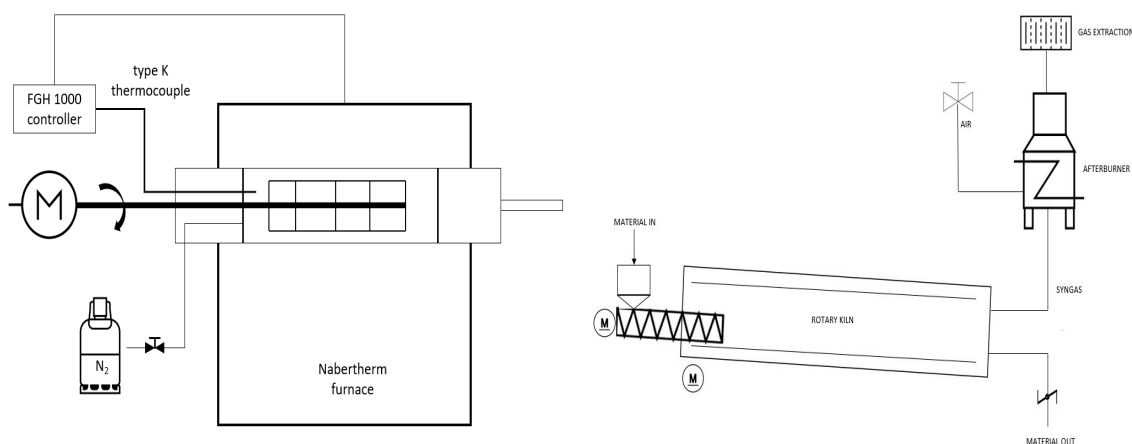
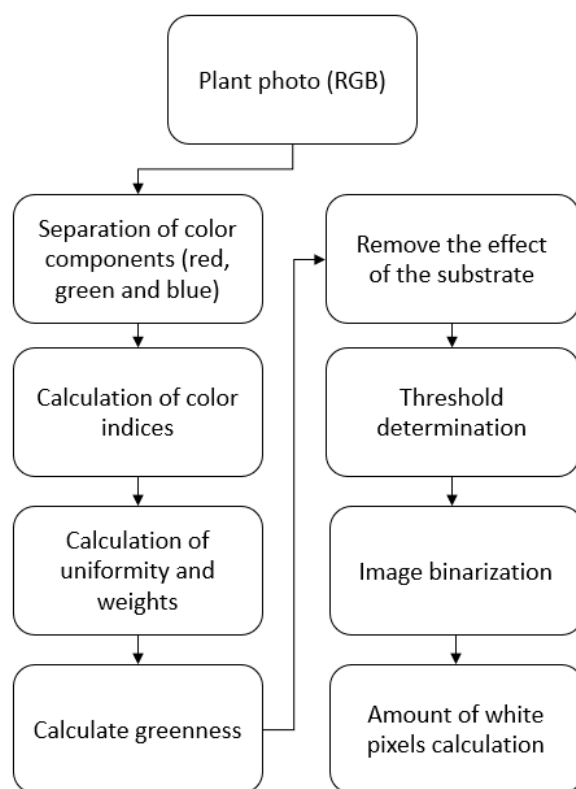


