# Bio-based opportunities for the chemical industry

## "Where bio-based chemicals meet existing value chains in Europe"


Authors:

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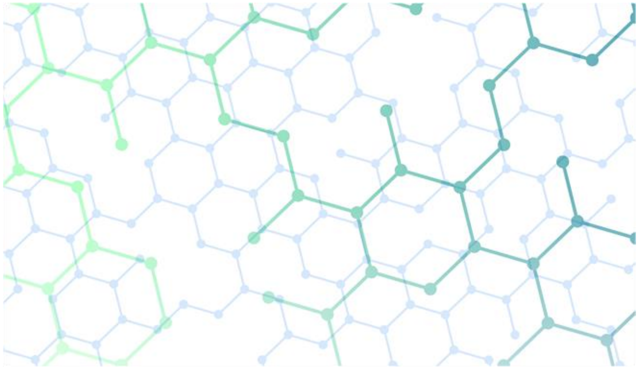
# Summary


- This report was prepared within the context of RoadToBio, an EU-funded project that will deliver a roadmap for the chemical industry. The roadmap will outline a path for achieving a 30 % share of bio-based products in the organic chemical industry by 2030. Here the results are described of a desk study of the following:
    1. The bio-based chemicals that are commercially available or close to commercialization
    2. The existing chemical markets and petrochemical value chains
    3. The interface between existing petrochemical value chains and bio-based chemicals

- In total more than 500 petrochemical value chains were analysed, which showed more than 1,000 entry points for bio-based chemicals. For 85 % of the existing petrochemicals at least one bio-based route was found that is available at either demonstration or commercial scale.

- This study provides the knowledge-base for the subsequent activities in the project, notably an assessment of the barriers as well as the most promising opportunities, and nine specific business case studies, which will together inform the roadmap for the chemical industry.

# Contents

# 1. Introduction

- **About RoadToBio**

  This report was prepared within the context of RoadToBio, which is an EU-funded project in HORIZON2020 that aims to pave the way for the European chemical industry towards a larger bio-based portfolio and competitive success, based on the benefits offered by the bioeconomy. The project will deliver a roadmap and action plan illustrating the 'sweet spots' for Europe's chemical industry towards the Bioeconomy over the coming decade, up to 2030.[1]

  The roadmap developed in RoadToBio will contain two main components: first, an analysis of the most promising opportunities for the chemical industry to increase its bio-based portfolio as well as the technological and commercial barriers and the hurdles in regulations and acceptance by society, governing bodies and the industry itself, and second, a strategy, action plan and engagement guide to overcome the existing and anticipated barriers and hurdles as mentioned above.

- **Goal and scope of this report**

  This report describes the results of a desk study with the purpose of creating a sound fact-base for the analysis of the most promising opportunities. The fact-base consists of:

  - An overview of the current status of the development of bio-based chemicals at demonstration or (semi-)commercial scale;
  - A map of the markets for chemical products, describing the existing value chains in the chemical industry;
  - An analysis of the interface between the bio-based chemicals and the existing value chains, to identify entry points for bio-based chemicals in the chemical industry.


**Notes:**
1. More information about the project, its goals and plans, and how you can contribute to this roadmap for the chemical industry can be found on www.RoadToBio.eu.

# 2 Overview of available bio-based chemicals

- **Introduction**

  An overview was prepared of the bio-based chemicals that are available on the market or close to commercialisation (TRL ≥ 6).[1] In recent years a number of reports have been published that describe the current status of bio-based chemicals. This overview is based on that body of literature as well as on the market intelligence of the project partners.[2]

  The goal of creating this overview was to gain insight where in the existing value chains of the chemical industry bio-based chemicals can play a role, as well as in the potential market size for these products. Therefore all bio-based products were classified according to the Eurostat - Prodcom classification system regarding their (potential) application.[3]

- **Results**

  A database was created with more than 400 bio-based chemicals that are currently on the market or under development. This database contains for all the chemicals (a.o.):

  - An assigned Prodcom-code with a potential market volume and market value estimation;
  - TRL ≥ 6: yes or no;
  - Classification: 'drop-in', 'smart drop-in', or 'dedicated' chemical, following RoadToBio definitions;[4]
  - Biomass feedstock options.

  From this database 120 bio-based chemicals were selected for an initial long list, on the basis that they should currently be at TRL ≥ 6 and show potential for the chemical industry in terms of market value.

