

Deliverable report

Deliverable Data		
Deliverable number	D1.4 including D1.1, D1.2	
Dissemination level	LignoCOST members	
Deliverable name	Operational WikiLignin, including D 1.1 and D 1.2	
Work group	WG1	
Lead WP/Deliverable beneficiary	B. Kurek, for the whole consortium	
Deliverable status		
Submitted (Author(s))	20/04/2023	B. Kurek T. Slaghek
Verified (WP leader)	20/04/2023	B. Kurek
Approved (Coordinator)	20/04/2023	R Gosselink

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Introduction

The main objective of **LignoCOST** is to jointly establish a network in which relevant information packages are produced with a focus on sustainable lignin production and valorisation at industrial level (<https://LignoCOST.eu/>).

The **LignoCOST** action has been structured in 5 working groups (WG) of which WG1 is dedicated to the development of a search tool, which should be available on the internet, dedicated to lignin information (nicknamed WikiLignin). This web tool should including information on lignin sources, lignin availability, lignin demand, lignin properties, available literature on lignin and a repository of state-of-the-art analytical methodologies and turnkey methods for the industry and academia.

WG1 has been organized into four tasks:

Task 1.1: Inventory of relevant information on lignin sources, availability, physicochemical and molecular composition, properties in the form of factsheets based on the input from participants.

Task 1.2: Overview and standardization of state-of-the-art analytical methodologies for characterization of lignin. Development of novel analysis techniques to contribute to fundamental knowledge of lignin.

Task 1.3: Mapping / analysis existing lignin production / valorization research infrastructure.

Task 1.4: Selection of relevant information to set up a repository of lignin data and designing / building a web tool called WikiLignin, including intellectual property and web hosting issues.

In the time line of **LignoCOST**, **WG1** had to deliver several items, which were:

- **An Overview existing lignin production/valorization research infrastructure. This has been achieved in October 2020 (D1.3)**
- **A WikiLignin operational webtool, combining the collected and available data on lignins (type, availability; main characteristics; D1.1) and on lignin characterization techniques (D1.2), consolidating some information from D1.3. This will be was achieved for May 3rd, 2023 (D1.4)**

This report on deliverable **D1.4** will present the operational WikiLignin webtool as a whole.

It will include **D1.1** and **D1.2**, because the factsheets are components of the web tool, within a knowledge book (KBook).

The strategy used to construct the webtool and its main functionalities will be explained.

WikiLignin is accessible through the LignoCOST web site <https://lignocost.eu/>

Summary

WG1 is dedicated to the development of a web tool-based lignin information portal on the internet, named WikiLignin. The tool is constituted of two web modules, accessible through specific hyperlinks directly or from the Lignocost website portal (<https://lignocost.eu/>).

The first web module is a keyword searchable database, with around 4000 new and relevant lignin publications covering years 2019 to 2023, which has been updated weekly. Some important papers from prior 2019 and down to 1984 are also included in the database. The tool is hosted by the WUR library (NL; <https://www.wur.nl/en/library.htm>) and is complementary to the core collection of books available on the lignin topic. It is also accessible directly through the following permalink : **<https://library.wur.nl/WebQuery/lignin?collection=lignine>** .

The second web module is a knowledge book (KBook). This electronic media is representing graphically: i/ the main lignin value chains investigated within LignoCOST and ii/ the main concepts and factsheets for structure and characteristics of industrial and pilot scale available lignins (deliverable D1.1) and iii/ the main concepts and factsheets for analytical techniques and methods used in the development of new lignin applications (D1.2). The Knowledge book is hosted by INRAE (FR), accessible directly through a permalink which will be activated and accessible for the EC officers at May 3rd. At a later stage the permanent link will be provided.

Description of the operational WikiLignin tool

The research on lignin is very active within many moving scientific fields, as shown by the number of books and paper published every year. A query with the keyword "lignin" on google scholar retrieve more than 88 000 items, from years 2019 to 2023; the WUR library is referencing 98 books (paper; electronic) published during the last 5 years. This sustain the need of accessible but aggregated, and simplified but accurate informations, useful to the community of scientists and industrial targeting lignin valorization in new applications. The gathering of a complex, prolific and redundant information was a challenge within LignoCOST, addressed by the construction of the WikiLignin tool.