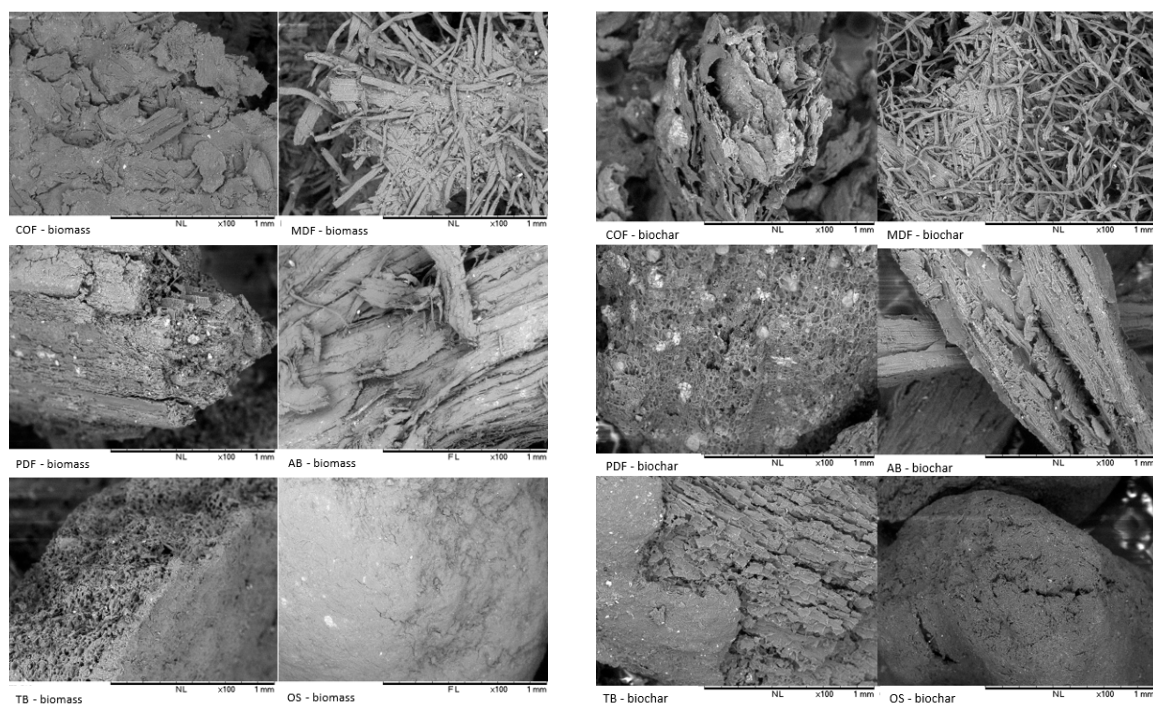
# An Experimentally Validated Selection Protocol for Biochar as a Sustainable Component in Green Roofs



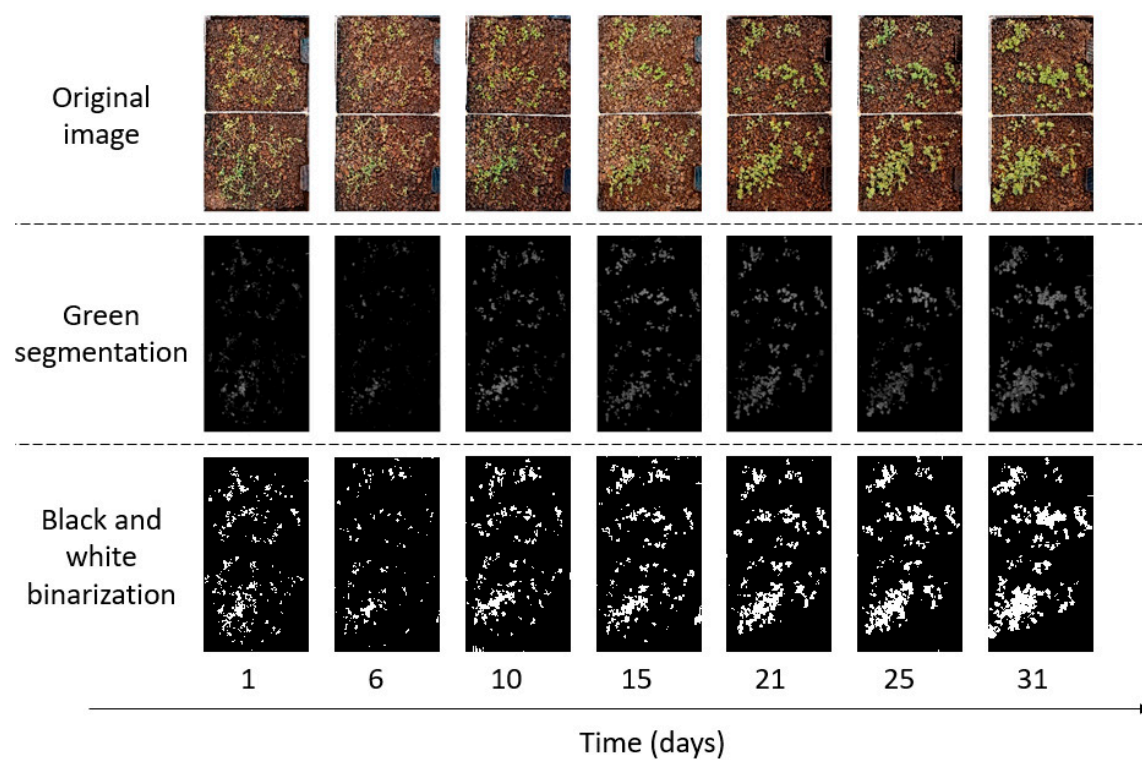
**Figure S1.** Schematic representation of the lab-scale batch reactor (left) and the pilot scale reactor (right) [1].



