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Data Article

Data set of green extraction of valuable chemicals from lignocellulosic biomass using microwave method

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A B S T R A C T

Lignocellulosic biomass is a promising alternative for the replacement of limited fossil resources to produce various chemical compounds, such as 5-hydroxymethylfurfural, furfural, vanillin, vanillic acid, ferulic acid, syringaldehyde, and 4-aminobenzoic acid. However, the complex biomass structure is a limitation to making effective use of this naturally found feedstock. This research presents a data set of different compounds obtained directly from forest residues, with special emphasis on achieving effective utilization of the biomass. The extraction method and the catalyst are considered as the two main factors in this valorization process.

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Specifications Table

Subject area	Chemistry
More specific subject area	Biomass, bioproducts, biorefining, forestry residues.
Type of data	Tables, figures, and text file.
How data was acquired	- Planetary ball mill (PM100; Retsch Corporation). - Microwave-assisted extraction (MAE) instrument (Perkin-Elmer Anton Paar Multi-Wave Sample Prep System, USA). - Thermo Scientific Liquid TSQ Quantum Access Mass Spectrometer (Thermo Scientific, Mississauga, Canada).
Data format	Raw and Analyzed data set
Experimental factors	- Data set for different compounds were obtained from forestry residues using microwave-assisted extraction. - The compound analysis was carried out directly from the liquid hydrolysate.
Experimental features	- Forestry residues from hardwood and softwood were used for products obtention. - Experiments in batches were performed to evaluate the reaction time, temperature and catalyst concentration effect. - Data was analyzed using a response surface model (Box-Behnken) in a Minitab® Software version 17.
Data source location	Quebec city, Quebec province, Canada
Data accessibility	Data are available in article

Value of the data

- Lignocellulosic biomass was used as a feedstock to obtain the data of valuable chemical compounds. Therefore, the data might contain valuable information in a sustainable frame to approach and suggest the exploitation of this renewable feedstock.
- Data from alkaline-microwave assisted extraction shown that is an efficient method to obtain valuable chemical compounds from lignocellulosic biomass. Additionally, the data can be used as a base to develop scale-up experiments.
- Data can offer an overview of the importance and application of these valuable compounds in the market and their use in different industries.

1. Data

Figs. 1 and 2 show desirability plots for the optimal conditions to increase the concentration of different compounds from hardwood and softwood sawdust (respectively).

Fig. 3 from the data showed that vanillic acid, vanillin, and ferulic acid its present in high concentration in softwood sawdust compare with hardwood sawdust, where 4-aminobenzoic acid and syringaldehyde was found in highest concentrations. On another hand, 5-HMF and furfural not showed a significative difference (p-value = 0.32) in both feedstocks.

Finally, data that are shown in the table with characteristics of each of the compounds can suggest their possible uses in the industry as precursors for other compounds (see Table 1)

2. Experimental design, materials, and methods

Hydrophilic compounds derived from sawdust of hardwood and softwood were obtained after processing in microwave-assisted extraction in the presence of an alkaline catalyst (NaOH). Compounds were extracted separately for each type of wood. A response surface methodology (Box-Behnken) was used to validate the effect of three different factors: temperature (65, 80 and 95 °C), time (15, 30, and 45 minutes) and NaOH concentration (1, 4, and 7% v/v) on levulinic acid, 5-hydroxymethylfurfural, furfural, 4-aminobenzoic acid, vanillic acid, vanillin, syringaldehyde and ferulic acid concentration.

