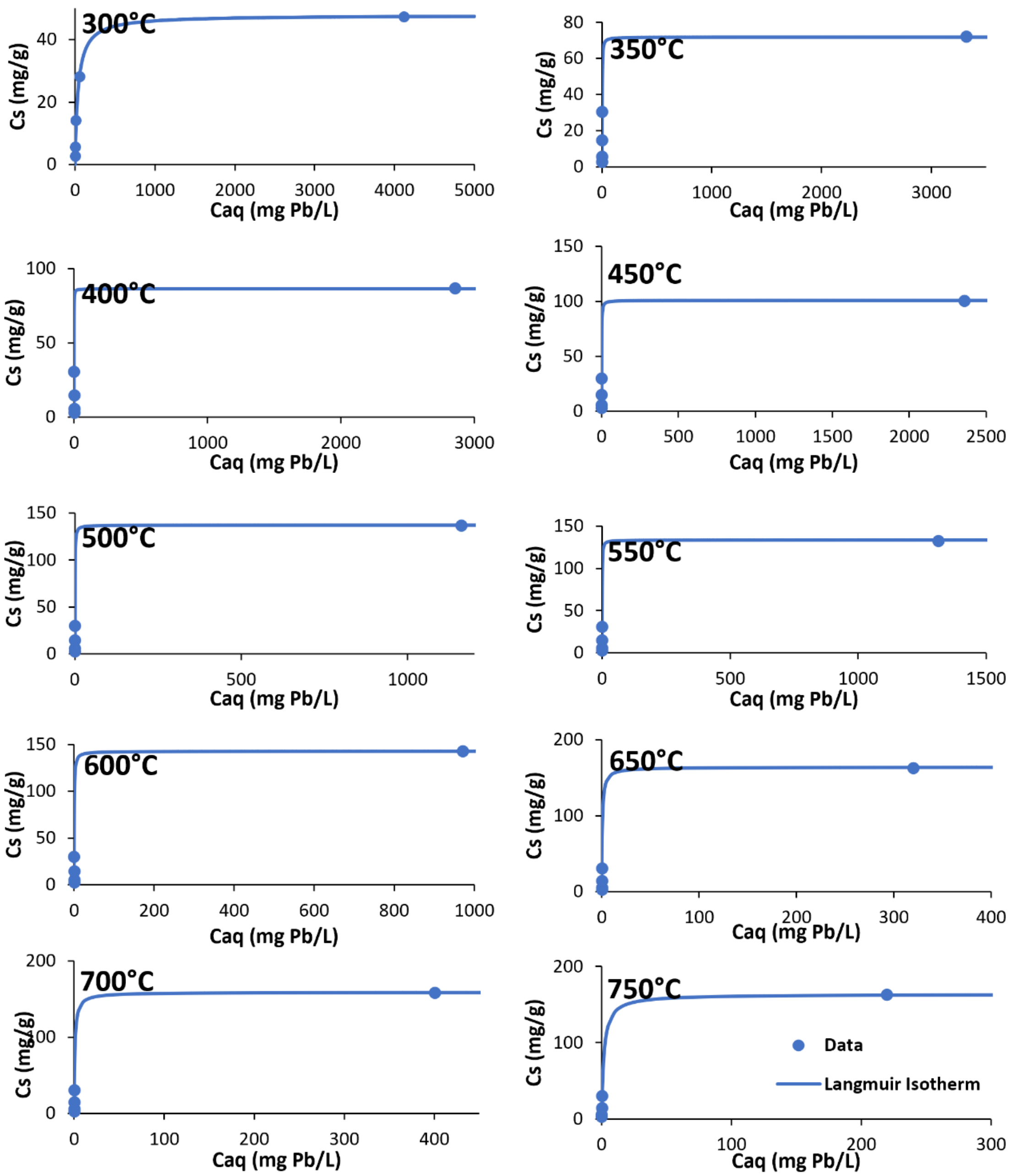


**Figure S-2; Sorption isotherm for wheat straw biochars pyrolyzed at 300 °C, 350 °C, 400 °C, 450 °C, 500 °C, 550 °C, 600 °C, 650 °C, 700 °C, and 750 °C shaken with 100, 200, 500, 1000, and 5000 mg/L of Pb and fitted to a Langmuir sorption isotherm model**