**Figure S2.** Flow diagram for green segmentation strategy.



**Figure S3.** SEM images of biomasses and biochars produced in the pilot scale reactor (T = 450 °C).



**Figure S4.** Growth process of *Sedum Hispanicum* approached as surface green coverage on substrate with 5 wt. % of biochar during 31 days. Top: original image, middle: image after green segmentation and bottom: image after black and white binarization.

**Table S1.** Band assignments of FT-IR spectra of the different biomass samples. Results of FT-IR for MDF were previously published [2].

Wavenumber (cm <sup>-1</sup> )	COF	MDF	PDF	AB	TB	OS	Peak shape	Band assignment	Source
3600-3100	x	x	x	x	x	x	Very broad	Multitude of OH stretching in the phenolic and aliphatic structures of cellulose, hemicellulose and lignin. When N is present in higher concentrations (COF, MDF and AB), NH stretching vibrations are also found.	[3]
2950,2925 and 2850	x	x	x	x	x	x	Shoulder + sharp double peak	Symmetric and asymmetric C-H stretching vibrations	[3, 4]
1736	x	x	x	x	x	x	Broad	C=O stretch hemicellulose	[4]
1643	x	x	x	x	x	x	Broad	OH-bending of absorbed water	[5]
1608	x	x	x	x	x	x	Broad	C=C symmetric stretching of aromatic ring systems	
1539	x	x		x		x	Weak	C=C stretch in a nitrogen based ring	[6]
1513	x	x	x	x	x	x	Weak	Aromatic ring vibration in lignin	[5]
1455	x	x	x	x	x	x	Weak	CH <sub>3</sub> and CH <sub>2</sub> deformation	[3, 5]
1425	x	x	x	x	x	x	Weak	HCH and OCH in plane bending vibration of cellulose	[3]
1371	x	x	x	x	x	x	Weak	CH and OH bending	[3]
1321	x	x	x	x	x	x	Weak	CH <sub>2</sub> wagging in cellulose and hemicellulose or OH bending	[3]
1262	x	x		x	x		Sharp	aromatic ring vibration of guaiacyl lignin	[3]
1240	x	x	x	x	x	x	Broad	C-O stretch and O-H in plane bending in polysaccharides and syringyl lignin	[4]
1155	x	x	x	x	x	x	Shoulder	C-O-C band vibration in cellulose and hemicellulose	[3, 5]
1106	x	x	x	x	x	x	shoulder	O-H band vibration in cellulose and hemicellulose	[3, 5]
1050	x	x	x	x	x		Shoulder	C-O stretching in holocellulose	[7]
1033	x	x	x	x	x	x	Very sharp	aromatic C-H in plane deformation of guaiacyl lignin and C-O deformation	[3–5]
893	x	x	x	x	x	x	Weak	COC, CCO and CH deformation in cellulose and hemicellulose	[5]
808	x	x	x	x	x	x	Weak	C-H bending	
772	x	x	x	x	x	x	Weak	C-H bending	
718	x	x	x	x			Weak	Ca-O bonds	[8]

**Table S2.** Band assignments of FT-IR spectra of the different biochar samples, adapted from [2, 9–12]. Results of FT-IR for MDF were previously published [2].

