This article is part of the

Proceedings of the 16th Minisymposium Verfahrenstechnik and 7th Partikelforum (TU Wien, Sept. 21/22, 2020)

Title:
Bioactive compounds as main economic drivers for sustainable biorefineries

Corresponding author:
Sebastian Serna-Loaiza (TU Wien - ICEBE), sebastian.serna@tuwien.ac.at

Date of submission:
28.07.20

Date of revision:
08.09.20

Date of acceptance:
08.09.20

Chapter ID:
MoP3-(01)

Length:
4 pages

ISBN (full book):
978-3-903337-01-5

Bioactive compounds as main economic drivers for sustainable biorefineries

Sebastian Serna-Loaiza [1], Anton Friedl [1]

1: Institute of Chemical, Environmental and Bioscience Engineering, Technische Universität Wien, 1060 Vienna, Austria
sebastian.serna@tuwien.ac.at

Keywords: Bioactive Compounds; Biorefineries; Hemp; Sustainability; Wheat Straw

Abstract

This document describes a PhD proposal framed in a doctoral college entitled "PhD program TU Wien bioactive - Technologies for Drug Discovery and Production". This project focuses on two main core thematic units: discovery of novel bioactive substances and sustainable production of pharmaceuticals. The first thematic unit focuses on discovering new bioactive substances with pharmaceutical application potential from fungi and plants. The second thematic focuses on the development of a sustainable production process for pharmaceuticals. The present PhD proposal is embedded in this second thematic unit. The presented PhD project is entitled: "Bioactive compounds as main economic drivers for sustainable biorefineries". The main goal is to use a renewable plant biomass as nutrient source for the bioprocesses of the fungal expression hosts and set up a sustainable biorefinery for maximal resource utilization of the remaining components of the plant biomass.

Introduction

The necessity of changing the economy and society in general from oil-based to bio-based is a topic that has been already in discussion for the last decades [1]. In the last Global Energy & CO2 Status Report 2018, the International Energy Agency stated "*robust sustainability frameworks are key to bioenergy growth. Only bioenergy that reduces GHG emissions while avoiding unacceptable social, environmental and economic impacts has a future role in decarbonising the energy system*" [2]. Since 2015, the Sustainable Development Goals (SDG) of the United Nations established a route map in order to achieve a more sustainable society, aiming at reaching these goals by 2030 [3]. This context pushes the industry to aim at sustainable production processes and biorefineries have been studied as the technological scheme to process integrally renewable resources and add value to biomass [4]. A great variety of feedstocks, technologies and products have been researched in recent years, given that a shift into a bioeconomy requires not only the production of energy, but also of products used in different industrial and daily life applications [5]. Among these, the so-called "bioactive" compounds have been of high interest, given their high added value and their application in pharmaceutical, health, and cosmetics, among many other fields [6].

However, despite of the applicability and economical interest in these compounds, there are still certain elements that need to be analyzed and connected in order to consider them economic drivers of sustainable production processes. First, bioactive compounds can be produced from many sources, either by extraction from their natural matrix, or producing substrates and obtain them via fermentation, among others. Therefore, it is important to identify raw materials that can be used for this purpose. Second, for the production process to be sustainable, not only the extraction/production of the bioactive compound itself should be considered, but also the valorization of the remaining components of the raw material. Hence, identifying the components of the matrix of the feedstock becomes of great importance, as the composition determines the possible products to be obtained. Finally, the availability of the feedstock plays an important role, because it directly affects the scale of the process. Generally, fine/specialty chemicals have high sales prices, which allows producing them at small scales, but considering aspects as the transport and logistics associated to the availability is important as it strongly influences the feasibility.

Based on the aforementioned elements, this PhD consists of designing sustainable biorefineries at small-scale with bioactive compounds as main economic drivers. Using feedstocks from different origins, the aim is to show that the extraction of high added-value and bioactive compounds coupled with the subsequent valorization of the remaining fractions of the feedstock will result in a sustainable biorefinery, identifying the scale at which it can operate and the respective energy-supply scheme.