**Notes:**

1. "Technology Readiness Level"; following the European Commission definitions, p.29, TRL 6 means "technology demonstrated in industrially relevant environment".
2. Important references are:
   - E4tech *et al.*, "From the sugar platform (...)", 2015
   - nova Institute, "Bio-based building blocks (...)", 2016
   - S.N. Jogdand, "Current status of bio-based chemicals", 2015
   - L. Nattrass *et al.*, "The EU bio-based industry (...)", 2016
   - BIO, "Advancing the Biobased Economy (...)", 2016
   - M.J. Biddy *et al.*, "Chemicals from biomass (...)", NREL 2016
   - Biofuels Digest, 2017
   - World Bio Markets, Conference proceedings, 2017

   *A complete list of references is available within appendix A.*
3. Eurostat 2017
4. See the recent RoadToBio paper by Carus *et al.*, 2017.

# 2.1 Long-list of bio-based chemicals with Prodcom code

| Bio-based chemical | Prodcom code | Bio-based chemical | Prodcom code | Bio-based chemical | Prodcom code |
|---|---|---|---|---|---|
| Acetaldehyde | 20146113 | Ethylene chloride (aka vinyl chloride) | 20141371 | Phenol formaldehyde resin | 20165650 |
| Acetic acid | 20143271 | Ethylene glycol | 20142310 | Poly(butylene adipate-co-terephthalate) - PBAT | 20164080 |
| Acetic anhydride | 20143277 | Ethylene oxide | 20146373 | Poly(butylene succinate) - PBS (aka 'Bionolle') | 20164090 |
| Acetone | 20146211 | Farnesene | 20141190 | Poly(butylene terephthalate) - PBT | 20164080 |
| Acrylic acid | 20143310 | Fatty alcohols | 20142100 | Poly(ethylene furanoate) - PEF | 20164080 |
| Acrylonitrile[1] | 20144350 | Fatty amines | 20144119 | Poly(ethylene glycol) - PEG | 20164015 |
| Adipic acid | 20143385 | Fumaric acid | 20143381 | Poly(ethylene terephthalate) - PET | 20164062 |
| Alkanes (iso-) | 20141120 | Furan | 20145225 | Poly(ethylene) - PE | 20161035 |
| Alkyl polyglucosides (APG) | 20412090 | Furandicarboxylic acid (2,5-) (FDCA) | 20145225 | Poly(hydroxyalkanoate) - PHA | 20164090 |
| Alkyl polypentosides (C5-surfactants) | 20412090 | Furfural | 20145215 | Poly(hydroxybutyrate) - PHB | 20164090 |
| Azelaic acid (aka nonanedioic acid) | 20143381 | Furfuryl alcohol | 20145215 | Poly(isosorbide) | 20164090 |
| Bio-'Naphtha' | 20592000 | Glucaric acid / Sodium glucarate | 20143381 | Poly(lactic acid) - PLA | 20164090 |
| Butadiene | 20141160 | Glycerol | 20411000 | Poly(methyl methacrylate) - PMMA | 20165350 |
| Butanediol (1,2-) | 20142337 | Glycerol carbonate | 20411000 | Poly(propiolactone) - PPL | 20164090 |
| Butanediol (1,4-) | 20142338 | Glycolipids | 20165960 | Poly(propylene) - PP | 20165130 |
| Butanediol (2,3-) | 20142337 | Guayule | 20165960 | Poly(tetrahydrofuran) - PTHF (aka PTMEG) | 20164020 |
| Butanol (iso-) | 20142240 | Heptanoic acid (aka enanthic acid) | 20143280 | Poly(trimethylene terephthalate) - PTT | 20164080 |
| Butanol (n-) | 20142230 | Heptanol | 20142265 | Poly(urethane) - PUR | 20165670 |
| Butene (iso-) | 20141150 | Hyaluronic acid | 20165960 | Poly(vinyl chloride) - PVC | 20163010 |
| Butyric acid | 20143220 | Hydroxymethylfurfural (5-) (HMF) | 20145225 | Propane | 20141120 |
| Capric acid (aka decanoic acid) | 20143280 | Hydroxypropionic acid (3-) | 20143475 | Propanediol (1,3-) | 20142337 |
| Caproic acid (aka hexanoic acid) | 20143280 | Isoprene | 20141160 | Propylene | 20141140 |
| Caprylic acid (aka octanoic acid) | 20143280 | Isosorbide | 20142337 | Propylene glycol (aka 1,2-propanediol) | 20142320 |
| Carboxymethyl cellulose | 20165940 | Itaconic acid | 20143381 | Propylene oxide | 20146375 |
| Cellulose | 20165940 | Lactic acid | 20143475 | Rayon | 20602120 |
| Cetylic alcohol | 20142265 | Lactide | 20143475 | Ricinoleic acid (aka 12-Hydroxyoctadec-9-enoic acid) | 20143475 |
| Chitin/Chitosan | 20165960 | Lauric acid (aka dodecanoic acid) | 20143280 | Sebacic acid (aka decanedioic acid) | 20143381 |
| Citric acid | 20143473 | Lauryl alcohol | 20142265 | Sophorolipids | 20412050 |
| Dimethyl ether (DME) | 20146310 | Levulinic acid | 20143475 | Sorbitan | 20145225 |
| Dimethyl isosorbide | 20145225 | Limonene | 20141215 | Sorbitol | 20595770 |
| Docosahexaenoic acid | 20143280 | Malic acid | 20143381 | Squalene | 20141190 |
| Dodecanedioic acid | 20143381 | Methane | 20141120 | Starch | 10621111 |
| Epichlorohydrin | 20146379 | Methanol | 20142210 | Stearic acid (aka octadecanoic acid) | 20143235 |
| Epoxy resins | 20164030 | Methyl methacrylate (MMA) | 20143340 | Succinic acid | 20143381 |
| Esterquats | 20412030 | Methyl tert-butyl ether | 20146310 | Terpenes | 20141190 |
| Ethanol | 20147400 | Octadecanedioic acid (1,18-) | 20143381 | Tetrahydrofuran (methyl-) | 20145225 |
| Ethyl acetate | 20143215 | Octanol (2-) | 20142263 | Tetrahydrofuran (THF) | 20145215 |
| Ethyl lactate | 20143475 | Oleic acid | 20143350 | Turpentine | 20147140 |
| Ethyl tert-butyl ether (ETBE) | 20146310 | Palmitic acid (aka hexadecanoic acid) | 20143235 | Undecanoic acid (aka undecylic acid) | 20143280 |
| Ethylene | 20141130 | Pelargonic acid (aka nonanoic acid) | 20143280 | Xylene (para-) | 20141245 |