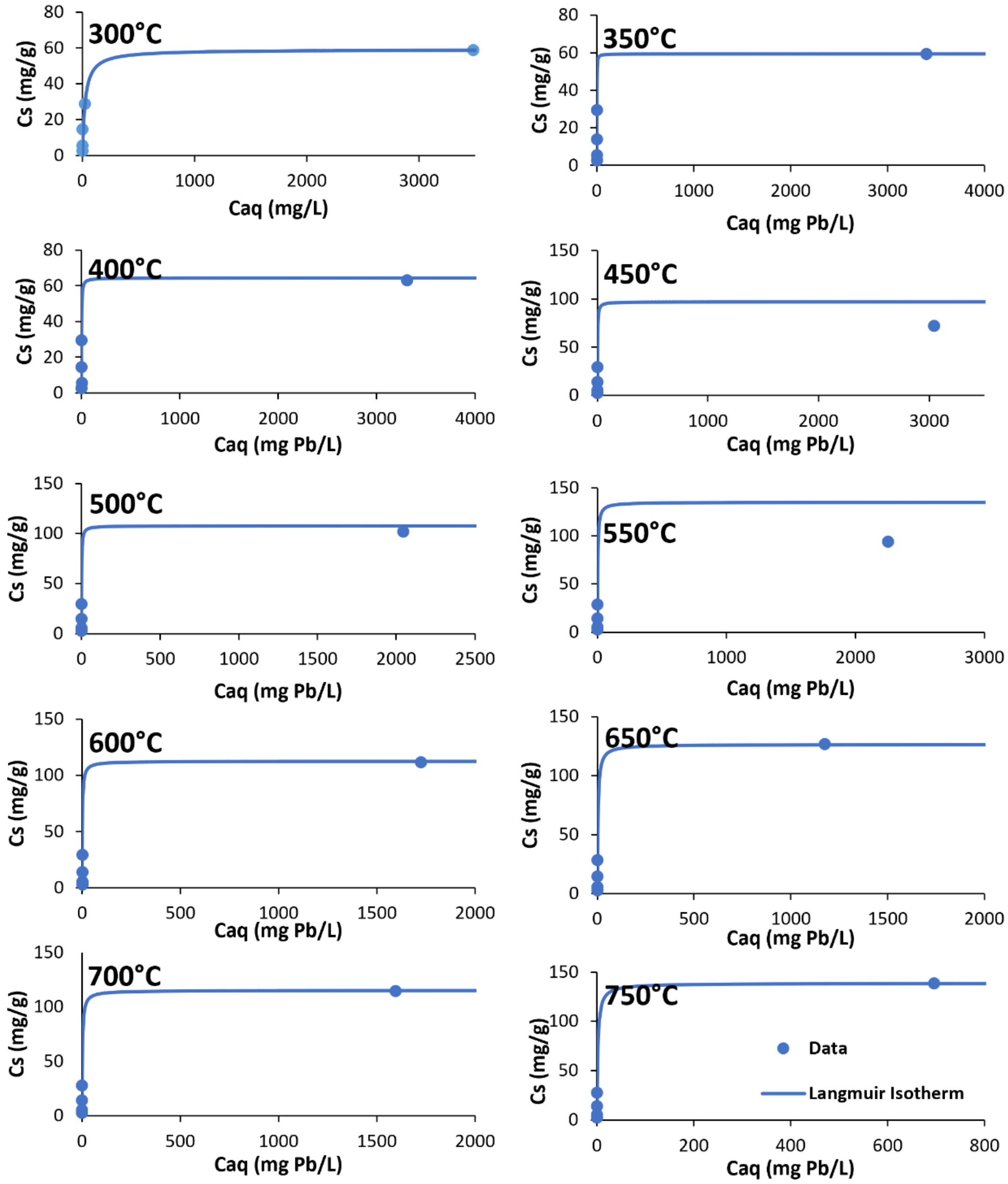


**Figure S-3; Sorption isotherm for coco coir biochars pyrolyzed at 300 °C, 350 °C, 400 °C, 450 °C, 500 °C, 550 °C, 600 °C, 650 °C, 700 °C, and 750 °C shaken with 100, 200, 500, 1000, and 5000 mg/L of Pb and fitted to a Langmuir sorption isotherm model**

