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Getting your hands dirty: A data digging exercise to unearth the EU's bio-based chemical sector

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ABSTRACT

Under the auspices of the EU's new Circular Economy Action Plan and Bioeconomy Strategy, the usage of sustainably renewable biomass for bio-based chemicals is a part-solution for addressing the multidimensional challenges of (*inter alia*) growth and employment, food and energy security, climate change and biodiversity. Unfortunately, the lack of a formal system of European data classification and collection presents a major obstacle to measuring, monitoring and *ex-ante* modelling of the bio-based chemicals sector, which clouds the ability to make science-based policy and legislative judgements. Employing a combination of different data sources and plausible assumptions, this paper seeks to overcome some of these data gaps through the compilation of a meaningful set of economic and sustainability indicators for specific bio-based chemical activities and products. Due to the variety of data sources employed for each indicator, a data quality index is constructed, whilst rigorous comparisons with other studies and further critical discussion reaffirms the general observation of poor data quality. Subject to these data and methodological limitations, this paper analyses the performance of bio-based chemical industries. As long as official data sources lack adequate information systems, the current paper serves as a springboard for lowering the data 'entry costs' behind this intricate sector, encouraging further knowledge-sharing and serving as a replication template for other regions.

1. Introduction

The European Green Deal [1], presented in 2019, reflects the increased and substantiated efforts of the EU in the pursuit of a more sustainable and circular economy, departing sharply from the traditional 'take-make-dispose' linear model of economic growth, as also supported by the new Circular Economy Action Plan [2]. Launched in 2012 and updated in 2018, the EU's Bioeconomy Strategy [3,4] plays an integral role promoting sustainably renewable biomass to meet the multiple challenges of (*inter alia*) food and energy security, climate change and biodiversity.

In this context, a key tenet of this EU approach towards sustainability, known as the 'cascading' use model, is to prioritise biomass to maximize its economic value over its production lifespan [5], while keeping the usage for food as the highest priority. Typically, this implies the production of higher-value added bio-based products before recycling into lower value–added applications,[1] with a final conversion to energy. Within this paradigm, a clear candidate for high value-added production is the promotion of biomass for bio-based chemical applications. Indeed, this drive toward bio-based chemicals is recognised in the Chemicals Strategy for Sustainability [7], released in 2020, which aims to accelerate the green transition of the chemical industry and its value chains. Moreover, as the world is struggling with the COVID-19 pandemic, the strategic importance of biotechnological and bio-based chemical products has come to the fore. Under the auspices of the Green Deal, the EU recovery plan provides opportunities for investments into sustainable and long-term systemic solutions, whilst the European

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[1] An exception is the process of *upcycling*, i.e., the conversion of by-products and waste into products of higher quality and value [6]. A relevant example of upcycling is the transformation of PET bottles into textiles of higher value.

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Abbreviations and nomenclature:

BBI-JU	Bio-based Industries Joint Undertaking
CEFIC	European Chemical Industry Council
CGE	Computable General Equilibrium
CN 2016	Combined Nomenclature 2016
CPA	European Classification of Products by Activity
DG RTD	Directorate General for Research and Innovation
EU	European Union
EUR mln	million euro
EUR/kg	euro per kilo
GHG	Green House Gases
ha	hectares
ha/t	hectares per tonne
JRC	Joint Research Centre
KCB	Knowledge Centre for Bioeconomy
kt	kilotonne (1,000,000 kg)
LCA	Life-Cycle Assessment
NACE	nomenclature statistique des activités économiques dans la Communauté européenne
PE	Poly(ethylene)
PET	Poly(ethylene terephthalate)
PLA	Poly(lactic acid)
Prodcom	PRODuction COMmunautaire
QI	data Quality Index
t	tonne (1000 kg)
TRL	Technology Readiness Level
UAA	Utilized Agricultural Area

Circular Bioeconomy Fund[2] is another instrument to support bio-based innovations, not least in the area of the chemical sector.

It is estimated that 96% of all manufactured goods require inputs from the chemical industry [8]. With 1.14 million employees and sales of €507 billion in 2016, the European chemical industry is one of the largest industrial sectors in the European Union and a leading source of direct and indirect employment in many regions [9]. Crucially, the chemical industry in its entirety is also characterised as a highly energy intensive activity, constituting a large source of greenhouse gas emissions [10,11], although bio-based alternatives offer potential solutions for decarbonising chemical activities.

Thus, the channelling of biomass into chemical applications is a potentially lucrative outlet for sustaining growth and employment prospects for product diversification within biorefineries [12,13] and for the contemporary bioeconomy as a whole. Moreover, with the potential to (partially) substitute conventional fossil technologies with bio-based equivalents, there also lies the opportunity to alleviate climate change concerns [8,9,14]. A related issue, however, is the sustainability of promoting said technologies in the EU, where the usage of biomass of agricultural origin and its implications for third-country leakage effects is currently under debate [15,16]. Moreover, within the EU there is a disconnect between its strategy recommendation and public policy support [17,18]. The latter biases biomass usage toward energy generation [12,19], thereby running the risk of crowding-out investments in, and production of, 'higher-value' materials [20,21].

Taking a scientific evidence based approach to evaluate the sustainability criterion associated with different biomass sources, optimise economic growth and employment and assess the thorny issue of bioeconomy policy coherence, requires a mixture of expert insight, *ex-post* key indicator analysis and *ex-ante* modelling assessments. Since 2017, the Joint Research Centre (JRC) of the European Commission (EC) launched a platform to compile these different sources of knowledge, called the Knowledge Centre for Bioeconomy (KCB), with public access to data sources for researchers, policy makers and other interested parties to monitor the bioeconomy in Europe.[3] For EU bio-based chemical activity, however, the picture is still highly incomplete owing to data scarcity, which severely hampers meaningful monitoring and performance analysis. The EU's statistical office, Eurostat, provides insightful manufacturing statistics based on official activity and product classifications (e.g., NACE, CPA, CN 2016 and Prodcom), although the activity and product line definitions are not adequate for extracting values and quantities originating from bio-based production pathways. In their revision of the literature examining sustainability indicators for bio-based chemicals, it has been observed that hitherto economic indicators are typically inferred or 'constituent' upon other indicators, rather than being explicitly reported or calculated [22]. An additional complication arises from the high number of different chemical products, estimated to reach more than 75,000 chemicals and more than 15, 000 consumer products [23].

In the absence of appropriate statistics, scientists have elaborated methodologies for estimating the production quantity of bio-based chemicals or the economic size (in terms of turnover or value added) of the bio-based component of the chemical industry. Such methodologies are classified as input- or output-based methodologies [24]. Input-based methodologies estimate the proportion of bio-based inputs in total inputs for the production of bio-based chemicals, with examples for the Netherlands [25], Germany [26] and the EU25 [27]. The European Chemical Industry Council (CEFIC) publishes data on the share of renewable raw materials in the total organic raw material demand of the EU chemical industry [28]. Output-based methodologies estimate the biomass content of bio-based chemicals. Employing Eurostat data as a primary source and expert knowledge, output-based bio-based shares at product level have been estimated and subsequently extrapolated to sectoral level to calculate the values of bioeconomy-related activities (including chemicals) [29]. Supporting *ex-post* indicators (employment, value added and turnover) are calculated for the whole EU and individual Member States and annually updated [30–34]. Similar output based studies including chemical activity, have also been carried out for the Lithuanian [35], Dutch [36] and Norweigan [37] economies. More recently, Kuosmanen et al. (2020) [38] propose a hybrid framework combining input- and output-based approaches for estimating the size of the European Bioeconomy.

The above efforts have also played a role in opening official national accounts, which are employed in economy-wide assessments of the bioeconomy. For example, a representation of bio-based chemical activities within a system of macroeconomic national accounts for all EU Member States [39], has paved the way for their inclusion within linear multiplier analysis [40,41] and medium to long-term computable general equilibrium (CGE) simulation modelling studies [42,43]. In these studies, however, bio-based chemical activity is restricted to two 'promising value chains'[4] supported by bottoms-up engineering estimates, whilst a fully comprehensive characterisation of 'current' bio-based chemical technologies remains elusive. A related CGE study [44] splits out bio-based plastics from the national accounts to examine the impact of increased adoption of bio-based plastics on conventional feedstocks and land use driven GHG emissions.

This paper critically builds on earlier work [45] in the construction of a set of key *ex-post* indicators for bio-based chemicals (i.e.,

[2] https://circulareconomy.europa.eu/platform/en/news-and-events/all-news/european-fund-support-circular-bioeconomy.

[3] https://ec.europa.eu/knowledge4policy/bioeconomy_en.