**Notes:**

1. A few bio-based chemicals on this long-list have not reached TRL 6 yet. If there is a clear development pathway available that provides such chemicals with the opportunity to move through the development funnel very rapidly (to TRL 9 before 2025), because of e.g. a bio-based drop-in precursor that is (semi-) commercially available, they were still included in the long-list. An example of this would be acrylonitrile made from bio-based propylene.
2. The long-list including main feedstock options and potential market values and volumes is available in Appendix A, including the list of bio-based chemicals in the database that are not on the long-list.

# 3. Mapping the chemical markets

- **Introduction**

  The European chemical industry is extremely complex, therefore it is impossible to create a single map that covers all value chains in the entire industry. Given that the goal of this task was to investigate the interface between existing value chains and bio-based products, nine product groups were selected that cover a range of different NACE classes[1] and Prodcom groups and with that a significant part of the chemical industry. The selected product groups were:

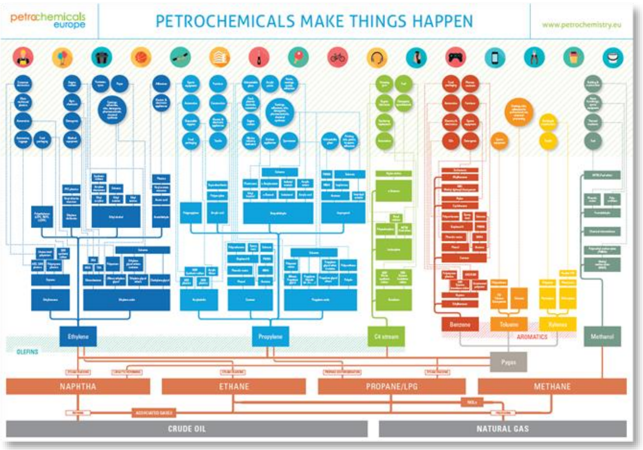
  - Adhesives
  - Agrochemicals
  - Cosmetics
  - Lubricants
  - Man-made fibres
  - Paints / Coatings / Dyes
  - Plastics / Polymers
  - Solvents
  - Surfactants

- **Value chain descriptions**

  For each of these product groups a range of different products were identified, and for each product the petrochemical value chain was mapped back to basic building blocks such as ethylene, propylene, benzene, etc. This was inspired by the 'petrochemicals flow chart' of Petrochemicals Europe.[2]

  A schematic overview of this approach is shown on the next page.