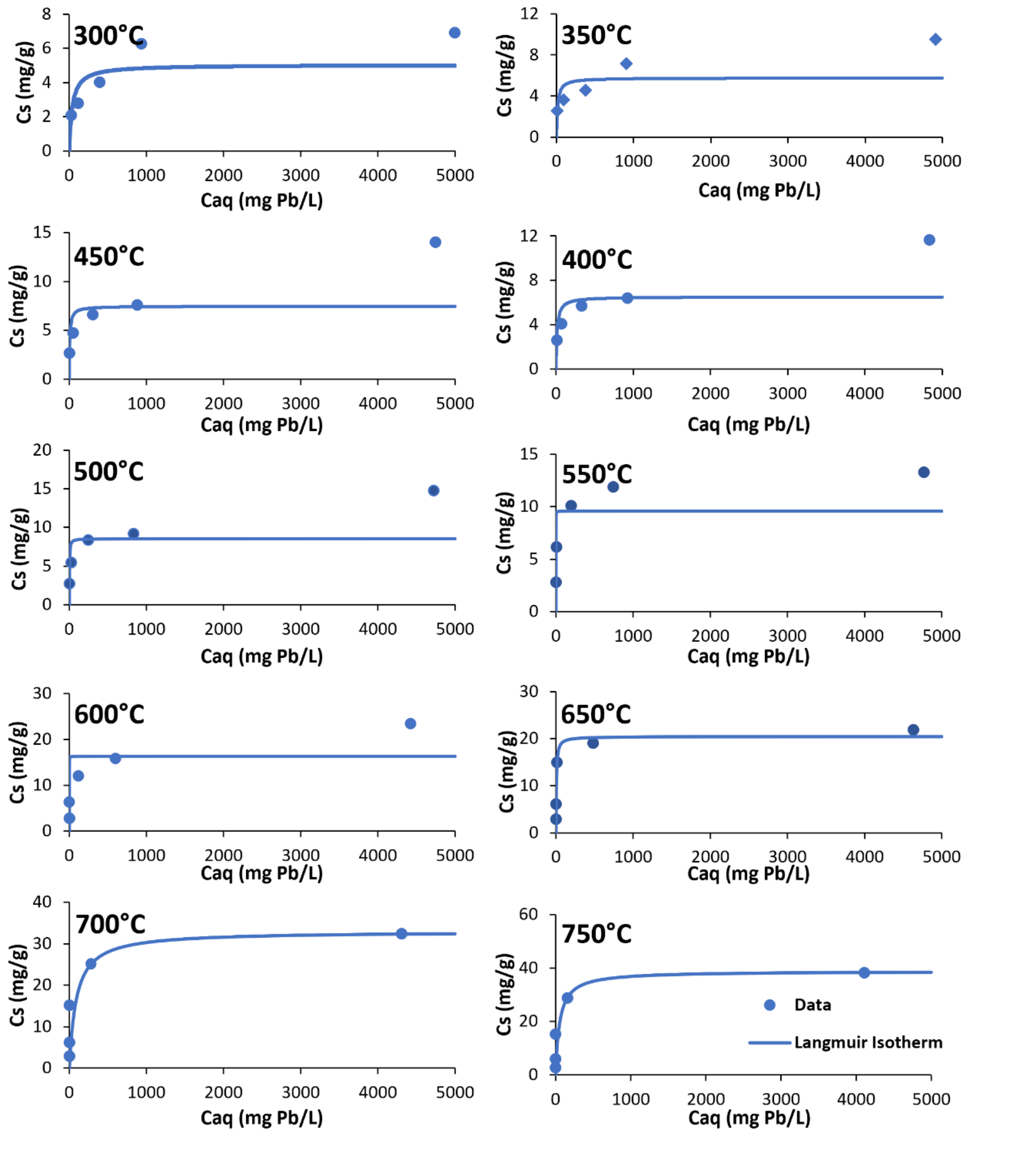


**Figure S-4; Sorption isotherm for pine bark biochars pyrolyzed at 300 °C, 350 °C, 400 °C, 450 °C, 500 °C, 550 °C, 600 °C, 650 °C, 700 °C, and 750 °C shaken with 100, 200, 500, 1000, and 5000 mg/L of Pb and fitted to a Langmuir sorption isotherm model**