[4] These two value chains are polylactic acid and polyethylene.

production, consumption, price, trade, feedstock and land use indicators). In order to provide a higher level of detail than what is currently available in published input- and output-based approaches (i.e. below the Prodcom 8-digits level), official statistics from Eurostat are combined with secondary data sources such as specialist market data suppliers, specialist literature, and individual companies and expert interviews, while accounting for the data quality of each source.

A further objective of the paper is to highlight the main assumptions and key challenges to be addressed in the compilation of such a detailed assessment. Moreover, we describe the strategies adopted to overcome these challenges together with their strengths and weaknesses. To the extent possible, the numbers and methodologies in the paper are also compared with available statistics from other literature.

Insofar that official statistics lack adequate coverage of the flows and value of bio-based products and their biomass needs [29,46], the methodology proposed here could be taken as a blueprint for further understanding the complexities of other contemporary bio-based sectors and stimulate further actions in the construction of a more comprehensive information system.

The rest of the paper is structured as follows. Section 2 explains the key methodologies, indicators of bio-based chemical markets, assumptions and uncertainties underlining the analysis. Section 3 presents the results, whilst the final section provides some discussion and concludes.

2. A data digging exercise

2.1. Scope and methodology

In this description of the chemical sector, the focus is only on non-energy and non-traditional bio-based chemicals, either entirely or partially constituted by renewable raw materials from biomass. By adopting the EC definitions on Technology Readiness Levels (TRLs) [47] only those products that are commercially available are examined, i.e., that have a TRL equal to or above eight. The exclusion of products with a lower TRL facilitates both data collection and comparison with other studies such as Nattrass et al. [48].

The methodology is composed of three main steps. In the first step, ten representative application categories were defined. The second step was to select a representative subset of bio-based chemicals from the RoadToBio longlist of bio-based products [49] to reflect the application categories derived from step one. Finally, a set of indicators was compiled using the collected information. A graphical representation of the chemicals selection procedure is provided in Fig. 1.

2.2. Data aggregation challenges in official statistics

One of the main challenges in using official statistics to describe the bio-based chemical sector is represented by the classifications intrinsic to the official coding system (for example, the NACE classification [50]) which does not capture the nature of bio-based chemical products. More specifically, bio-based chemical products can be divided into two main classifications. The first classification is *drop-in chemicals*, defined as bio-based variants of already existing petrochemicals. The second classification, denominated as *dedicated bio-based chemicals*, describes chemicals which can only be produced via a biomass-based pathway, without having petrochemical counterparts [51]. These classifications pose challenges for the extraction of relevant information from official production and trade statistics. For *drop-in* chemicals, even at the most disaggregated 8-digit Prodcom/CN 2016 codes, it is not possible to distinguish between pathways that are bio-based and fossil based. Thus, the aggregation of bio-based pathways is not feasible. As *dedicated* bio-based chemicals have no petrochemical equivalent, the aforementioned aggregation issue for dedicated bio-based chemicals from official databases is not a problem, although there are two other data aggregation considerations. The first is that the 8-digit identifier could potentially represent a whole bundle of products rather than a single commercial tradable product. Thus, when bundled products are represented by a single Prodcom/CN 2016 code, the task of discerning the share attributable to bio-based production becomes unwieldy and thus, statistics may suffer from aggregation problems. The second issue is that bio-based chemicals - both drop-in and dedicated - may be obtained as mixtures of bio-based and fossil-based feedstock and retrieving the percentage of each feedstock source might require complex assessments. Thus, even in those cases where official production and trade statistics were available for a dedicated bio-based product with a one-to-one mapping with a Eurostat code, in the absence of additional assumptions or data sources, it is still difficult to extract the 'true' bio-based portions from those statistics.

2.3. Defining the boundaries of chemical sectors

The bio-based chemicals market is a complex mix in terms of the number of products, and the complexity and novelty of their value chains [45]. One way of capturing some of these complexities, is to describe the sector in terms of application categories (e.g., platform chemicals, solvents, polymers, etc.). These application categories are groups of chemicals that share similar properties and final uses, whilst providing a synthesised representation of the market. Even though the use of application categories may mask some important heterogeneity and requires some assumptions regarding the number of categories and their definition, it allows one to synthesise the representation of such a complex segment.

The choice of these application categories is non-trivial but can be performed by taking into account the main end-uses of the chemical products represented. Thus, ten categories are selected following the NACE classification system in order to maximize present and future links with official statistics. Table 1 presents these ten categories.

A related issue, however, is that even defining each of these application categories in terms of specific chemical products is not a straightforward task. To illustrate, in Table 2, three of these application categories with their respective representative chemicals, are presented. For each of the bio-based chemicals presented, both the selected application category as well as other potential application categories, are shown.

Table 2 highlights the challenges posed by the level of aggregation of official classification system and by the complexity of the value chains in the chemical sector. Each chemical is assigned to only one category. However, due to their chemical characteristics, many of the selected chemicals could, in principle, be included in several application categories. For example, propylene glycol is classified as a platform chemical but it could have been assigned to either one of the groups solvents or paints. On the contrary, butanol(-iso) is classified as a solvent, while it could also have been classified as a platform chemical or as a paint. Polyethylene, as several other chemicals classified as polymers for plastics, could have been treated as a man-made fibre instead.

The full correspondence table between products and application categories is presented in Table A1 of Annex A. The decision of the classification of each product into a specific application category has been based on a series of theoretical and practical considerations. The distribution of chemicals into application categories was done in such a way to capture a fuller diversity in the feedstock requirements (i.e., starches/sugars versus vegetable oils) within each category while guaranteeing that categories were assigned chemicals with different characteristics (alkenes, alcohols, polyols, etc.). However, a different choice in the definition of the application categories and their composition would have had an impact on the final assessment of the bio-based chemicals market.

In addition, despite being based on a series of technical considerations, the specific choices are subjective and also based on practical considerations such as data availability. Such a choice, as was the case for official coding systems, could have strong implications for the comparability and future classification of statistics. In fact, without an

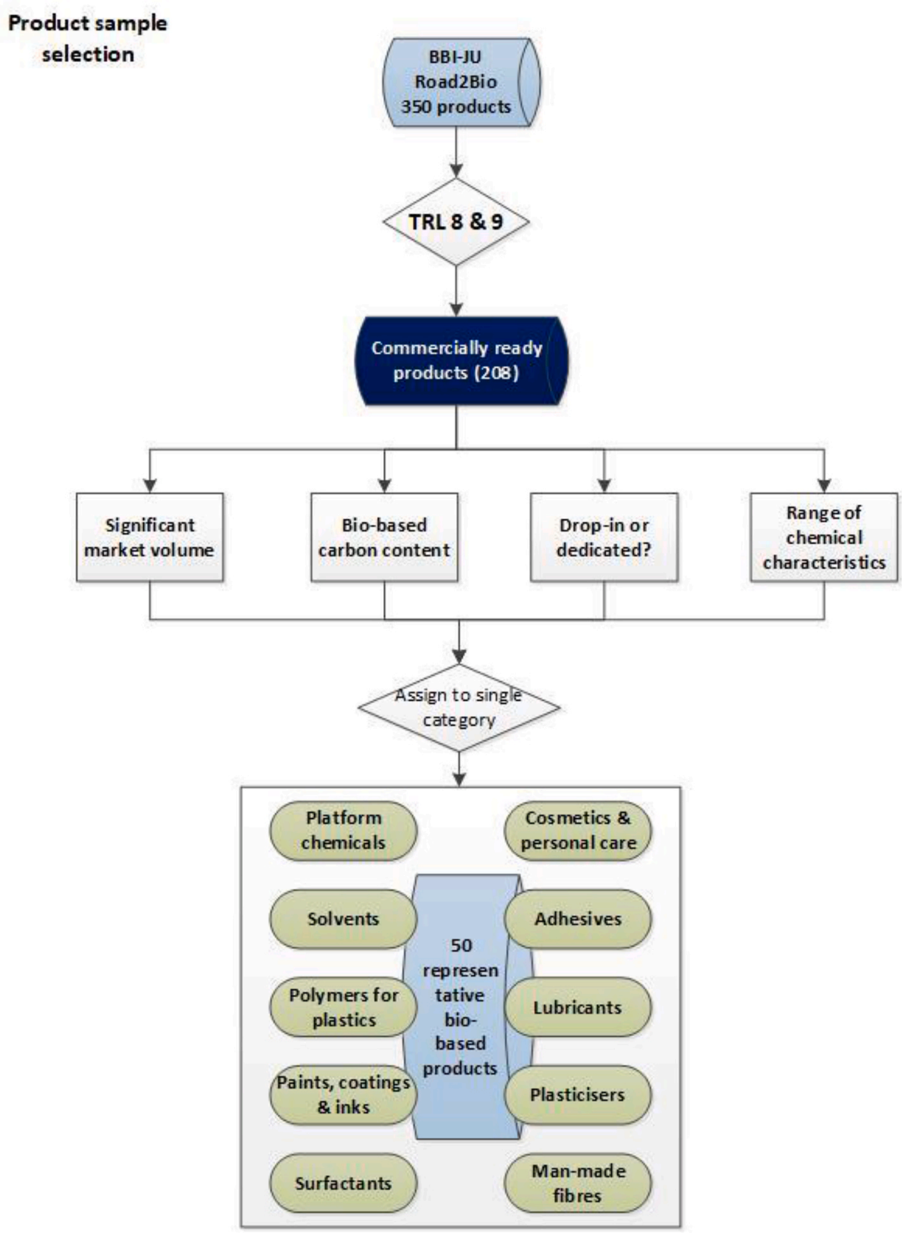

Fig. 1. Graphical representation of the product selection procedure.