The concept and work area of WikiLignin is based initially on the global lignin valorization schemes that has been designed by the participants of WG1 during the first LignoCOST meeting in Wageningen, in 2019 (**Figure 1**).



Figure 1. Original drawings resulting from WG1 session at the first Lignocost meeting, in Wageningen, 2019.

WikiLignin is the **deliverable D1.4**. It is composed of two different modules, dedicated to collection of information and to knowledge management, in line with the LignoCOST topics on lignin valorization.

The first module is a database, gathering the most recent papers and patents on lignin extraction, transformation and valorization, considering the value chains identified by WG1 participants. For that purpose, with the strong contribution of Corrie Snijder (NL) and Paulien Vredendaal (NL), librarian and information specialists at WUR, a weekly search was performed during all LignoCOST grant periods. The recorded papers and patents were then classified into eight categories by Ted Slaghek (WUR, NL), and Bernard Kurek (INRAE, FR), relatively to the main issues they address: i/ the feedstock, from which lignin is extracted or recovered; ii/ the lignin sources coming from industrial processes; iii/ the lignins coming from a lignin first approach; iv/ the applications, in which lignins or their fractions are tested and used; v/ the use of biotechnological conversion for applications; vi/ the use and development of analytical methods applied to lignins; vii/ the lignin properties viii/ the LCA methods applied to lignin valorization pathways.

The categorized papers were then indexed within a database, specifically elaborated by WUR. It allows a search by category, subject, author, year of publication, and by any word present in the title or the abstract or within the keywords of the published paper or patents (<https://library.wur.nl/WebQuery/lignin?collection=lignine> ; **Figure 2**).

Category

- Applications (18)
- Properties (4)
- Bioconversion (3)
- Lca and justification for lignin research (3)
- Lignin-first (3)

Subject

- Lignin (13)
- Bioeconomy (5)
- Life cycle assessment (3)
- Additives (2)
- Biomass (2)
 - more filters

Year of publication

- 2022 (13)
- 2021 (6)
- 2020 (1)

Author

- Bilal, M. (2)
- Iqbal, H.M.N. (2)
- Li, B.Z. (2)
- Liu, Z.H. (2)
- Yuan, Y.J. (2)
 - more filters

Type

- Article (16)
- Review (4)

Access Type

- Restricted Access (15)
- Open Access (5)

Language

- English (20)

Q bioeconomy Search ?

Records 1 - 20 / 20

Sort by Year of publication (Descending)

▼ Kraft lignin as a bio-based ingredient for Dutch asphalt: An attributional LCA	Science of the Total Environment	2022
▼ Next generation applications of lignin derived commodity products, their life cycle, techno-economics and societal analysis	International Journal of Biological Macromolecules	2022
▼ Ambient-pressure lignin valorization to high-performance polymers by intensified reductive catalytic deconstruction	Science Advances	2022
▼ Enhancing water repellency and decay resistance of wood by using water-soluble fractions separated from pyrolytic lignin of fast-pyrolysis bio-oil	Industrial Crops and Products	2022
▼ Ultra-refining for the production of long-term highly pH-stable lignin nanoparticles in high yield with high uniformity	Green Chemistry	2022
▼ Preparation of biomass-based gas separation membranes from biochar residue obtained by depolymerization of lignin with ZSM-5 to promote a circular bioeconomy	International Journal of Biological Macromolecules	2022
▼ A Comparison of Functional Fillers—Greenhouse Gas Emissions and Air Pollutants from Lignin-Based Filler, Carbon Black and Silica	Sustainability (Switzerland)	2022
▼ Creative biological lignin conversion routes toward lignin valorization	Trends in Biotechnology	2022
▼ Environmental Performance of Oxidized Kraft Lignin-Based Products	Sustainability (Switzerland)	2022
▼ Metal-based ionic liquids: effective catalysts in aqueous media for the selective production of vanillin from alkali lignin at room temperature	Green Chemistry	2022
▼ Lignin chemical derivatives in Brazilian sugarcane sector: An alternative to make 2C ethanol viable?	Journal of Cleaner Production	2022
▼ Biospecting lignin biomass into environmentally friendly polymers—Applied perspective to reconcile sustainable circular bioeconomy	Biomass Conversion and Biorefinery	2022
▼ Molecular Engineering of Biorefining Lignin Waste for Solid-State Electrolyte	ACS Sustainable Chemistry and Engineering	2022
▼ Transformation of Corn Lignin into Sun Cream Ingredients	ChemSusChem	2021
▼ Understanding lignin micro- And nanoparticle nucleation and growth in aqueous suspensions by solvent fractionation	Green Chemistry	2021
▼ Lignin valorization for protocatechuic acid production in engineered: <i>Saccharomyces cerevisiae</i>	Green Chemistry	2021