  All intermediate chemicals across the petrochemical value chains associated with the nine product groups were mapped and assigned a Prodcom code, in order to be able to match all involved petrochemicals to the bio-based chemicals on the long-list. In this way the possible entry points for bio-based chemicals could clearly be defined.




**Notes:**

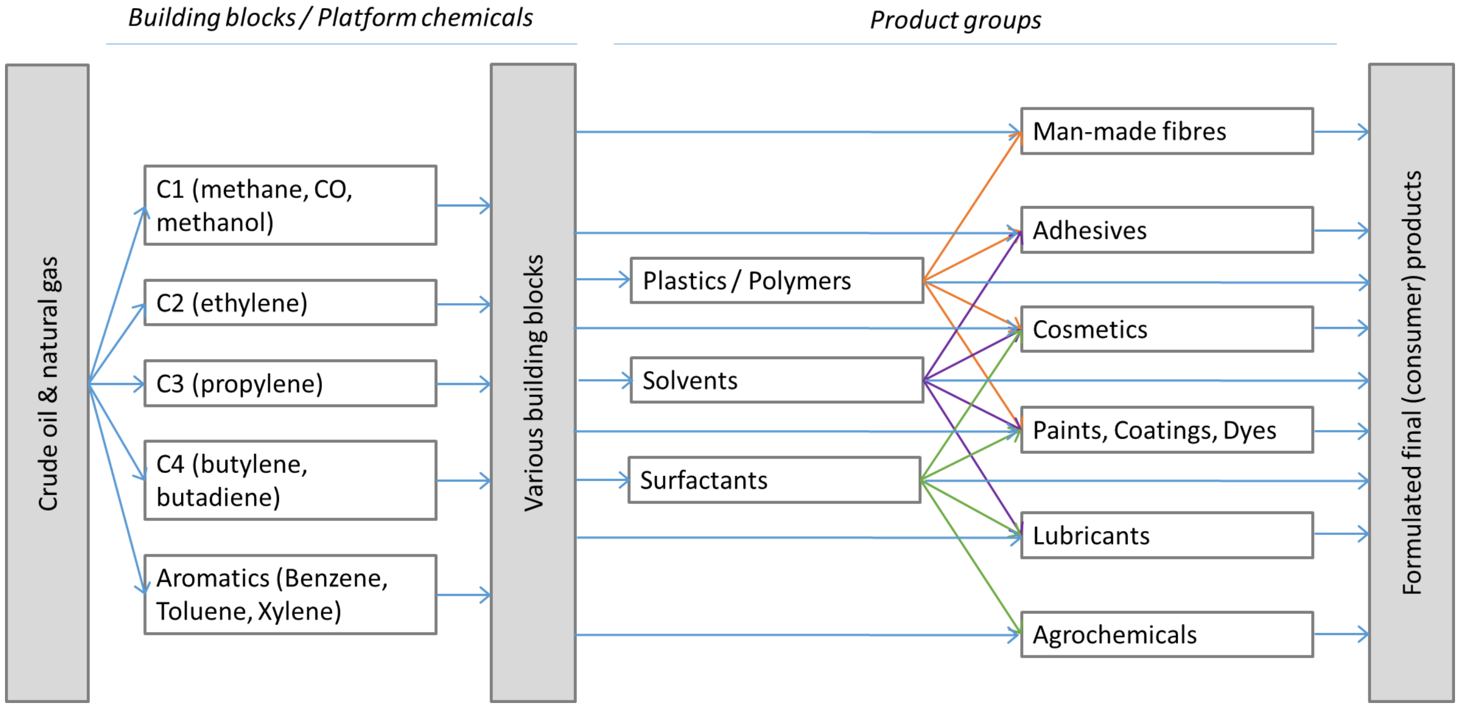
1. NACE ("Nomenclature statistique des Activités économiques dans la Communauté Européenne"), is the industry standard classification system used in the European Union. The first four digits of the code, which are the first four levels of the classification system, are the same in all European countries. They classify industrial products according to their type. The NACE classes within division 20 (Manufacture of chemicals and chemical products, classes range from 20.11 to 20.60) describe the different sectors of the chemical industry.
2. Petrochemicals Europe, 2015