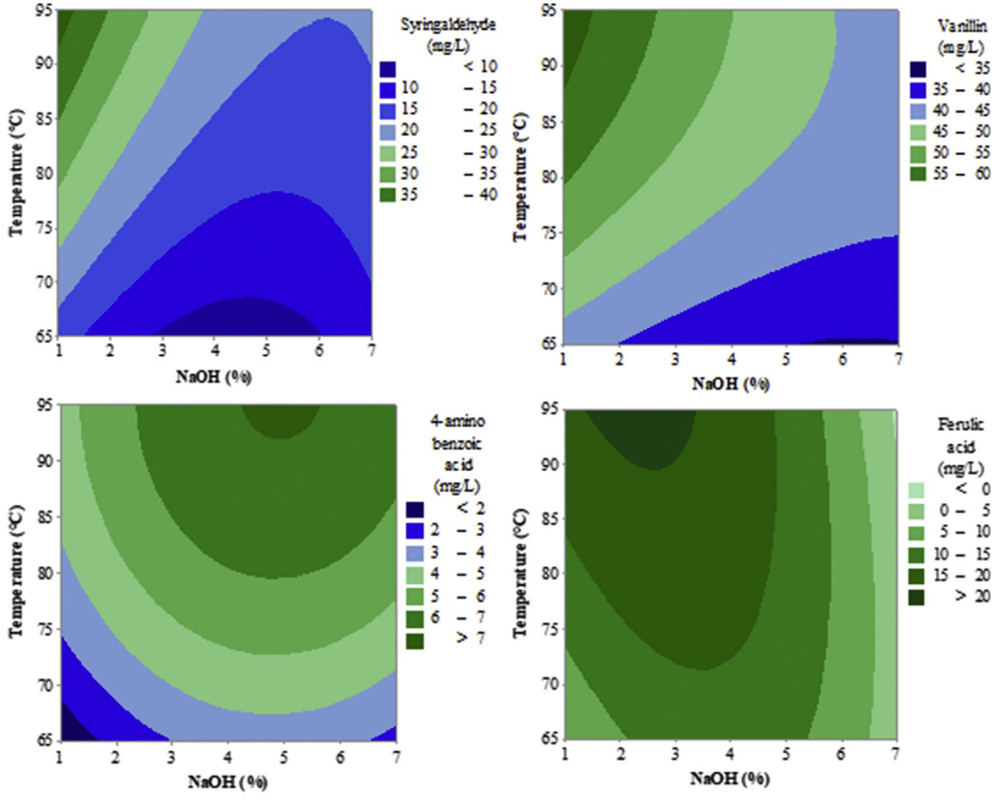

Fig. 1. Desirability plots for different compounds obtained from hardwood sawdust.

Sawdust softwood (35% White Spruce and 65% Fir) and hardwood (100% Maple wood), was kindly provided from Quebec Forest Industry Council (QFIC). Both materials were dried at 60 °C for 12 hours and ground in a planetary ball mill (PM100; Retsch Corporation) for 15 min at 500 rpm. The resulting milled feedstock was fractioned in a range of 1 mm–300 μm. After that, samples were uniformly mixed and used for the preparation of test samples. Sawdust samples (200 mg) for both kinds of wood were treated with MAE at 1000 W of power. After MAE, samples were centrifuged at 9000g for 15 min at room temperature and the supernatant and solids were keep separately in sterile tubes to 4 °C for further experiments. To determine furfural, 5-HFM, levulinic acid, vanillin, vanillic acid, ferulic acid, syringaldehyde, and 4-aminobenzoic acid a Thermo Scientific Liquid TSQ Quantum Access Mass Spectrometer (LC-MS) equipped with a BetaBasic-18 100 mm × 2.1 mm; 3 μm column heated at 30 °C, was used. Water: methanol (80:20 v/v) was used as a sample diluent and water: acetic acid (0.1%), methanol: acetic acid (0.05%), in a ratio of 82.5:17.5 (respectively) as mobile phase with a flow of 0.3 mL/min, and 20 μL as total injection volume. The mass detector was operated in a mode SRM of a positive detection. Finally, 20 μL/mL of phenylethanol-D5 was used as an internal standard. All green chemical compounds were determined and quantified by comparing peak areas and the retention times with their similar standard compound provided from Sigma-Aldrich, USA. All the experiments were carried out in duplicates and the average and standard deviation for data set were calculated.