Table 1
List of application categories.

Application category
Adhesives
Cosmetics and personal care products
Lubricants
Man-made fibres
Paints, coatings, inks and dyes
Plasticisers
Platform chemicals
Polymers for plastics
Solvents
Surfactants

agreed definition on the boundaries of the bio-based chemical sectors, the comparability of production and trade data can always be challenged, as has been the case for some official classification systems such as NACE. Moreover, part of the bio-based chemical sector is still in development. In response to rapidly increasing demand for sustainable products and policy driven mandates, it is expected that a proliferation of new products, both dedicated and drop-in, will be available on the market in the coming years. To provide comparable statistics over time and to monitor the evolution of the bioeconomy, the classification system for the bio-based chemical sector should therefore take into account the dynamic nature of the industry. The proposed approach (Table A1) should be considered as a proposal in this respect and as a starting point to define an agreeable, flexible definition of the bio-based chemical sector.

2.4. Indicators and data availability

A good set of indicators is a prerogative of an efficient monitoring system and the design of indicators should be targeted to capture synergies and trade-offs across multiple objectives and multiple scales [52]. To this end, a broad set of measures at different aggregation levels and different objectives should be established [52]. At the same time, the

Table 2
Selection of bio-based chemicals with selected and potential application categories.

Chemical name	Selected Category	Potential application categories								
		Platform chemicals	Solvents	Polymers for plastics	Paints	Cosmetics	Adhesives	Lubricants	Plasticisers	Man-made fibres
Ethylene	Platform chemicals	x								
Ethylene glycol		x	x		x					
Propylene glycol (aka 1,2-propanediol)		x	x							
Propanediol (1,3-)		x	x			x				
Acetic acid		x	x							
Acetic anhydride		x								
Sebacic acid (aka decanedioic acid)		x				x		x	x	
Lactic acid		x								
Epichlorohydrin		x								
Butanol (iso-)	Solvents	x	x		x					
Ethyl acetate		x	x		x		x			
Ethyl lactate		x	x		x	x	x			
Acetone		x	x		x	x	x			
Turpentine		x	x		x					
Poly(ethylene) – PE	Polymers for plastics			x						x
Poly(ethylene terephthalate) – PET				x						x
Starch used for polymers				x						
Poly(hydroxyalkanoates) – PHA				x						x
Poly(lactic acid) - PLA				x						x

Source: Spekreijse et al. [45].

choice of indicators is also dictated by data availability. In particular, when monitoring highly disaggregate sectors, a lack of data can be an important bottleneck in the creation of an efficient system of monitoring indicators. In those cases, basic indicators and proxies are typically favoured [52].

To describe the sustainability dimensions of the bio-based chemical sector, a number of quantitative indicators are identified that could be constructed using available data. Both economic and environmental indicators have been constructed at such a disaggregate level to allow for a detailed description of the impact of the bio-based chemical sector. Table 3 presents the indicators that have been used to describe the market for bio-based chemicals. Their estimation is achieved by combining data at category level with data obtained at the level of the representative chemicals.

The indicators are meant to describe the European market of bio-based chemicals in terms of supply side (production, prices and turnover) and demand side factors (consumption), the interlinkages with other bioeconomies (net trade and import dependence) and the environmental footprint (land use). These indicators are also part of the set of official key performance indicators provided in the Bio-Based Industries Joint Undertaking (BBI JU).[5]

For only two of the dedicated bio-based chemicals (rayon and cellulose acetate), was it possible to retrieve information on production, turnover, and trade data from Eurostat sources. For these two chemicals, their bio-based content is not reported at all in official statistics and has to be obtained from the specialised literature.[6]

Given the lack of official statistics, additional market data on production, price, consumption and trade were obtained from specialist market data suppliers, specialised literature and individual companies. Google Scholar, ISI Web of Knowledge and easily accessible online sources were accessed in the literature search to complement the data collection. For specialised market studies, only the free and publicly available data were used for this study. When no data could be obtained from market data suppliers or scientific literature, other sources were used, such as reports from consultancy firms, project reports or specialised websites.

Finally, in those cases where no relevant data could be found, a best estimate is provided and validated through expert interviews. Of course, the validity of a subjective measure obtained with best guesses can be debated. In fact, strong assumptions could lead to biased conclusions on some of the indicators presented. An example is represented by the price data associated to specific bio-based chemicals, where price data could not be found in the literature. In those cases, prices were assumed equal to their fossil-based counterparts. As bio-based compounds are typically more expensive than their fossil-based equivalents due to the novelty of their value chains, such an assumption may lead to an underestimation of turnover statistics of these bio-based chemicals. To flag up this potential bias due to data availability and assumptions, all data sources employed were classified according to their relative reliability (data quality indicator), ranging from one to four, that captures both the time frame to which the data refers and the degree of reliability of the source (see section 2.6).

Table 3
List of indicators.

Indicator	Description
EU bio-based production	Production of bio-based chemicals at category level
Total EU chemical production	Bio-based and non-bio-based production at category level
Bio-based share	Bio-based production divided by total chemical production
Prices	Production-weighted average price of representative chemicals
Turnover	Price multiplied by bio-based production
Consumption	Residually calculated from Eq. 1
Net Trade	Imports minus Exports
Products Import dependence	Net Trade divided by consumption
Land use	Hectares of land required to produce one tonne of a final chemical (see section 2.4)

Eq. 1: Production - Consumption + Import - Export + Stock Variation = 0, where Stock Variation is assumed to be zero.

[5] https://www.bbi-europe.eu/.

[6] The bio-based content of rayon and cellulose acetate is estimated to be 100% and 50% respectively [45].

2.5. Resource usage through value chain analysis

As the amount of resources to sustain the current and future development of the bioeconomy is still not well known in the literature [53, 54], the estimation of land requirements for the bio-based chemical sector represents an important data gap.

To this end, land usage associated with the current EU bio-based chemicals production and consumption is calculated through the use of value chains for the fifty individual products examined [45]. Value chains are representations of the conversion steps between primary biomass feedstock and final bio-based chemical products via bio-based intermediates. The value chains used in this work are described in a schematic way. Thus, for each tonne of final products, indicative amounts of feedstock and any intermediate products are reported together with average conversion yields. Average agricultural yields and specific literature based data on conversion coefficients are used to quantify materials requirements along the chains. For oil crops, an average of oil crops was used, with the exception of products that require a specific oil crop, e.g. castor oil.

Fig. 2 shows an example value chain used to transform bio-based production figures into feedstock usage and refers to the development of 1 tonne of ethylene glycol from 2.3 tonne of sugar originating from sugar and starch crops. The results of this analysis, in terms of land use requirements, are presented in section 3.3.

This is not the first time in the literature that value chains have been employed to calculate resource usage of specific products. In fact, the whole concept of product-related life-cycle assessment (LCA) is based on the idea of full representation of the production process coupled with the use of a series of technical coefficients to estimate resource usage and environmental impacts. However, to our knowledge there are no examples in the literature of an assessment of such a large number of different value chains for bio-based chemical products. With a sole focus on bio-based polymers for plastics, other studies [55–57] have adopted a similar value-chain approach to the estimation of resource usage.

When adopting such an approach to the measurement of resource usage, particular attention needs to be dedicated to the assumptions used in the definition of key transformation coefficients. For example, employing a sensitivity analysis, a series of factors important in the estimation of resource usages of bio-based polymers for plastics has been identified [57], foremost of which was biomass yield. As only part of the harvested biomass is diverted into the production of bio-based chemicals, as in the cases of polyethylene (PE), polyethylene terephthalate (PET) and polylactic acid (PLA), a yield correction factor to significantly reduce biased assessments of feedstock and land uses is estimated [57].