Research objectives and approach

The main research question leading this PhD is *Can bioactive compounds be the key elements for a shift into a bioeconomy?* Based on it, the following general objective was proposed: *to design sustainable biorefineries at small-scale with bioactive compounds as main economic drivers*. This implies both experimental and simulation work and the evaluation of different aspects covered within the framework of sustainability (technical/technological, economic, environmental, and energetic, among others).

In order to accomplish this main objective, the following Specific Objectives (SO) are proposed, as shown in **Figure 1**. Each SO also presents the respective research question to be answered and the novelty. For the development of the objectives, four tasks and four sub-tasks for the sustainability assessment are proposed, considering the wide range of topics to be covered (technical, economic, environmental, energy). **Figure 2** shows the respective tasks with a brief description of the overall activity for the task, the scale in case of being experimental work and the software to be used in case of being simulation work.

SO 1: To assess the influence of bioactive compounds in the sustainability of a biorefinery

Research Question	Novelty
Can biorefineries be sustainable if a bioactive compound is obtained as the economic driver?	Bioactive compounds as economic drivers of sustainable biorefineries

SO 2: To identify technology configurations for each feedstock that allow the process to be more sustainable at small-scale

Research Question	Novelty
Which technologies allow the process to be more sustainable at small-scale for a feedstock?	Relation of feedstock, technologies, sustainability and scale of the biorefinery

SO 3: To evaluate energy production schemes in a product-driven biorefineries to obtain bioactive compounds and identify energy self-supply schemes

Research Question	Novelty
Can product-driven biorefineries to obtain bioactive compounds be energy sufficient?	Energy self-supply of product-driven biorefineries to obtain bioactive compounds

SO 4: To identify the scale at which a biorefinery to obtain bioactive compounds is more sustainable

Research Question	Novelty
Which scale makes a product-driven biorefinery to obtain bioactive compounds more sustainable?	Scale at which a biorefinery to obtain bioactive compounds is more sustainable

Figure 1. Specific objectives for the development of the PhD project.

Task 1 — **Experimental extraction of products of interest (high added-value and bioactive compounds)**
Lab scale (1 L) and Pilot plant scale

Task 2 — **Valorization of remaining fractions of the biomass matrix – Experimental and simulation**
Lab scale; Simulation (Software: Aspen Plus V10.0);

Task 3 — **Sustainability assessment**

- **Task 3.1** — **Technical assessment: Technologies**
  Simulation (Software: Aspen Plus V10.0); Scenario Analysis: Selection of technological schemes in the biorefinery for the obtainment of the desired products
- **Task 3.2** — **Technical assessment: Energy production**
  Simulation (Software: Aspen Plus V10.0); Scenario Analysis: Identification of the most suitable energy production technology for the energy self-supply of the biorefinery
- **Task 3.3** — **Economic assessment**
  Simulation (Software: Aspen Plus V10.0); Determination of the Net Present Value of the biorefinery over the chosen lifetime for the project
- **Task 3.4** — **Environmental assessment**
  Life-Cycle Assessment (LCA) (Software: GaBi Professional); Identification of environmental impact indicators; Logistic and supply-chain preliminar analysis for the location

Task 4 — **Analysis of the scale**
Simulation; Determination of the scale at which a biorefinery to obtain bioactive compounds is more sustainable; Economic and LCA assessment at different scales (Softwares: Aspen Plus V10.0, GaBi Professional).

Figure 2. Planned tasks for the development of the research question

The proposed feedstocks to be used are wheat straw, hemp, and a third one to be selected. Each of these raw materials offer different specific features (composition, origin – agriculture, horticulture-, supply chain, availability) influencing the performance of the biorefineries. **Figure 3** shows the general scheme of the proposed biorefinery. The main sections are extraction of bioactive and added value compounds, platform valorization (cellulose, hemicellulose and lignin), substrate production and respective fermentation for the production of bioactive compounds, and effluent valorization through energy production. It is important to mention that the order of the stages and chosen technologies will depend on each raw material. The required methods and techniques will depend on the raw material. However, in general terms, some general methods will be used. **Table 1** describes some of the technologies as software that will be used on each of the tasks.