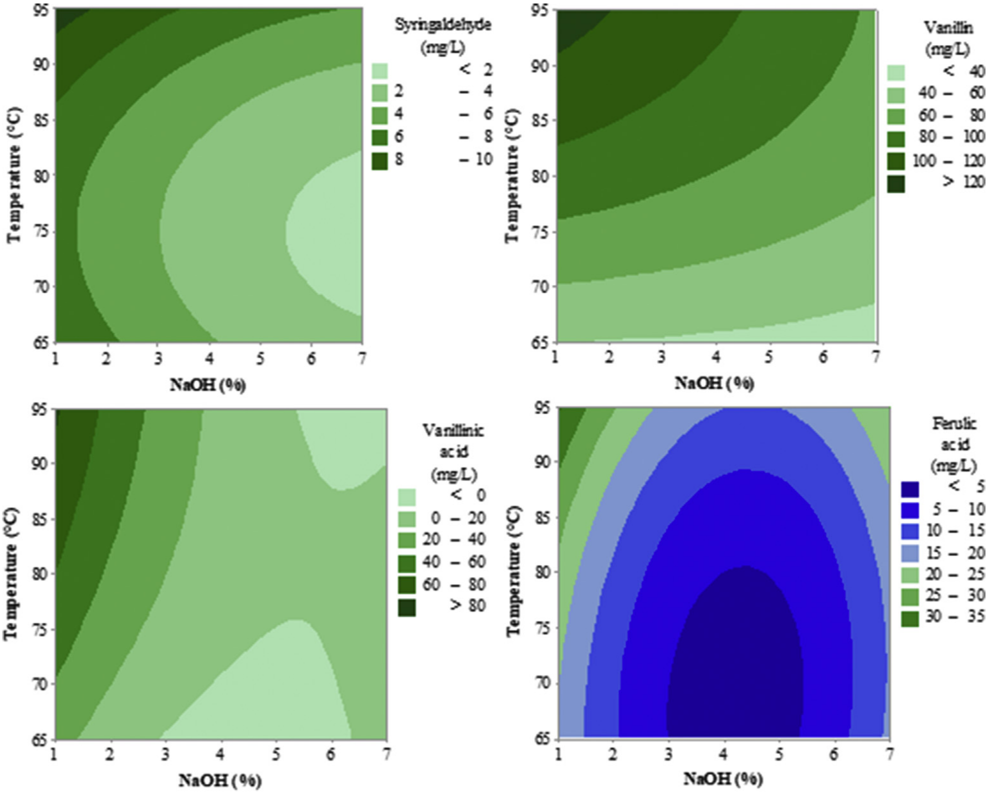

Fig. 2. Desirability plots for different compounds obtained from softwood sawdust.

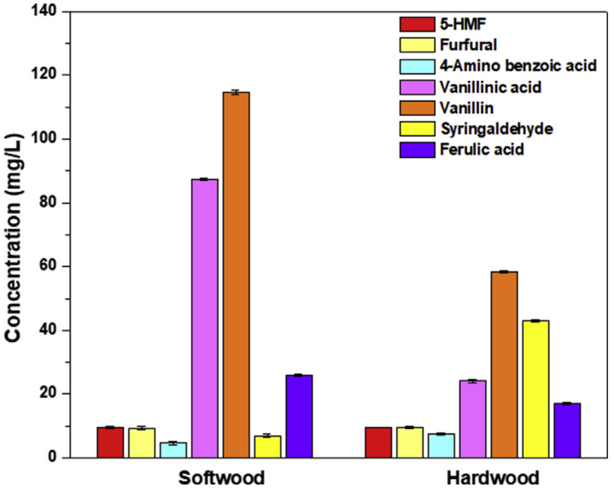

Fig. 3. Maximum values obtained for different green chemical compounds from lignocellulosic biomass.

Table 1
Features and different industrial uses of the compounds obtained from lignocellulosic biomass.

Compound	Characteristics	Industrial use	Reference
5-HMF	This compound is considered as a source of energy and a green chemical platform molecule with high added values. Its global consumption has been estimated at 100 tons per year. The most common production route for obtaining this compound is through the dehydration of C6 sugars, especially fructose.	Production of polymers and polyurethane foams, biofuels, polyethylene plastics, and food additives.	[1,2]
Furfural	Furfural production from lignocellulosic biomass is due to the dehydration of C5 sugars. This chemical compound is considered within of 30 building block chemicals by the US Department of Energy. Its annual production is approximately 200,000 tons per year.	Precursor molecule for the furfural alcohol. Used as a chemical additive in the preparation of adhesives, fungicides, and flavourings. Additionally, also has a wide implementation in the petrochemical industry.	[3,4]
4-Aminobenzoic acid	These compound come from lignin fraction in the biomass. Its biological activity has turned it into a compound of high expectations in different industries, the reason why its demand has been increasing during the last decade.	Main applications are in the biomedical industry as an anti-inflammatory drug, analgesic and antipyretic. On another hand, it's used in chemical, food, and agricultural industries as an intermediate, additive, or inhibitor compound.	[5]
Vanillin	The demand for this compound it's around 20,000 ton per year. This compound can be obtained from guaiacol oxidation group present in lignin fraction of biomass. Same previous compounds, vanillin its considerer as a top-priority renewable building block.	A most common use for this compound is in the food industry as a fragrance and flavoring ingredient. Also, used in the chemical industry as a building block, mainly in polymer production.	[6,7]
Vanillic acid	Obtained by the oxidation of two different compounds, guaiacol and vanillin, derived from lignin. Global annual production of the compound is about 18.9 megatons.	Widely used in the food and pharmaceutical industries as an antimicrobial, antibacterial, and antioxidant agent. In recent years, the interest for this compound has been increased, due to its capability to decrease oxidative stress on cardiovascular system following pathogenesis.	[8,9]
Syringaldehyde	Obtained directly from the oxidation of syringol group, a key component of lignin, as well as from oxidation of vanillin. The market price of this compound is reported to be about 22 USD per kilogram.	The compound is widely used in the food and cosmetic industries as a flavour and fragrance agent. However, has been used as a precursor in the chemical industry for second-generation products. Also used in the pharmaceutical industry as an antibacterial compound.	[10,11]
Ferulic acid	This compound can be obtained from two different sources: guaiacol oxidation group or 5-HMF dehydration group. The global market is valued in USD $ 53 millions.	It is used in food, pharmaceutical and personal care industry as an antioxidant as well as a photoprotective compound for other anti-oxidant such as ascorbic acid. Additionally, in recent years it has been used in polymer production.	[12–14]

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Conflict of interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.dib.2019.104347.

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