Figure 2. Screen shot of a typical page of the WikiLignin database. The search word was "bioeconomy", thus present or in the title or in the abstracts or in the keywords of the articles, and related to lignin research fields.

This pool of information (around 3800 papers, in April 2023) contain all needed information for scientist and industrials developing value chains on lignins. Still, the information is scattered within the database and links are only made through combinations of search words.

Among all, there are currently 2963 papers referenced within the category "applications", 716 within "properties", 564 within "lignin first", but only 25 "Life cycle analysis", for instance. 131 patents were also collected within the period 2016 to 2022, coping with extraction of lignins, derivatization/functionalization, use as nanoparticles, use as adhesives, use as dye, depolymerisation /transformation into BTX, uses as bulk compound, for instance.

The papers and patents retrieved are representative of the latest development for lignin applications, but not exhaustive, excluding all the aspect of lignification in plants, or the fate of lignin in the geo-environment. For instance, a query on the Web of Science (WOS) for article including "lignin" in title is sorting about 8050 items, a number to be compared to our resulting expert search and categorization, focused on lignin value chains from the feedstock to the products.

The second web module of the WikiLignin is a knowledge book (KBook). This hypermedia tool is specifically designed to facilitate the understanding of complex concepts and procedures in a specific scientific or technical field (see <https://ieeexplore.ieee.org/document/6166225>). It is constituted of standardised graphical representations of concepts, validated by experts, and illustrating all the most important knowledge of a particular topic. Such KBook approach to manage complex knowledge has been successfully used within a H2020 BBI European project on Humins and Lignins valorisation (Zelcor 2016-2021 ; <https://plastic-apps.transform.inrae.fr/zelcor/>), for instance.

The structure of the KBook has been designed with colleagues of INRAE Bordeaux (I2M research unit; FR), specialized in knowledge management (Christophe Fernandez; <https://www.i2m.u-bordeaux.fr/>) and thanks to the work of a post-doctoral scientist, Justine Padovani (INRAE UMR FARE, Reims, FR), to build and publish the final public version of the book.

Currently, the book is available for the Lignocost partners and the EC officers managing Lignocost from May 3rd, 2023 with the yet non-public link. It will be publicly accessible in a permanent way, at the latest in end of May 2023, after a final quality check and approval by EEC officers. The book will be accessible by direct permalink (indexed on google) or through the Lignocost website. The Lignocost website (www.lignocost.eu) will be available for at least the coming 5 years.

The KBook sections are organised in order to access to the main information by a general scheme with four chapters (*Materials/Analytical Methods/Processes/Sustainability and Value Chains*) and by a *detailed diagram*. This latter is, *in fine*, a graphical representation of the value chains of lignins addressed in all Lignocost working groups, and including the WG1 initial concept (see **figure 3**, and also **Figure 1 and annex**).

The entry page "**discover the book**" shows links to the Lignocost objectives overview, the different working groups and the link toward the WikiLignin database (*http switch*; central part, **Figure 3**).

The specific **deliverables of WG1, D1.1** (Materials hyperlinks switches) and **D1.2** (Analytical methods hyperlinks switches) are full part of the KBook.