An additional concern surrounds the measurement of the environmental footprint through the value chains [57]. In terms of feedstock demand, different types of feedstock can be used to produce the same bio-based chemicals. For example, ethylene could be produced both from the fermentation and dehydration of sugar and starches or from the conversion of vegetable oils. Examining feedstock supply, multiple crops could be used to derive the same feedstock. For example, sugar cane and sugar beet could both be used to obtain sugars to produce a specific bio-based product.

To address both of these aforementioned issues the approach adopted here is to first correct primary crop yields by the amount of usable biomass that can be extracted for the production of bio-based chemicals and secondly, derive composite yield indicators calculated as weighted averages of biomass-adjusted crop yields to account for multiple potential pathways. To do so, feedstock is classified into five categories (sugars, starches, vegetable oils, wood and oranges) and composite yield indicators are computed for each. The weights used in this calculation were equal to the share of the specific world production of the specific biomass composing each category [45].

While there are important advantages from the aggregation of feedstock categories, there are also obvious disadvantages in taking a simplified approach. One of the main drawbacks is that some of the important heterogeneity amongst alternative pathways could be masked. This issue is particularly evident when multiple raw material of the same type could be used in the production process of the same chemical compound. One example is represented by the production of acetic acid. This compound could be both obtained through fermentation of sugars or through oxidation of acetaldehyde. Both intermediate feedstocks are part of the same feedstock category, although the land use impact of these two pathways can be different. This concern is particularly evident by looking at the diversity of the bioeconomy in EU Member States in terms of endowments and productivity [34,54].

2.6. Data quality

A consideration of paramount importance in this study is that of data quality. Indeed, given the variety of data sources, their different scope, publication dates, and possibly conflicting figures, an indicator of 'data quality' is considered a useful tool to prioritise and select among data sources, as well as to assess the reliability of results.

As the pool of data sources used for this study is rather large, and as they have different degrees of uncertainty due to their diverse nature, a data quality index (QI) is applied to each of them, ranging from one (highest data quality) to four (lowest data quality). This data quality indicator is a relative indicator that can be used to compare competing data sources and to rank them according to their reliability. Thus, in those cases where company data is directly acquired from the company's internal sources, the QI is set to one (highest quality). The Prodcom and Easy Comext databases, given the incompleteness and inconsistencies identified in the few official statistics available, are assigned a QI value equal to two. The same value is also assigned to estimates extracted from market data when accompanied with a clear reviewing process. In the absence of this quality control filter, market data sources were awarded a QI equal to three. Finally, authors' estimates are eventually given the lowest quality measure, i.e., a value of four. A summary of this categorical scaling is presented in Table 4.

The quality indices were then adjusted to consider the age and consistency of the data sources. Recent data was considered of higher quality, thus the QI of a data source was reduced by one level for every 5 years of age of the data. Similarly, the QI was adjusted according to the consistency of data sources: 1 (higher QI) if there is convergence of multiple data sources, +1 (lower QI) if there is divergence of multiple data sources or data transformation needed. A more detailed view of the final adjusted QIs assigned to each data source is presented in Fig. B1 of Annex B. The data sources selected for this study were those associated with a highest degree of reliability among the available alternatives.

The scoring system used to define the quality of a specific data source is ad hoc and therefore, debatable. Different scoring systems and weights could be applied to improve the assessment of data quality and to make it comparable across studies. A different scoring system could in fact lead to a different ranking of data sources quality. However, the advantages of a relative scoring system attached to the available data source should not be underestimated. Not only does this provide transparency to the system of data collection by prioritising between competing, and sometimes conflicting information, but it also highlights the fundamental data gaps in monitoring the bioeconomy. As discussed in section 3.1, there are clear differences in the reliability of the data available for different indicators and for different subsectors.

3. Results

3.1. Reliability of results by indicator and application category

The development of QI indices by application category and by indicators can be useful for evaluating the reliability of the results obtained and for understanding the types of data gaps that characterise the bio-based chemical sector at a more fundamental level. Ranks the data quality (from highest to lowest) of the different indicators, Fig. 3 reveals

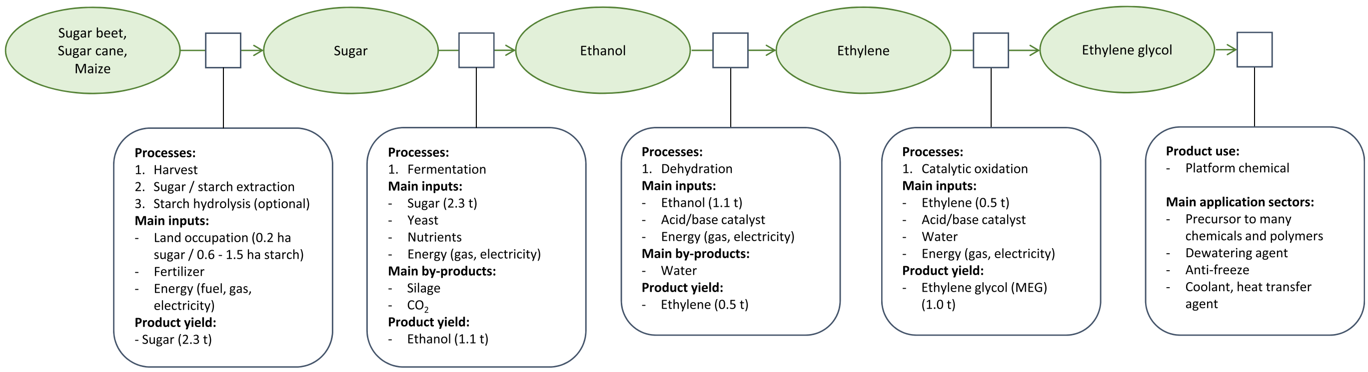

Fig. 2. Value chain for the platform chemical ethylene glycol.
Source: Spekreijse et al. [45].

Table 4
Data quality index (QI) for market data.

Variables	QI
Directly from companies	1
Scientific peer-reviewed literature	2
Prodcom and CN 2016 data	2
Market data specialists	2
Other reports and websites	3
Authors' estimates	4

that the quality of the data differs significantly across the different indicators. For example, production (bio-based production in particular) and price data showed higher levels of data quality across the 27 dedicated and 23 drop-in chemical products considered. In contrast, turnover and consumption data typically exhibited lower levels of data quality. In fact, of the 27 dedicated chemical products considered, over half (15) where considered to have price data in the top two QI categorisations. By contrast, for the indicators of net trade and turnover, this outcome was only apparent for 6 and 1 products, respectively. In the case of drop-in products, it is worth noting that the price for fossil-based equivalents appears to be one of the most reliable indicators with 17 of the 23 products associated with high data quality indicators.

Fig. 4 filters the QI results by grouping the selected bio-chemical products into application categories. It clearly highlights that platform chemicals and polymers for plastics are application categories that are based on sources of higher quality. For the other product categories, the proportion of data sources with greater uncertainty was much higher, particularly in the cases of cosmetics and personal care products. Surfactants is another application category with a higher proportion of unreliable data, despite the fact that all five surfactants selected for the analysis are dedicated products where a higher reliability of data would be expected.