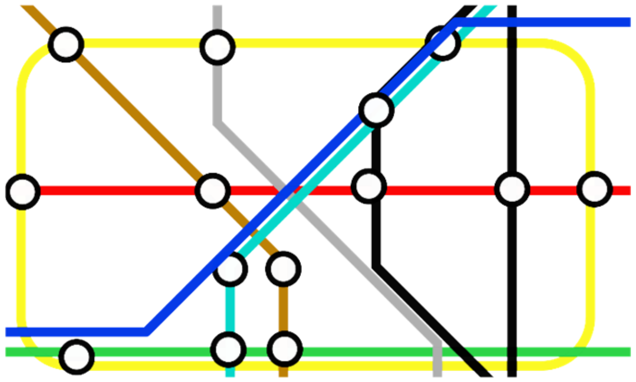
# 3.1 Mapping the product groups

- **Value chain descriptions**

  The scheme below shows a schematic view of the different value chains for the nine product groups.[1]

  Which products were mapped for each product group is discussed further on per product group. The intermediates for producing these products were mapped and are available in Appendix B.



**Notes:**

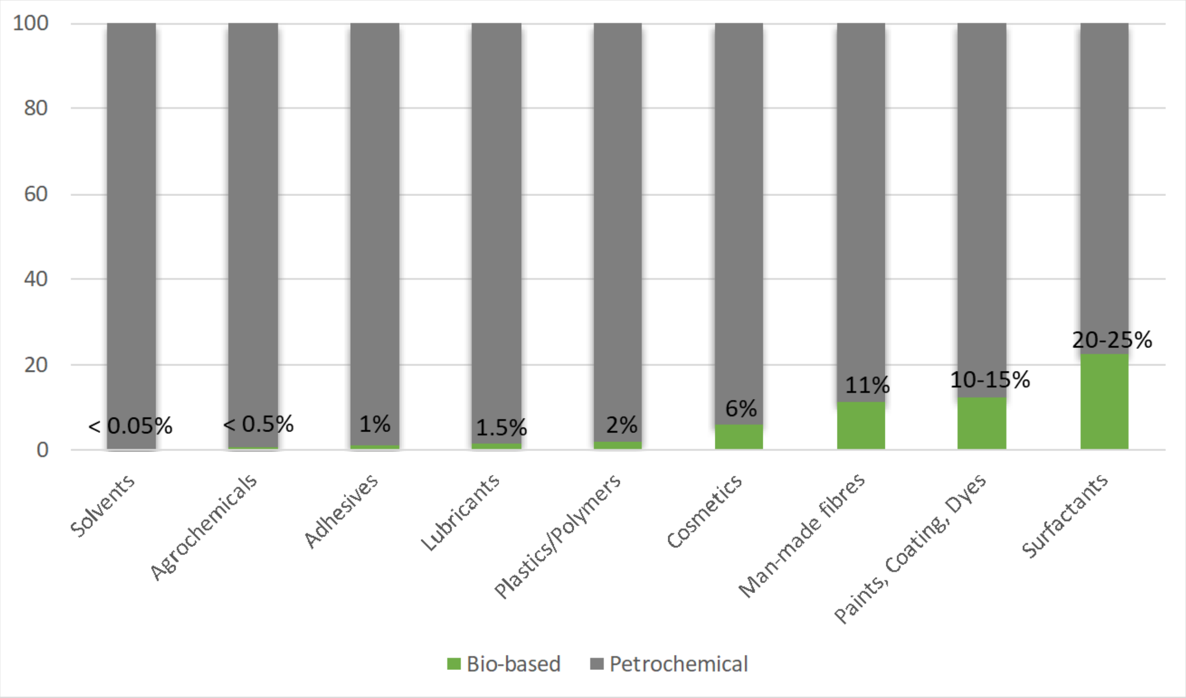
1. This flow chart is provided for clarification and does not pretend to be 100 % accurate regarding the relationships (arrows) between the different product groups.

# 3.2 Current bio-based portfolio in the chemical markets

- **Estimation of existing bio-based chemicals in each product group**

  The current bio-based portfolio of the different product groups was estimated on the basis of a combination of Eurostat data, literature and market analysis. This is depicted in the figure below.

  These data show that bio-based chemicals already form a significant share in some of the investigated product groups, while in other groups there are hardly any bio-based chemicals present.