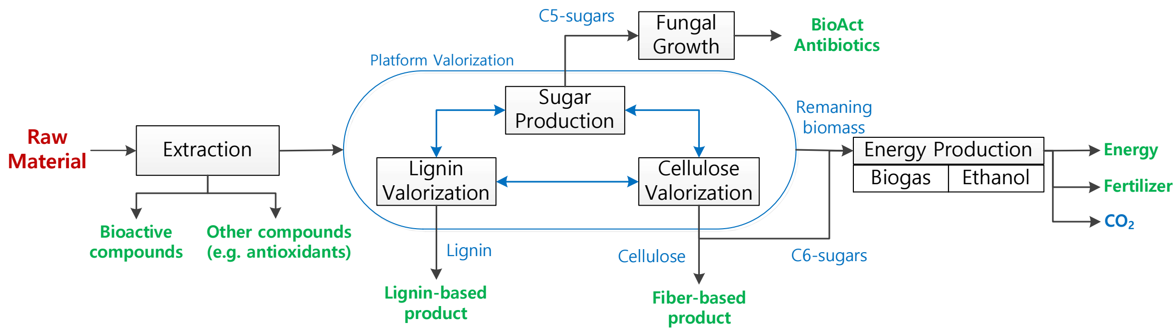

Figure 3. General scheme of the proposed biorefinery

Table 1. General methods and techniques for the development of the PhD

Task No.	Method / Technique	Remarks
1	Organosolv extraction	Pressurized liquid extraction to remove lignin and other compounds of interest. Temperature ranges from 100°C to 180°C depending on the feedstock. Solvent: Ethanol or Water-Ethanol mixture
	Product characterization	Bioactive compounds: HPLC, LC-MS
2	Lignocellulosic characterization	Characterization of the remaining solid after the extraction, to identify further possible uses (NREL/TP-510-42618 and NREL/TP-510-42623). - Cellulose; Structural carbohydrates (arabinan, galactan, glucan, xylan, mannan); Lignin; Ash
	Sugar production	Liquid hot water pretreatment for hemicellulose hydrolysis
	Fiber characterization and valorization	For fiber usage and valorization, techniques that are more specific can be necessary.
	Lignin valorization	Work associated with another PhD student from the research group (Johannes Adamcyk). Lignin precipitation and concentration. Product applications for different lignin formulations (solid, aqueous solution, ethanol-water solution).
1 2	Analytics	Determination based on the NREL/TP-510-42623 Sugars: HPIEC Degradation products (HMF, acetic acid, furfural): HPLC
3 4	Simulation and LCA	Simulation: Aspen Plus V10 LCA: GaBi Professional

Initial Results

The activities performed so far correspond to Tasks 1 and 2. The initial results obtained so far are presented as follows.

Raw material selection and characterization

Hemp threshing residues, grape vineshoots and wheat straw were selected as raw materials. A detailed description of the criteria used for the selection can be found on (Serna-Loaiza et al., 2019) [7]. The focus bioactive compounds of these raw materials are cannabinoids, flavonoids and lignin, respectively. Therefore, an initial characterization of the raw material was performed. This characterization is the base point for mass balances of the process. For hemp and grape vineshoots, the extractives content correspond to the fraction that contains the focus bioactive compounds. For wheat straw, lignin content was determined. **Table 2** shows the respective values obtained for the feedstocks.

Extraction of bioactive compounds

The extraction of cannabinoids was performed as a Pressurized Liquid Extraction (PLE) at 100°C for 100 min, using pure ethanol as solvent. The extraction was carried out in a stainless steel high pressurize autoclave (Zirbus, HAD 9/16, Bad Grund, Germany) with a capacity of 1 L and maximum temperature and pressure of 250°C and 60 bar, respectively. The agitation was set at 200 rpm. At these conditions, it was possible to obtain a raw extract with 1,25 g/L of cannabidiol, corresponding to an extraction yield of 15,1 mg of cannabidiol per gram of dry sample. The next step consists of testing different extractions time and temperatures, to identify the best extraction conditions and then proceed to initial concentration of the obtained extract.