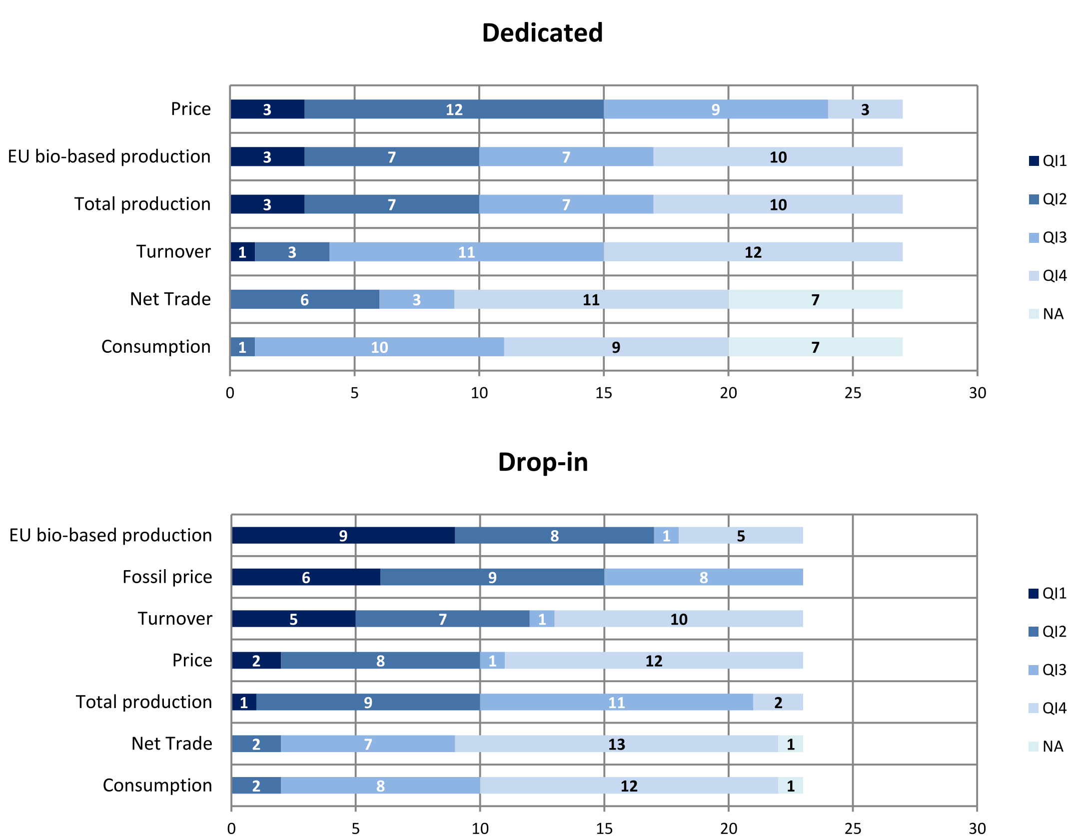

Fig. 3. QI by indicator. Source: authors based on Spekreijse *et al.* [45].

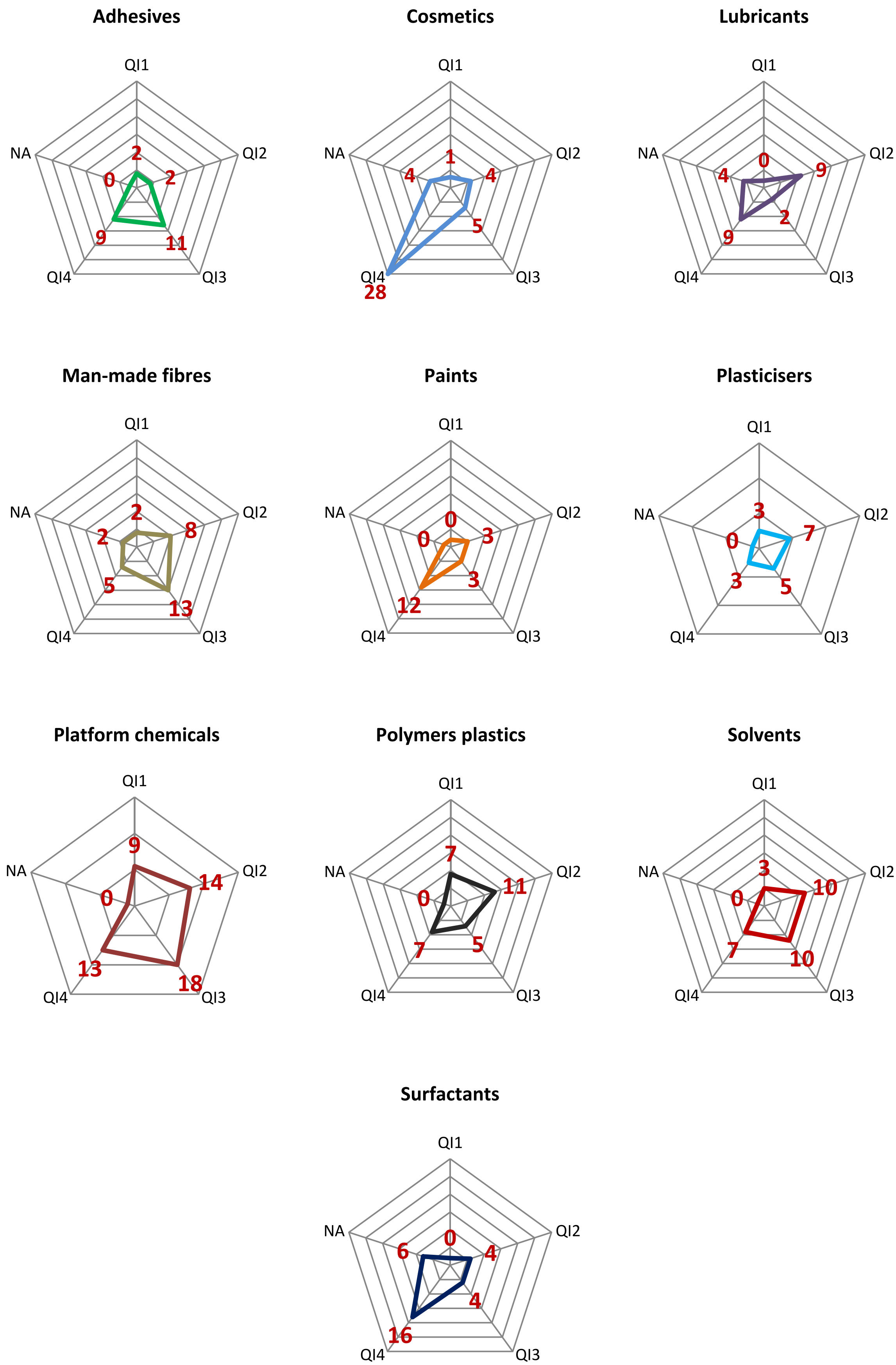

Fig. 4. QI by application category. Source: authors own elaboration.

3.2. Description of the market for bio-based chemicals

Table 5 presents a summary of the EU bio-based statistics of production, bio-based shares, prices, turnover, consumption, net-trade and import dependence at application category level.

The figures show that the market for bio-based chemicals is very diverse and in different stages of maturity. The factors that influence market growth may be very different from one chemical application group to another. Platform chemicals and polymers for plastics represent the largest categories in the chemical market, with an annual production of approximately 60,000 kt in the EU. However, the production shares corresponding to bio-based products for these two categories (0.3% and 0.4% respectively) are the smallest in the chemical market in the EU, indicating an opportunity for development.

Surfactants and cosmetics and personal care products are categories with high bio-based production shares (50% and 44%, respectively). The remarkable market development for surfactants is related to the fact that they are constituted in large part by oleo-chemicals that are typically considered bio-based. As it can also be seen by the QI of Fig. 4, it was more difficult to determine the bio-based share of cosmetics and personal care products, as a large number of products exist in this category and the data sources identified are associated with lower quality.

Price statistics are averages of product-level prices weighted by the corresponding bio-based production quantities. They were primarily employed in an indirect manner to estimate the turnover generated by industry. The results show the relatively large variations that characterise each sector: bio-based platform chemicals and solvents are associated with relatively low average prices in the range of 1–1.48 EUR/kg, whilst bio-based cosmetics and plasticisers are associated with generally higher prices in the range of 2–3.6 EUR/kg.

Indicators of turnover, consumption and net-trade are associated with higher uncertainties and care should be taken when interpreting the results of the figures. However, what emerges is that the EU's net trade position is very much a function of the specific chemical under consideration. The EU is a net exporter of bio-based polymers for plastics and lubricants, while it is a net importer of bio-based plasticisers and solvents. Moreover, the EU is a net importer of bio-based chemicals that are associated with a higher consumption levels, such as paints and surfactants. Given the fact that these latter two categories rely mostly on oleo-chemicals from vegetable oils, the EU's third country import dependence for vegetable oils might have a noticeable impact (i.e., leakage effect) on those developing economies from where this feedstock is typically sourced.

A comparison of our findings with other studies is complicated by the chosen definition of the boundaries of the bio-chemicals sector. For example, employing an output-based approach for assessing the importance of the EU bioeconomy, the value share of bio-based chemicals to overall chemical production has been estimated, whilst also considering the relative importance of major bio-based chemicals through the Prodcom codes [32]. As noted in section 2.1, however, the use of official coding systems with their associated data aggregation issues, renders the cross-mapping of chemicals and subsequent comparison of production values with [32] impossible.

With a focus on 'promising' biochemical technologies, another study [13] presents data for prices and production volumes for the US market. In terms of quantities, a comparison with the current study is obscured by the limited overlap of products across the studies. Moreover, in Ref. [13] it is noted that production volume data often requires assumption based inference from production "capacity" estimates. In terms of prices, better quality data enables some degree of comparison between EU and US markets. More specifically, for ethyl lactate, lactic acid, propanediol (1,3) and propylene glycol, average market prices are broadly comparable, differing by +5.3%, −5.1%,-1.7%, and +12.3%, respectively.