**Notes:**

1. These numbers are estimations based on different sources and market analysis and can therefore not be considered to be 100% accurate.
2. References:
   - http://ec.europa.eu/eurostat/web/prodcom/data/excel-files-nace-rev.2
   - European Man made Fibers Association, http://www.cirfs.org
   - www.european-bioplastics.org
   - Handbook of Natural Colorants, Edited by Thomas Bechtold and Rita Mussak, John Wiley & Sons 2009
   - nova-Institute, "Bio-based Building Block and Polymers – Global Capacities and Trends 2016-2021", 2016

# 4. The interface between bio-based and petrochemical

- **Introduction**

  The previous chapters described how a long-list of bio-based chemicals that are close to the market was established and how we mapped the value chains within nine petrochemical value chains. By assigning Prodcom codes to both the bio-based chemicals and all final chemicals and intermediates, the shape of the interface becomes visible, where bio-based chemicals can enter the existing value chains.

- **Methodology of the interface analysis**

  The 'interface' of bio-based chemicals and a petrochemical value chain was defined as all the entry points where bio-based products can enter that specific value chain. Therefore the entire value chain towards a certain final product can have multiple entry points up and down the chain. Each petrochemical in each value chain of each product group was compared to each bio-based chemical on our long-list, to see where the petrochemical could be replaced by a bio-based chemical. Wherever such a replacement could take place, we called that an 'entry point'. This approach does not take other factors into account, such as production costs or replacing the function of fossil products.

  The data was handled in a semi-automated fashion because of the quantity,[1] therefore only the processed and analysed results will be shown in this report.

  In the next section of this report the results that were obtained per product group will be analysed. For each product group first the characteristics of the map of its value chains will be described, followed by an analysis of the potential interface between the bio-based chemicals and the petrochemical value chains.

**Notes**

1. This was done using MS Excel and an in-house created MS Visual Basic programme. The programme matches the bio-based chemicals and petrochemical value chains by Prodcom code and produces a table with the new value chains in which the bio-based chemicals are integrated into the petrochemical value chains. Subsequently a manual check was performed to remove any errors or artefacts.

# 4.1 Adhesives map

- **Introduction**

  For the adhesives value chains, three distinctly different types of components were distinguished, which together typically form an adhesive. These different components are solvents, plasticisers, and polymers (or monomers in some cases).[1]

  For each of these components, the value chains of a number of representative final chemicals were mapped by identifying the intermediates in the value chain from the final chemical back to the basic building blocks.

- **Adhesive solvents**

  Typical solvents were analysed: ethyl acetate, ethylene glycol ethers, ethylene glycol, diethylene glycol, acetone, and isophorone.

- **Adhesive plasticisers**

  Also typical plasticisers were analysed: benzoates, diisobutylphthalate, adipate plasticiser, epoxy, and phenol sulphonic amide.

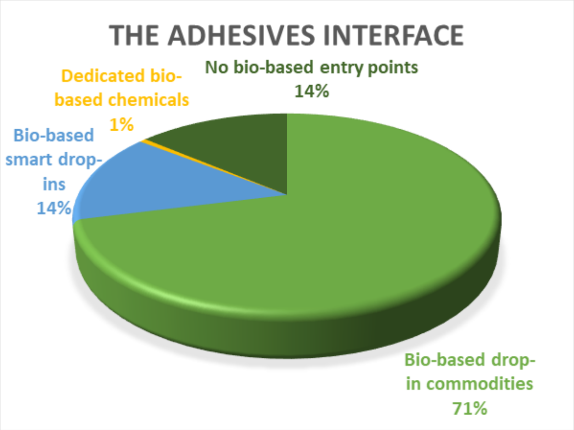
- **Adhesive polymers**

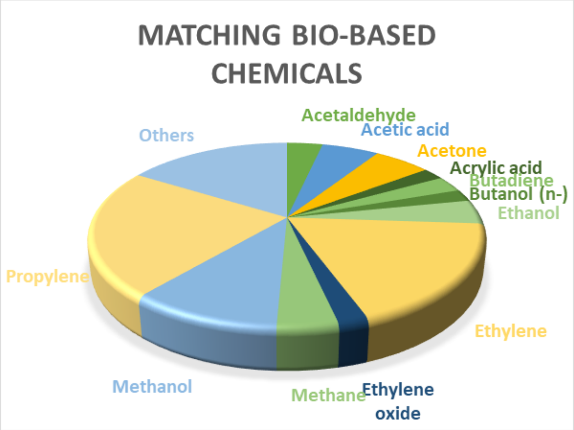
  Here different polymeric chemicals were analysed: various synthetic rubbers, vinyl polymers, acrylates, resins, etc.