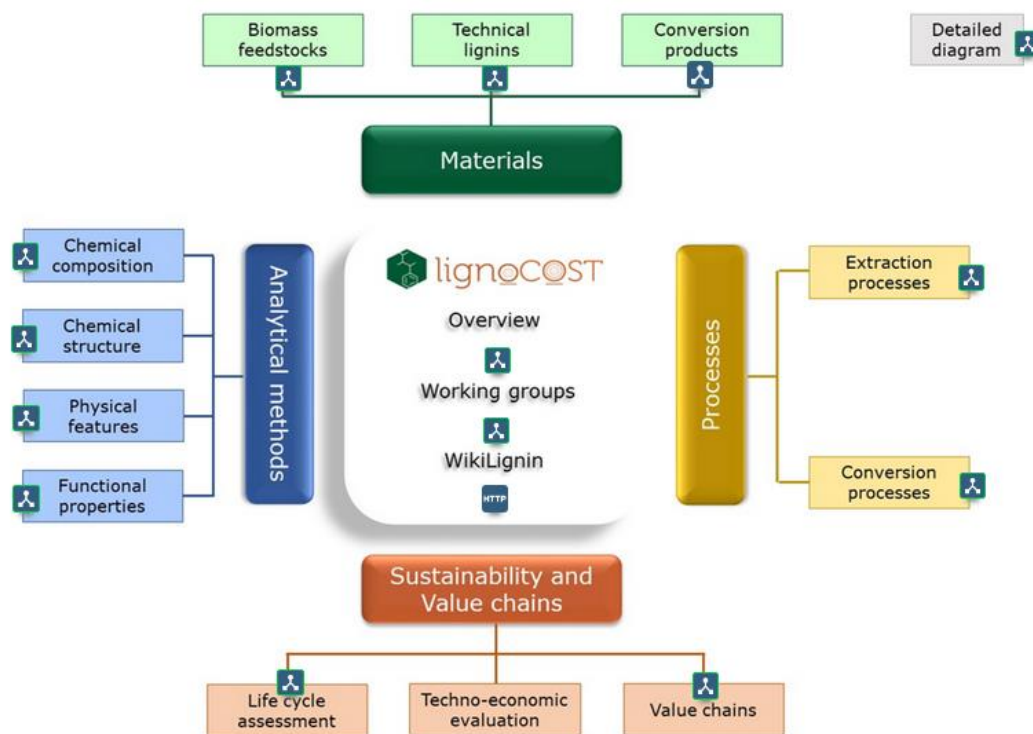




Figure 3. Entry page of the KBook

Description of the deliverable 1.1 - Lignin data factsheets

The **Deliverable 1.1** is composed by the concept maps of technical lignins (C-maps; hyperlink symbol ), where factsheets are attached (hyperlink symbol ).

A total of **12 factsheets** on the main characteristics of technical lignins are attached to the concept map shown in **Figure 4**. They described specifically the main characteristics of the Kraft family, liginosulfonates, soda lignins, organosolv lignins, DES lignins, pyrolysis lignins, etc...