A further literature search shows that even global figures on total production of bio-based chemicals are scarce. Global production capacity statistics for 2018 and their forecast to 2023 on a selected number of bio-based chemicals have been estimated [58]. The chemicals comparable to those provided in the current study were limited to epoxy resins, polyhydroxyalkanoates (PHA), polylactic acid (PLA), polytrimethylene terephthalate (PTT), cellulose acetate (CA), polyurethanes (PUR). However, the comparisons between world production capacities of selected biochemical with EU production figures could lead to a misleading picture. A further study [59] also provides global figures, with data for production volumes, prices, and turnover[7] of selected bio-based chemicals. Their estimations are used in Table 6 to draw loose comparisons between the EU figures and the world.

According to Table 6, column 3, in only a handful of bio-based chemicals is the EU a key player on the world stage. EU world production shares are high for lactic acid (53.8%), succinic acid (46.0%) and furfuryl alcohol (13.3%), with a non-trivial share observed for 1,3-Propanediol (5.5%) and PLA (3.9%). In general, prices seem to be higher in the EU. On a product basis for this relative measure, EU prices of acetic anhydride (+60%), furfuryl alcohol (+42%), ethylene glycol (+29%) and propylene glycol (+28%) are particularly high, where in two cases (furfuryl alcohol and succinic acid) the EU retains a substantial share of world production despite the higher price. Only for ethyl acetate (−17%), lactic acid (−5%), and ethyl lactate (−4%), are producer prices in the EU lower than world prices. Comparing both sets of observations, there is an apparent non-significant negative correlation[8] between EU price ratios and the shares of world production.

3.3. From land to product

Quantifying feedstock and land use for the production of bio-based chemicals represents an important step in addressing the sustainability challenges raised by the Bioeconomy Strategy. The value chains discussed in section 2.5 were developed to infer resource usage for each of the described bio-based chemicals. From the initial bio-based feedstock, these value chains describe the steps that are followed to produce each bio-chemical product.

Fig. 5 presents the results of the estimation of land requirements for the 50 representative bio-based products considered. Land requirement varies from zero to 3 ha per tonne of bio-based product. Clearly, bio-based products made out of waste material have very low land requirements. Examples of these are N-acetyl glucosamine, made out of fisheries waste (0 ha/t bio-based product), limonene (d-), made from orange by-products (0.1 ha/t) and furfuryl alcohol, made from sugar cane waste. Wood-based products also tend to have a moderate land impact (0.3–0.6 ha/t). At the other end of the spectrum, each tonne of glycolipids production requires 3 ha of oil crops.

For every application category, bio-based products are ranked by decreasing land use. Adhesives, lubricants and solvents are the categories with the lowest land requirements (less than 0.7 ha/t of bio-based products) while surfactants, man-made fibres and plasticisers show the highest heterogeneity in terms of land use (0.2–3 ha/t in the case of surfactants).

Sustainability comparisons for this indicator based on other literature was only possible for three bio-based chemicals (PE, PTA and PLA. In fact, a similar value-chain approach has been adopted [55] but with a sole focus on bio-based polymers for plastics. Moreover, their focus was on a limited number of bio-based chemicals and their aim was to estimate resources in terms of land and water requirements. Other literature [56,57] also presents estimates on land-uses for a few bio-based polymers for plastics and have highlighted the strong sensitivity of the approach to specific technical coefficients assumed in the assessment.

[7] Turnover statistics for the world market are obtained by multiplying average prices and market volumes provided in Ref. [59].

[8] A spearman correlation coefficient of −0.12 associated with a 0.66 p-value has been calculated.

Table 5
Statistics on EU production volume, value, consumption, net trade, and import dependence by application category.

Application category	EU bio-based production (kt/year)	EU bio-based share (%)	Bio-based price (EUR/kg)	Bio-based Turnover (EUR mln/year)	Consumption (kt/year)	Bio-based net trade (kt/year)	Bio-based import dependence (%)
Platform chemicals	181	0.3	1.48	268	197	16	9
Solvents	75	1.5	1.01	76	107	32	43
Polymers for plastics	268	0.4	2.98	799	247	−21	−8
Paints, coatings, inks and dyes	1002	9.7	1.62	1623	1293	291	29
Surfactants	1500	50.0	1.65	2475	1800	300	20
Cosmetics and personal care products	558	44.2	2.07	1155	558	0	0
Adhesives	237	8.8	1.65	391	320	83	35
Lubricants	237	3.5	2.33	552	220	−17	−8
Plasticisers	67	5.2	3.60	241	117	50	74
Man-made fibres	600	13.3	2.65	1590	630	30	5

Source: authors based on Spekreijse et al. [45].

Table 6
The EU in a global context: production, prices and turnover of specific bio-based chemicals.

Application category	Product	EU share of world production	EU Price/World Price	EU share of world turnover
Adhesives	Furfuryl alcohol	13.3%	1.42	19.0%
Plasticisers	Succinic acid	46.0%	1.24	57.1%
Platform chemicals	Lactic acid	53.8%	0.95	51.5%
Platform chemicals	1,3-Propanediol	5.5%	1.27	7.2%
Platform chemicals	Propylene glycol	1.0%	1.28	1.3%
Platform chemicals	Acetic Anhydride	0.4%	1.60	0.6%
Platform chemicals	Acetic acid	0.3%	1.06	0.3%
Platform chemicals	Ethylene	0.0%	1.27	0.0%
Platform chemicals	Ethylene glycol	0.0%	1.29	0.0%
Polymers for plastics	Polylactic acid - PLA	3.9%	0.94	3.7%
Polymers for plastics	Polyethylene - PE	0.0%	1.05	0.0%
Solvents	Ethyl Acetate	1.1%	0.83	0.9%
Solvents	Ethyl Lactate	0.0%	0.96	0.0%
Solvents	Isobutanol	0.0%	1.19	0.0%

Fig. 6 shows the comparisons with [55,57]. The coloured bars represent the hectare per tonne of product from the current results, while the vertical lines represent the range of estimates provided in the aforementioned cited studies. Fig. 6 reveals that the current estimates fall within the ranges provided by the literature, although in the case of PET, this is very much a lower range estimate.

This value-chain approach for the estimation of resource usage can also be applied at the product level using the weighted average of land use per tonne of product at product category level. This weighted average per category is constructed by weighting land uses per tonne associated to each product of a specific category by its corresponding EU production. Results of these calculations at application category level can be found in Table 7.

According to the estimation at application category level, paints, coatings, inks and dyes are the application category with the lowest impact in terms of land-use (0.35 ha/t). A similar land use is estimated for polymers for plastics (0.36 ha/t) and for man-made fibres (0.38 ha/t). Lubricants, platform chemicals and adhesives have estimated land use impacts ranging between 0.48 and 0.49 ha/t. Solvents and surfactants are associated to 0.56 and 0.59 ha/t respectively. The two categories with the largest impacts are plasticisers and cosmetics with 0.64 and 0.77 ha/t, respectively.

Given these estimates on the land use and the data on total and bio-based production in the EU at the level of application categories, it could be possible to estimate the actual land use dedicated to the production of categories of bio-based chemicals.

At present, land requirements for the production of bio-based polymers for plastics in the EU is negligible [60]. The current results confirm that this is the case also for other bio-based chemical application categories. The production of bio-based surfactants - the application category with the largest land use - currently requires approximately the 0.49% (Table 8) of the total utilized agricultural area (UAA).[9] Cosmetics and personal care products are the application category with the second largest estimated land use followed by paints, coatings, inks and dyes and by man-made fibres. These four application categories have an estimated land use impact of 0.24%, 0.20% and 0.13% respectively. All remaining application categories have an estimated land use impact lower than 0.10% of total UAA.

4. Discussion

Given the challenges of data collection, a key contribution of this work is the assessment of the quality of the available data. Our results suggest that the data coverage of the chemical markets differs significantly by application category and by type of indicators. Accordingly, the variation in data reliability impacts on the value of some of the indicators presented and the conclusions that can be drawn from them.

While production data (both total and bio-based) appears to be relatively more reliable, trade and consumption data show deficiencies. Improving the quality of data in those areas would enable a better analysis throughout the value chains of bio-based chemical products, especially considering that the EU is import dependent for feedstock in most bio-based chemical application categories. Similarly, some categories of bio-based chemicals are better documented than others. Platform chemicals and polymers for plastics are the categories that show the lowest data uncertainty levels, while surfactants and cosmetics and personal care products are categories that could benefit from more reliable data.

The analysis of data on chemical application level could inform policy makers of those categories with the highest impact potential. For example, platform chemicals and polymers from plastics are the highest production sectors in the EU, but both present a relatively low share of bio-based products. Any action in these sectors could potentially have a big impact in the overall bio-based chemical market.