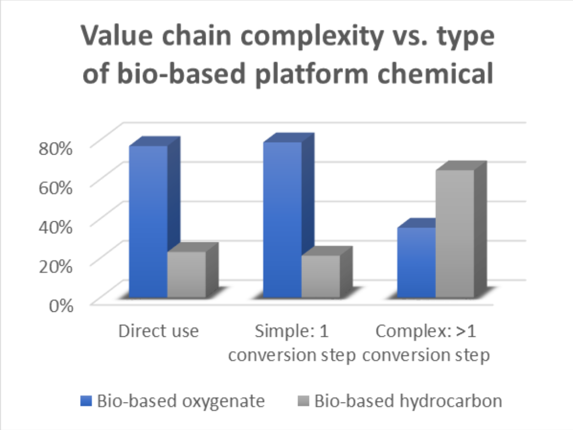
**Notes**

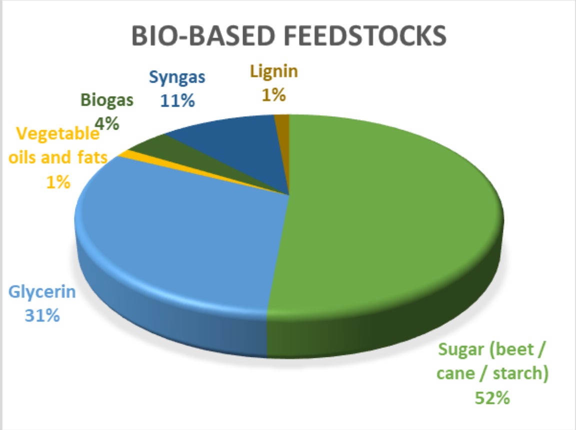
1. Main reference: Ullmann's Encyclopedia of Chemical Technology, 'Adhesives', 2012

# 4.1 Adhesives interface




- **Results**
  - 58 petrochemical adhesives were analysed; at least one entry point for a bio-based chemical in the value chain was identified for 86% of the adhesives, the majority being drop-in commodities.
  - 30 different bio-based chemicals could enter the value chains at 142 entry points that were found. Ethylene, propylene and methanol were the most prevalent options.
  - The analysis of the complexity[1] of the remaining value chains showed that, in general, bio-based oxygenates can enter the adhesives value chains further downstream than bio-based hydrocarbons, leading to less subsequent conversion steps.
  - The main feedstock platforms[2] that can currently provide these bio-based chemicals are the sugar platform,[3] the glycerin platform, and the syngas platform.

**Notes:**

1. If a bio-based chemical directly matched a final chemical product of a petrochemical value chain, we called that 'direct use'; if there was still one conversion step or co-reagent necessary to turn the bio-based chemical into the desired final chemical product, we called that a 'simple value chain'; if there was more than one subsequent conversion step still necessary to produce the desired final chemical from the bio-based chemical, we called that a 'complex value chain'.
2. Following IEA task 42 biorefinery platforms, 2012. Here we distinguish between glycerine and vegetable oils and fats. IEA task 42 adds them together in the 'oil' platform.
3. Ethylene was assumed to be made from the most common route, which is via sugar-based ethanol. There are other routes possible, for example via steam-cracking of vegetable oils, which were left out of scope here.

# 4.2 Agrochemicals map

- **Introduction**

  Agrochemicals may include pesticides, disinfectants, as well as fertilisers. Fertilisers were out of scope, because they consist almost exclusively of inorganic elements. NACE group 20.20, “agrochemical products”, was used as starting point for the selection of the value chains. Because many different pesticides exist, a selection was made of eleven products from ten different Prodcom groups, in order to cover a broad spectrum of agrochemicals.