For the case of the grape vineshoots, the extractives obtained from the stage of characterization were used for the identification of components. These results correspond to two fractions: water and ethanol. **Table 3** summarizes the concentration of components of interest that may have bioactive applications determined in the samples. Both quercetin and Shikimic acid have significant concentrations that may be of interest for extraction and purification.

The next step for these two feedstocks consists of testing different extractions time and temperatures, to identify the best extraction conditions and then proceed to initial concentration of the obtained extract. For the case of wheat straw and lignin, previous studies have been carried out already in the Research Group to extract the lignin using Organosolv [8]. For this reason, the focus with this feedstock will be on the valorization of the remaining solid and the combination of pretreatment stages (e.g. Organosolv combined with Liquid Hot Water) to enhance the production of lignin and other products of interests (e.g. sugars).

Table 2. Characterization of the raw materials

Plant Part	**Hemp Threshing Residues**			**Grape Vineshoots**			**Wheat Straw**		
Variety	*Finola*			*Grüner Veltliner*			-		
Determined Component	*Weight percentage (%wt)*								
Extractives	55,13	±	0,53	44,74	±	0,71	52,42	±	1,48
Lignin	9,79	±	0,57	5,79	±	0,31	17,71	±	0,72

Table 3. Characterization of the extracts obtained from the Grape Vineshoots.

Fraction	**Water**	**Ethanol**
Component	**Concentration [µg/mL]**	
Myo-Inositol	746,81	ND
Quercetin	228,22	ND
Shikimic acid	183,38	ND
β-sitosterol	ND	19,98
Inositol	46,88	ND
Gallic Acid	37,77	ND

ND: Not Detected

Outlook

The results obtained so far indicate the potential for the extraction of the selected bioactive compounds. After the optimization of the extraction conditions, the next steps to be considered are:

- Evaluation of a concentration stage to recover the solvent and have the raw extracts in a concentrated form.
- Valorization of other fractions of the feedstocks. Combination of the extraction stage with the sugar production stage (Liquid Hot Water) to determine, which order provides simultaneously a higher extraction yield of the given bioactive compound and sugar.
- Identification of possible applications of the remaining solids after the stages of extraction and sugar production.

References

[1] M. Palmeros Parada, P. Osseweijer, and J. A. Posada Duque, “Sustainable biorefineries, an analysis of practices for incorporating sustainability in biorefinery design,” *Ind. Crops Prod.*, vol. 106, pp. 105–123, Nov. 2017, doi: 10.1016/j.indcrop.2016.08.052.

[2] International Energy Agency (IEA), “Global Energy & CO2 Status Report 2018,” Paris, France, 2019.

[3] United Nations Development Program, “The 2030 Agenda for Sustainable Development,” 2015. https://sustainabledevelopment.un.org/?menu=1300 (accessed May 22, 2019).

[4] S. Serna-Loaiza, C. A. García-Velásquez, and C. A. Cardona, “Strategy for the selection of the minimum processing scale for the economic feasibility of biorefineries,” *Biofuels, Bioprod. Biorefining*, vol. 13, no. 1, pp. 107–119, 2019, doi: 10.1002/bbb.1941.

[5] B. Kamm and M. Kamm, “Principles of biorefineries,” *Appl. Microbiol. Biotechnol.*, vol. 64, no. 2, pp. 137–145, 2004, doi: 10.1007/s00253-003-1537-7.

[6] V. Oreopoulou and C. Tzia, “Utilization of Plant By-Products for the Recovery of Proteins, Dietary Fibers, Antioxidants, and Colorants,” in *Utilization of By-Products and Treatment of Waste in the Food Industry*, Berlin, Germany: Springer, 2007, pp. 209–232.

[7] S. Serna-Loaiza, A. Miltner, M. Miltner, and A. Friedl, “A Review on the Feedstocks for the Sustainable Production of Bioactive Compounds in Biorefineries,” *Sustainability*, vol. 11, no. 23, 2019, doi: 10.3390/su11236765.

[8] S. Beisl, P. Loidolt, A. Miltner, M. Harasek, and A. Friedl, “Production of micro- and nanoscale lignin from wheat straw using different precipitation setups,” *Molecules*, vol. 23, no. 3, 2018, doi: 10.3390/molecules23030633.