Wavenumber (cm <sup>-1</sup> )	COF	MDF	PDF	AB	TB	OS	Trend with increasing temperature	Band assignment
3600-3100	x	X	x	x	x		--	Multitude of OH-stretching frequencies in phenolic and aliphatic structures of degradation products of cellulose, hemicellulose and lignin or N-H stretching in biomasses with enhanced N content
3025		X	x				++	C <sub>sp2</sub> -H stretching vibration of aromatic structures
2950,2925 and 2850	x	X	x	x		x	--	C-H symmetric and asymmetric bond stretching in aliphatic and alicyclic components
2175	x						++	Nitrile groups
1700-1600	x	x	x	x		x	--	C=O stretching vibrations as found in degradation products of hemicellulose
1580		x	x	x	x	x	Normalized	C=O stretching of aromatic moieties
1435		x					++	C=C stretching of aromatic moieties
1420	x		x		x		++	CaCO <sub>3</sub> and other carbonates like K <sub>2</sub> CO <sub>3</sub>
1375		x		x			--	C-H deformation
1300-1100	x					x	--	C-N and C-O functionalities
1160			x		x	x	--	C-O stretching
1107			x				++	Si-O bonds*
1020		x		x		x	++	Aromatic ethers
875 (High ash biomass)	x		x		x		++	CaCO <sub>3</sub> and other carbonates like K <sub>2</sub> CO <sub>3</sub>
875 (Low ash biomass)		x		x		x	++	Aromatic C-H bending
810		x		x	x	x	++	Aromatic C-H bending
755		x	x	x	x	x	++	Aromatic C-H bending
718	x		x		x		++	CaCO <sub>3</sub> and other carbonates like K <sub>2</sub> CO <sub>3</sub>
675		x	x	x	x	x	++	Aromatic C-H out of plane bending
620	x	x	x		x		++	Aromatic C-H out of plane bending

**Table S3.** Heavy metal concentrations in all biochars.

	As (mg/kg)	Cd (mg/kg)	Cr (mg/kg)	Cu (mg/kg)	Hg (mg/kg)	Ni (mg/kg)	Pb (mg/kg)	Zn (mg/kg)
COF350	<100	<10	<20	213 ± 12	<100	<20	<100	108 ± 2
COF450B	<100	<10	<20	235 ± 10	<100	<20	<100	108 ± 5
COF500	<100	<10	<20	292 ± 3	<100	<20	<100	122 ± 1
COF550	<100	<10	<20	248 ± 5	<100	<20	<100	110 ± 1
COF450C	<100	<10	<20	195 ± 2	<100	<20	<100	91 ± 2
MDF350	<100	<10	<20	24 ± 1	<100	<20	<100	28 ± 1
MDF450B	<100	<10	<20	19 ± 1	<100	<20	<100	27 ± 1
MDF500	<100	<10	25 ± 2	32 ± 4	<100	<20	<100	52 ± 4
MDF550	<100	<10	<20	50 ± 1	<100	<20	<100	57 ± 4
MDF450C	<100	<10	<20	21 ± 1	<100	<20	<100	<20
PDF350	<100	<10	105 ± 1	<20	<100	121 ± 8	<100	<20
PDF450B	<100	<10	39 ± 6	<20	<100	<20	<100	<20
PDF500	<100	<10	30 ± 1	<20	<100	<20	<100	<20
PDF550	<100	<10	108 ± 5	<20	<100	<20	<100	<20
PDF450C	<100	<10	<20	28 ± 2	<100	<20	<100	69 ± 1
AB350	<100	<10	124 ± 4	87 ± 1	<100	481 ± 11	488 ± 10	485 ± 49
AB450B	<100	<10	135 ± 1	123 ± 7	<100	524 ± 42	534 ± 40	572 ± 36
AB500	<100	<10	135 ± 4	105 ± 1	<100	589 ± 50	599 ± 60	553 ± 25
AB550	<100	<10	155 ± 5	149 ± 11	<100	1372 ± 20	1402 ± 26	976 ± 34
AB450C	<100	<10	141 ± 2	161 ± 8	<100	<20	321 ± 27	315 ± 19
TB350	<100	<10	<20	31 ± 1	<100	<20	<100	159 ± 7
TB450B	<100	<10	<20	27 ± 1	<100	<20	<100	145 ± 4
TB500	<100	<10	24 ± 2	33 ± 7	<100	<20	<100	135 ± 8
TB550	<100	<10	25 ± 3	42 ± 5	<100	<20	<100	130 ± 2
TB450C	<100	<10	<20	29 ± 1	<100	<20	<100	148 ± 3
OS350	<100	<10	<20	26 ± 1	<100	<20	<100	<20
OS450B	<100	<10	<20	25 ± 1	<100	<20	<100	<20
OS500	<100	<10	67 ± 13	29 ± 2	<100	<20	<100	<20
OS550	<100	<10	73 ± 14	50 ± 3	<100	55 ± 1	<100	21 ± 2
OS450C	<100	<10	<20	22 ± 1	<100	<20	<100	<20