[9] UAA refers to the total Utilized Agricultural Area in the EU 28 (2013–2020) for 2018 (Eurostat).

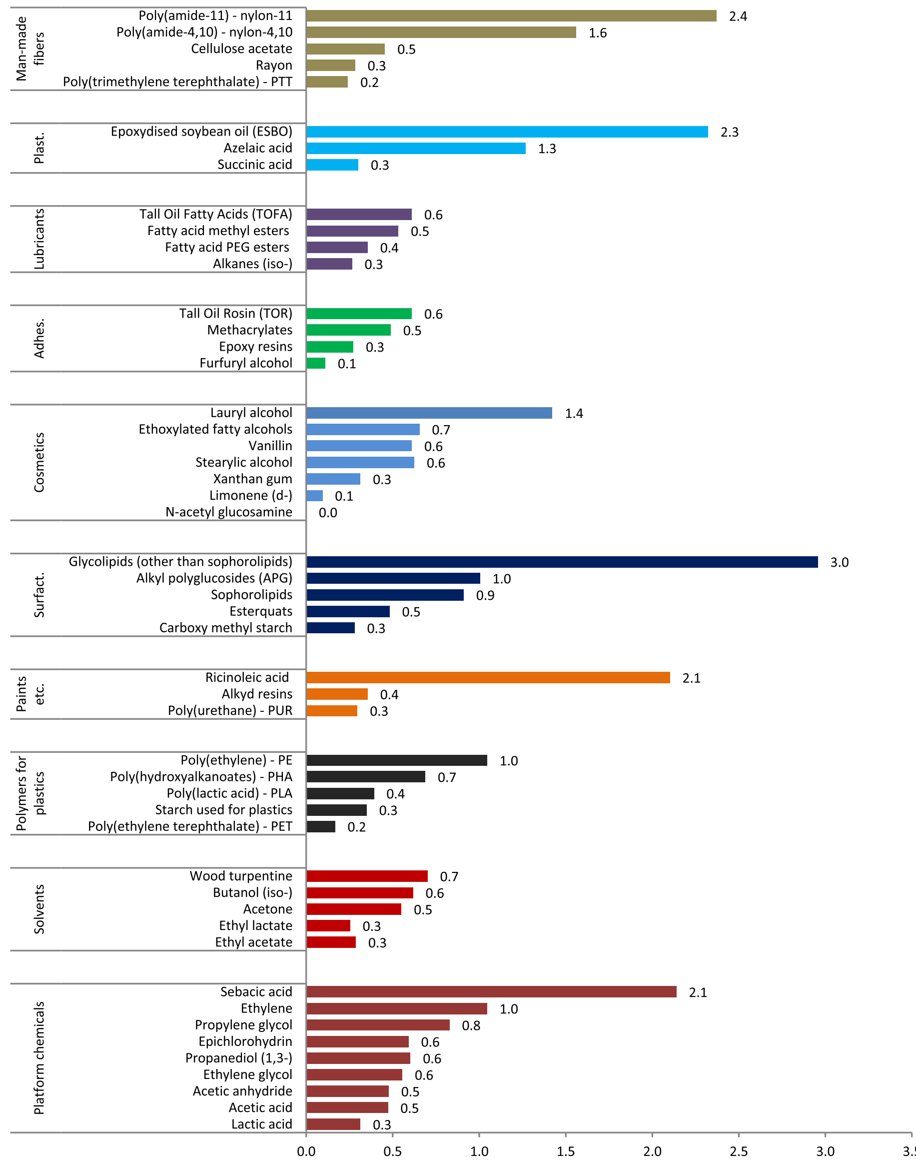

Fig. 5. Land use in hectares for every tonne (ha/t) of bio-based chemical.
Source: authors own elaboration

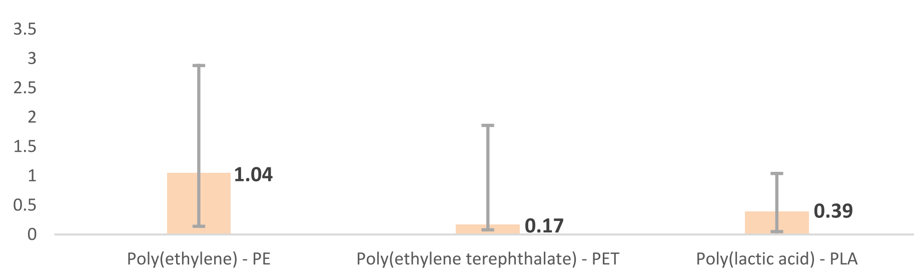

Fig. 6. Land use in hectares for every tonne (ha/t) of bio-based chemical. comparison with bounds provided by Refs. [55,57].

Table 7
Land use in hectares for every tonne (ha/t) of bio-based chemical.

Application category	ha/t
Paints, coatings, inks and dyes	0.35
Polymers for plastics	0.36
Man-made fibres	0.38
Lubricants	0.48
Platform chemicals	0.49
Adhesives	0.49
Solvents	0.56
Surfactants	0.59
Plasticisers	0.64
Cosmetics and personal care products	0.77

Source: authors own elaboration

Table 8
Land use in hectares (ha) for every application category.

Application category	Land use (1000 ha)	Share of EU total UAA
Surfactants	885	0.49%
Cosmetics and personal care products	429.66	0.24%
Paints, coatings, inks and dyes	350.7	0.20%
Man-made fibres	228	0.13%
Adhesives	116.13	0.06%
Lubricants	113.76	0.06%
Polymers for plastics	96.48	0.05%
Platform chemicals	88.69	0.05%
Plasticisers	42.88	0.02%
Solvents	42	0.02%

Source: authors own elaboration

With the currently available data sources, a picture of the EU bio-based chemical sector could be provided. However, several limitations make comparisons with other studies difficult. For an effective future monitoring of the bioeconomy and thereafter evidence-based decision making, the creation of a tailored monitoring system for bio-based products is therefore highly recommended, where these products are assigned their own specific CN 2016 and Prodcom codes. For the EU, such a paucity of data can only be addressed and overcome by a concerted action on the part of the official statistical offices of each of the Member States and Eurostat. This will solve many of the data challenges presented and, in particular, will help solve data aggregation issues. Nevertheless, the issue of the definition of chemical products will remain an open question that will have to be tackled to create a coherent and consistent policy-support system.

In the current paper, the description of value chains has helped to better understand the link between feedstock usage and production data. With additional information, it could also be extended to estimate the overall cost structure of specific biomass conversion processes. In addition, it may provide insight on the feasibility of future sustainability targets such as reductions in energy usage for the production of chemicals as well as the feedstock and land needs to cover additional expected demand.

5. Conclusions

Placed as a high value application of biomass within the cascading model, bio-based chemicals offer an opportunity to promote a competitive and environmentally friendly strategy for sustainable development within the EU's circular economy. Unfortunately, the absence of an official coherent data framework for measuring, monitoring and modelling this diverse collective of activities, presents a major obstacle toward the recommendation of policy strategies and the implementation of legislation, both at pan-European and national level. Indeed, official statistics do not provide adequate coverage of biomass-based conversion processes or the products they produce, nor do they keep pace with data needs, which in part relates to data confidentiality issues, as well as the dynamic nature of the biochemical industry owing to the emergence of new value chains.

Nevertheless, this study is an attempt to bridge the data gaps for the bio-based chemical market and provides a methodology that can, in principle, be applied to other sectors of the bioeconomy that suffer from the same data deficiency. Using various data sources, a series of key *ex-post* indicators has been constructed. The presented statistics show that the market for bio-based chemicals is very diverse and that this diversity may be the result of different technological and economic drivers. Therefore, an important conclusion of this exercise is that a one-size-fits-all approach is not expedient. Each of the application sectors requires a different set of measures to stimulate its market development as each sector shows its own specificities.

Acknowledging that the EU's environmental footprint needs to be reduced while striving toward an inclusive, carbon-neutral circular economy, several strategies under the umbrella of the Green Deal outline key elements on how legal, policy and financing measures could drive the transition to sustainable consumption and production. For example, the EU has increased its greenhouse gas emissions reductions ambition [61], targeting a reduction of at least 55% by 2030 compared with 1990 levels. Moreover, important potential feedstocks for the production of bio-based chemicals are waste and residue streams [62], which in addition avoid any competition with biomass usage for food. As a final point, concrete steps are now being implemented to prepare a policy framework for bio-based plastics and biodegradable or compostable plastics [63], where a central element within the transformation will be the role of sustainable biorefineries [4,64].