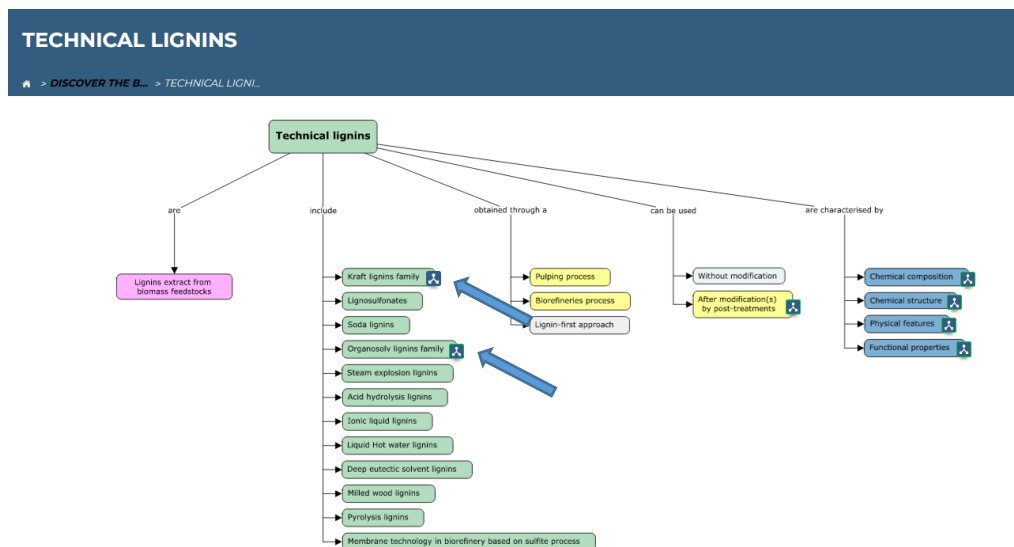


Figure 4 - Draft of the concept maps of technical lignins, where factsheets constituting D1.1 are attached. In this static draft version, clicking on the C-maps symbols (blue arrow) will open a second level of C-maps, where specific factsheets will be available, as exemplified in the next **Figure 5**.

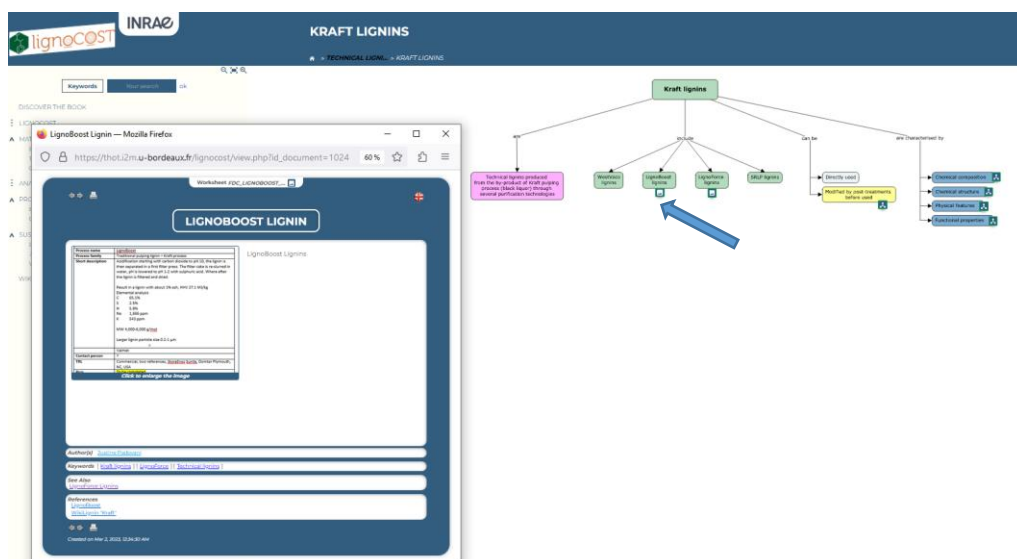



Figure 5. Example of a factsheet appearing by clicking the *lignoboost* hyperlink factsheet switch (, see arrow), from the *kraft lignin* concept maps (final version may differ in appearance).

Description of the deliverable 1.2 - Overview of the state-of-the-art analytical lignin characterization techniques

The Deliverable D1.2 on lignin characterization methods are presented in a same manner as D1.1 in the KBook. Figure 6 is showing for example a static draft version of the concept maps for chemical characterization.