## References

1. Haeldermans T., Lataf M.A., Vanroelen G., et al. Numerical prediction of the mean residence time of solid materials in a pilot-scale rotary kiln. *Powder Technol.* **2019**, 354, 392–401. <https://doi.org/10.1016/j.powtec.2019.06.008>
2. Haeldermans T., Claesen J., Maggen J., et al. Microwave assisted and conventional pyrolysis of MDF – Characterization of the produced biochars. *J. Anal. Appl. Pyrolysis* **2019**, 138, 218–230. <https://doi.org/10.1016/j.jaap.2018.12.027>
3. Xu F., Yu J., Tesso T., et al. Qualitative and quantitative analysis of lignocellulosic biomass using infrared techniques: A mini-review. *Appl. Energy* **2013**, 104, 801–809. <https://doi.org/10.1016/j.apenergy.2012.12.019>
4. Acquah G.E., Via B.K., Fasina O.O., Eckhardt L.G. Rapid Quantitative Analysis of Forest Biomass Using Fourier Transform Infrared Spectroscopy and Partial Least Squares Regression. *J. Anal. Methods Chem.* **2016**, 2016, 1–11. <https://doi.org/10.1155/2016/1839598>
5. Müller G., Bartholme M., Kharazipour A., Polle A. FTIR-ATR spectroscopic analysis of changes in fiber properties during insulating fiberboard manufacture of Beech Wood. *Wood Fiber Sci.* **2008**, 40, 532–543
6. Lyman D.J., Benck R., Dell S., et al. FTIR-ATR analysis of brewed coffee: Effect of roasting conditions. *J. Agric. Food Chem.* **2003**, 51, 3268–3272. <https://doi.org/10.1021/jf0209793>
7. Lao W., Li G., Zhou Q., Qin T. Quantitative analysis of biomass in three types of wood-plastic composites by FTIR spectroscopy. *BioResources* **2014**, 9, 6073–6086. <https://doi.org/10.15376/biores.9.4.6073-6086>
8. Galván-Ruiz M., Hernández J., Baños L., et al. Characterization of Calcium Carbonate, Calcium Oxide, and Calcium Hydroxide as Starting Point to the Improvement of Lime for Their Use in Construction. *J. Mater. Civ. Eng.* **2009**, 21, 694–698. [https://doi.org/10.1061/\(ASCE\)0899-1561\(2009\)21:11\(694\)](https://doi.org/10.1061/(ASCE)0899-1561(2009)21:11(694))
9. Liu Y., He Z., Uchimiya M. Comparison of Biochar Formation from Various Agricultural By-Products Using FTIR Spectroscopy. *Mod. Appl. Sci.* **2015**, 9, 246–253. <https://doi.org/10.5539/mas.v9n4p246>
10. Zhao L., Cao X., Mašek O., Zimmerman A. 2013 Heterogeneity of biochar properties as a function of feedstock sources and production temperatures. *J. Hazard. Mater.* **2013**, 256, 1–9. <https://doi.org/10.1016/j.jhazmat.2013.04.015>
11. Molenda J., Swat M., Osuch-Słomka E. Effect of Thermal Conditions of Pyrolysis Process on the Quality of Biochar Obtained from Vegetable Waste. *Eng. Prot. Environ.* **2018**, 21, 289–302. <https://doi.org/10.17512/ios.2018.3.7>
12. Dai L., Tan F., Li H., et al. Calcium-rich biochar from the pyrolysis of crab shell for phosphorus removal. *J. Environ. Manage.* **2017**, 198, 70–74. <https://doi.org/10.1016/j.jenvman.2017.04.057>