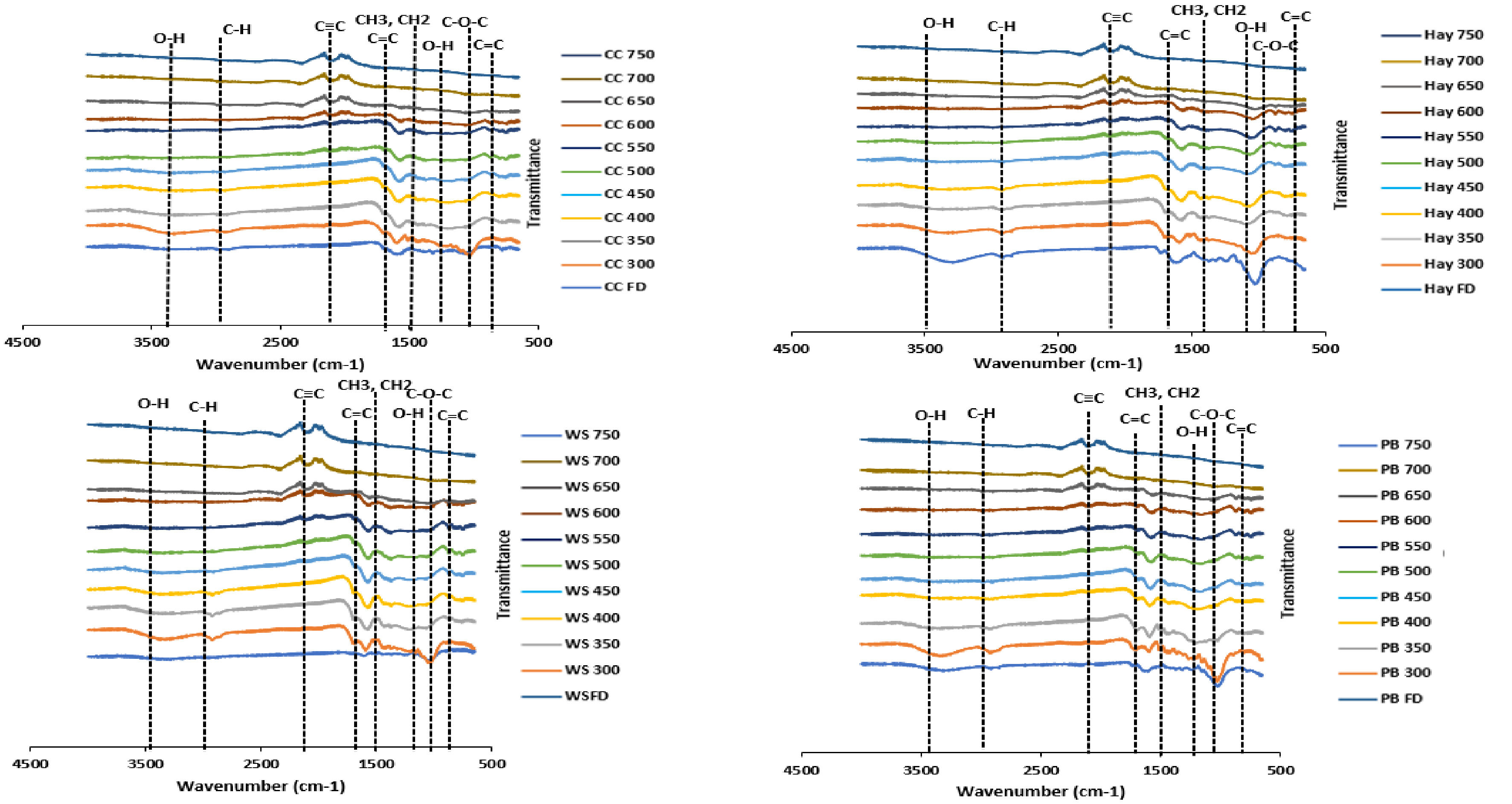


**Figure S-5. FTIR spectra for feedstocks (FD) and biochars made from coco coir (CC), hay, wheat straw (WS), and pine bark (PB) at pyrolysis temperatures between 300°C and 750°C**