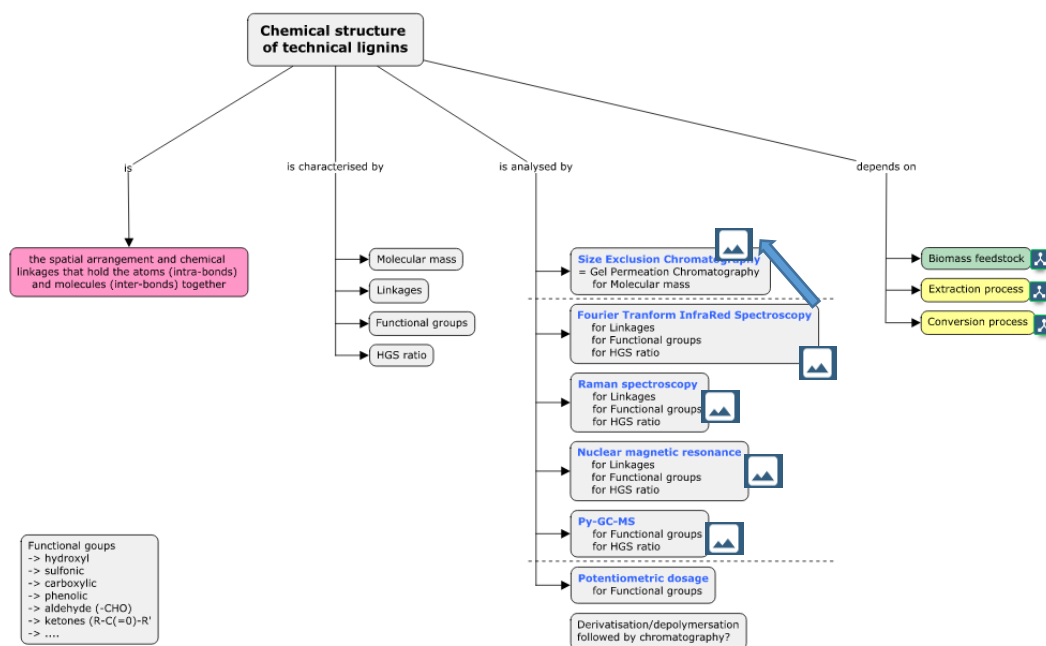


Figure 6. Concept maps for methods used to characterize the chemical structure of technical lignins. The factsheets are constituting D1.2; hyperlinks switches will point to each factsheet, as shown in the previous **Figure 5**.

The **D1.2** is constituted by **25 factsheets**, that are linked to relevant sections: chemical composition; chemical structure, physical features. As an example, **Figure 7** shows the factsheets on *size exclusion chromatography* of the section illustrated in **Figure 6** (arrow).

- Size Exclusion Chromatography -

The size exclusion chromatography (SEC) also called gel permeation chromatography (GPC) is a liquid chromatography experiment that aims to determine the molecular mass distribution of the sample.

The solubilized sample is eluted through a column stationary phase which is a porous gel matrix with specific pore size. The role of the column is to sort the molecules by their size. Indeed the smallest molecules penetrate more easily into the pores of the column causing a higher retention time than the larger molecules.

Several detectors can be used with SEC :


- **Refractive index detector (RI)**: This detector is the most common and allows to determine in continue the specific refractive index increment parameters (dn/dc) for determine the concentration of each molecules. The dn/dc is useful for interpreting results obtained with other detectors. Each molecule have a specific dn/dc resulting of the difference between the RI of molecule with the RI of eluent. The chromatogram obtained is a graph of the concentration in function of elution time. The signal is proportional to the concentration of molecules. With the help calibration curve obtained by analysis of suitable mass range of standards, the SEC experiment can provide several structural parameters of the technical lignins such as the molecular weight (M_w), the molecular number (M_n) and subsequently the polydispersity index ($PI = M_w/M_n$).

Complementary detection modules can be added to obtain further data such as:

- **Photodiode array detector (Pda)**: This detector measures in continue the UV absorption of the molecules and provide addition information about chemical composition notably aromatic molecules and functional groups.
- **Multi angle (laser) light scattering (MALS or MALLS) detector**: This detector measures the scattering intensity of the sample and provides additional information about chemical structure such as the mass concentration, the conformation (linear, aggregate...) or the gyration which inform about the size and shape of the molecule . This detector is more suitable for large and heterogeneous molecules like technical lignins.

As the experiment happens in liquid environment, this implies that the lignin sample are soluble in the solvent used which is the same of that the eluent (mobile phase) of the column. To improve the solubilisation of technical lignins, they can be derivated by acetylation.

Author(s)	Justine Padovani ; Bernard Kurek
Keywords	Size exclusion chromatography; SEC; Gel permeation chromatography; GPC; molecular mass; RI ; PDA ; MALS ; MALLS ; structure
See Also	text
References	WikiLignin "SEC" https://library.wur.nl/WebQuery/lignin?q=sec

Figure 7. Example of a factsheet appearing by clicking on the factsheets switches ( see arrow in Figure 6; final online version may differ in appearance).