Authorship statement

Authors have developed the paper jointly. Nevertheless, contributions can be identified as follows: EB: data collection, conceptualization, writing, supervision. GP: conceptualization, literature review, writing, supervision. JS: data collection, data analysis, literature review. PG: conceptualization, data visualization, writing. TL: data collection, literature review. CP: conceptualization, literature review. TR: conceptualization, literature review. MV: literature review. RB: conceptualization, literature review, writing.

Declaration of competing 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.

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Annex A.

Table A1
List of application categories, representative products and codes

Application category	Chemical name	Drop-in/Dedicated	Prodcom	CN 2016
Platform chemicals	Ethylene	Drop-in	20 14 11 30	29 01 21 00
	Ethylene glycol	Drop-in	20 14 23 10	29 05 31 00
	Propylene glycol (aka 1,2-propanediol)	Drop-in	20 14 23 20	29 05 32 00
	Propanediol (1,3-)	Drop-in	20 14 23 37	39 05 39 28
	Acetic acid	Drop-in	20 14 32 71	29 15 21 00
	Acetic anhydride	Drop-in	20 14 32 77	29 15 24 00
	Sebacic acid (aka decanedioic acid)	Dedicated	20 14 33 81	29 1713 10
	Lactic acid	Dedicated	20 14 34 75	29 18 11 00
	Epichlorohydrin	Drop-in	20 14 63 79	29 10 30 00
Solvents	Butanol (iso-)	Drop-in	20 14 22 40	2905 14 90
	Ethyl acetate	Drop-in	20 14 32 15	29 15 31 00
	Ethyl lactate	Dedicated	20 14 34 75	29 18 11 00
	Acetone	Drop-in	20 14 62 11	29 14 11 00
	Turpentine	Dedicated	20 14 71 40	38 05 10 30
Polymers for plastics	Poly(ethylene) - PE	Drop-in	20 16 10 35	39 01 10 10
	Poly(ethylene terephthalate) - PET	Drop-in	20 16 40 62	39 07 60 20
	Starch used for polymers	Dedicated	10 62 11 70	35 051 0
	Poly(hydroxyalkanoates) - PHA	Dedicated	20 16 40 90	39 07 99 90
	Poly(lactic acid) - PLA	Dedicated	20 16 40 90	39 07 70 00
Paints, coatings, inks and dyes	Ricinoleic acid (aka 12-Hydroxyoctadec-9-enoic acid)	Dedicated	20 14 34 75	29 18 19 98
	Poly(urethane) - PUR	Drop-in	20 16 56 70	39 09 50 90
	Alkyd resins	Dedicated	20 16 40 50	39 07 50 00
Surfactants	Glycolipids (other than sophorolipids)	Dedicated	20 16 59 60	39 13 90 00
	Esterquats	Dedicated	20 41 20 30	34 02 12 00
	Sophorolipids	Dedicated	20 41 20 90	34 02 19 00
	Alkyl polyglucosides (APG)	Dedicated	20 41 20 50	34 02 13 00
	carboxy methyl starch	Dedicated	20 16 59 60	39 13 90 00
Cosmetics and personal care products	Limonene	Dedicated	20 14 12 15	29 02 19 00
	Lauryl alcohol	Drop-in	20 14 22 65	2905 17 00
	Stearylic alcohol (1-octadecanol)	Drop-in	20 14 22 65	29 05 17 00
	Vanillin	Drop-in	20 14 61 35	29 1241 00
	Xanthan	Dedicated	20 16 59 60	39 13 90 00
	Ethoxylated fatty alcohols	Drop-in	20 41 20 50	34 02 13 00
	N-acetyl glucosamine	Dedicated	21 10 20 60	29 24 19 00
Adhesives	Methacrylates	Drop-in	20 16 53 90	3906 90 90
	Furfuryl alcohol	Dedicated	20 14 52 15	29 32 13 00
	Epoxy resins	Drop-in	20 16 40 30	39 07 30 00
	Tall Oil Rosin (TOR)	Dedicated	20 14 71 50	38 06 10 00
Lubricants	Alkanes (iso-)	Drop-in	20 14 11 20	29 0110 00
	Tall Oil Pitch (TOP)	Dedicated	20 14 71 70	38 06 10 00
	Fatty acid methyl esters (e.g. methyl palmitate, stearate, laurate)	Dedicated	20 59 20 00	15 18 00 91
	Fatty acid PEG esters (e.g. polyoxyethylene oleate, palmitate)	Dedicated	20 59 20 00	15 18 00 91
Plasticisers	Azelaic acid (aka nonanedioic acid)	Dedicated	20 14 33 81	29 17 13 90
	Succinic acid	Drop-in	20 14 33 81	29 17 19 20
	Epoxydised soybean oil (ESBO)	Dedicated	20 59 20 00	15 18 00 91
Man-made fibres	Poly(trimethylene terephthalate) - PTT	Drop-in	20 16 40 80	39 07 9190
	Rayon	Dedicated	20 60 21 20	55 02 00 10
	Poly(amide-11) - nylon-11	Dedicated	20 16 54 50	39 08 10 00
	Poly(amide-4,10) - nylon-4,10	Dedicated	20 16 54 90	39 08 90 00
	Cellulose acetate	Dedicated	20 60 21 40	55 02 00 40

Source: Spekreijse et al. (2019) [45].

Annex B.

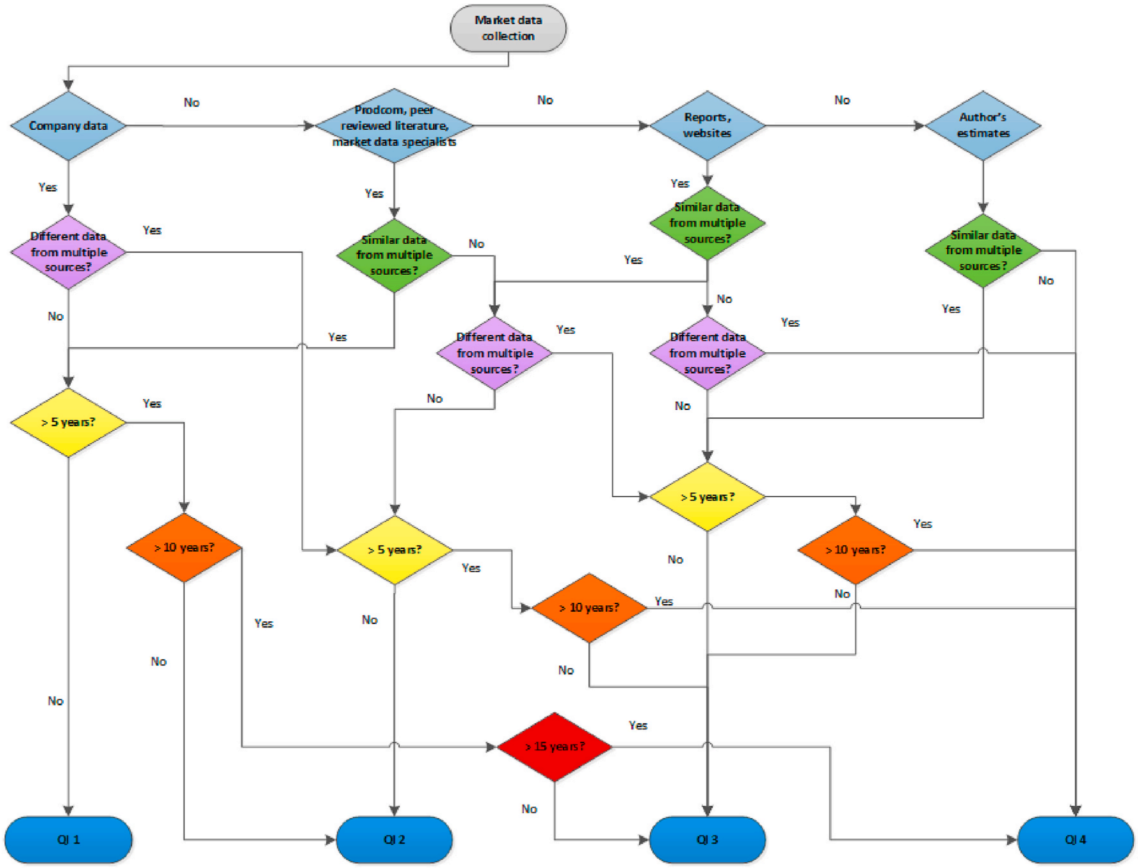

Fig. B1. Decision tree to estimate quality of data. Source: authors based on Spekreijse et al. [45].

Disclaimer

The views expressed are those solely of the authors and should not in any circumstances be regarded as stating an official position of the European Commission.

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