Functional properties of lignins are reported in the KBook, but not detailed into factsheets, being out of the scope of WG1. Nevertheless, the 16 most relevant methods used to characterize functional properties of lignins and their products were listed. More information can be found within the 250 categorized "functional properties" papers from the WikiLignin database, as well as in deliverables from other LignoCOST Working Groups and alternatively in the Zelcor KBook, where some generic methods of lignins functional properties are described (<https://plastic-apps.transform.inrae.fr/zelcor/navig.php?idoc=1037>).

Limits of the WikiLiLignin webtool and further dissemination and valorization

The WikiLignin is an original way to gather information and to disseminate knowledge on lignins value chains. The web tool, hosted jointly by WUR (NL) and INRAE (FR) will guarantee permalinks over the time. The book can be evolutive, and new information can be added, if necessary. In particular, it is planned to add hyperlinks in the *detailed diagram* pointing to the deliverables from the other WG of LignoCOST (see text *ks*

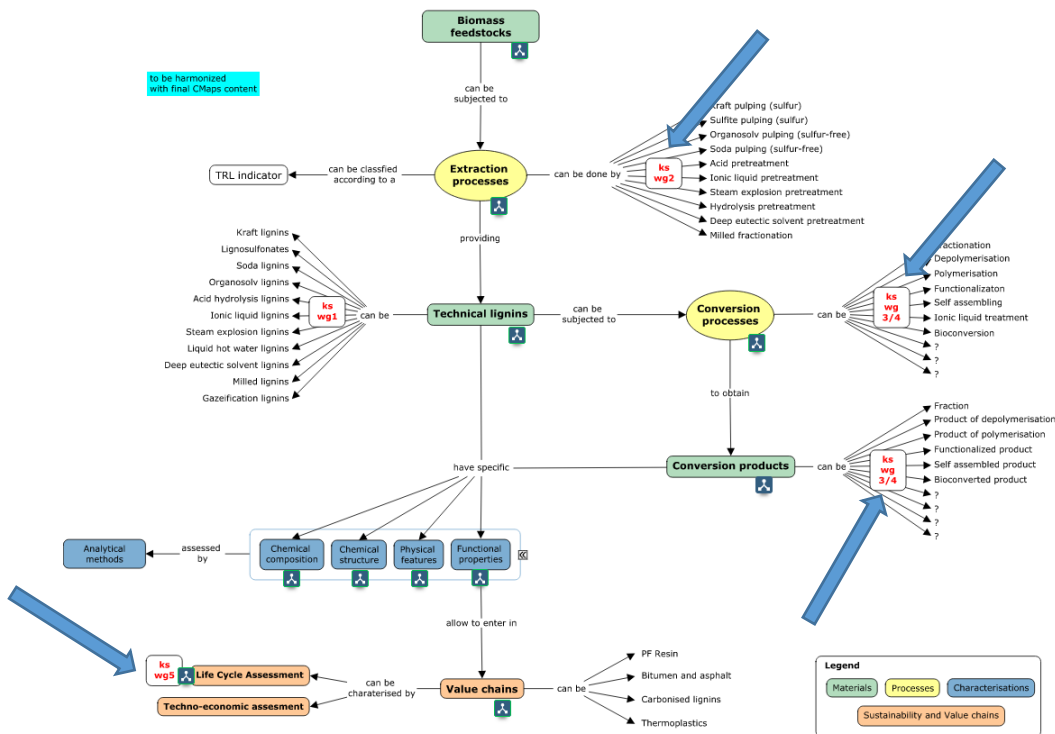
wg2, 3, 4 and 5 in red in the web page - see annex), allowing a complete overview of this collaborative network project.

The main limit of the WikiLignin tool is its focusing on the network activity. It is not covering exhaustively the scientific and patent literature on lignins. Nevertheless, this portal to knowledge is unique, accurate and will be updated the next 5 years, according to a *gentleman agreement* between Lignocost WUR and INRAE members, for the benefit of the community.

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ANNEX

Possible hyperlinks switches (labelled *ks wgx* or *ks wgx/y* - see arrows) pointing toward all WG 2, 3 4 and 5 deliverables in the detailed diagram section of the WikiLignin KBook.



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