- **Fungicides**

  The chosen fungicides were Captan, a common foliar nonsystemic fungicide, Epoxiconazole, a typical azole-based fungicide and Mancozeb, a dithiocarbamate that is used as fumigant for a variety of crops.[1]

- **Herbicides**

  Herbicides that were analysed include Glyphosate, a very common phosphate-based non-selective systemic herbicide, 2,4-Dichlorophenoxyacetic acid, a typical phenoxy-phytohormone,[2] and Linuron, a urea-based, selective, systemic herbicide.[3]

- **Insecticides**

  The insecticides that were mapped were Permethrin, Dimethoate, and Mineral oil.[4] The first being a pyrethroid, the second an organophosphorous insecticide, and the latter a pesticide that has rapidly been gaining market share over the last years and that is often used in organic farming.[5,6]

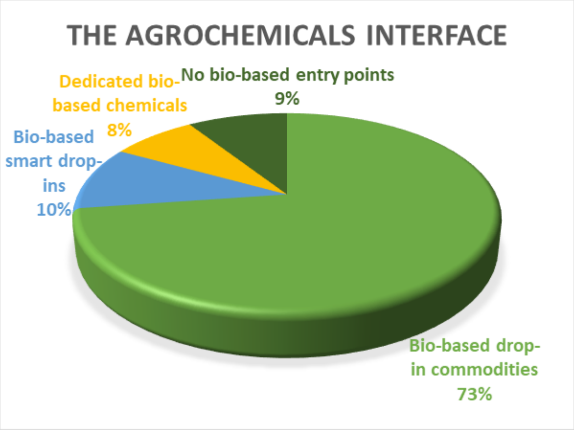
- **Disinfectants**

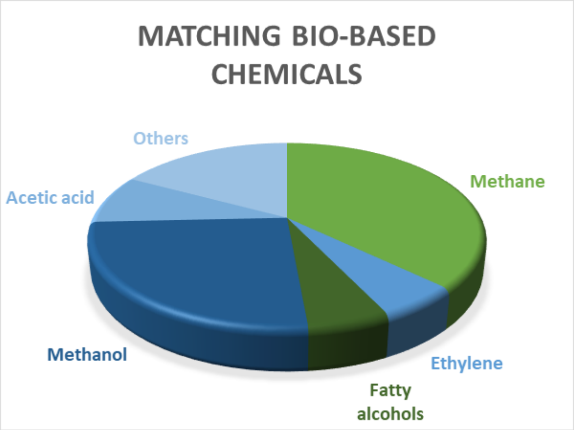
  Didecyldimethylammonium chloride and Benzalkonium chloride were selected, both quaternary ammonium salts.[7]

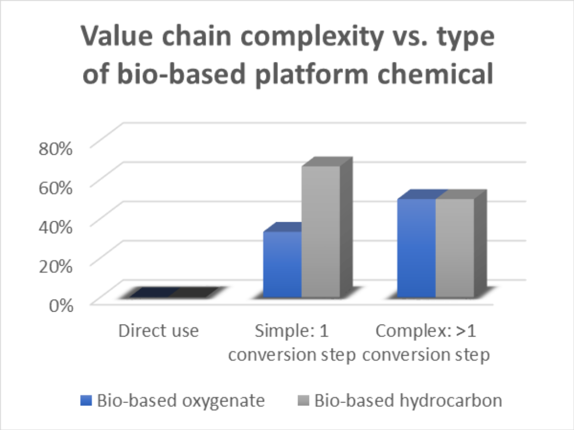
**References:**

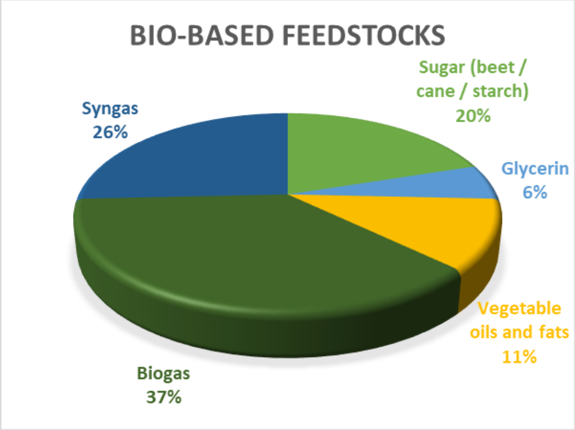

1. F. Müller *et al.*, “Fungicides, Agricultural, 2. Individual Fungicides”, in: *Ullmann’s Encyclopaedia of Industrial Chemistry*, Wiley 2012
2. F. Müller *et al.*, “Weed Control, 2. Individual Herbicides”, in: *Ullmann’s Encyclopaedia (…)*, Wiley 2012
3. T.A. Unger, “Linuron”, in: *Pesticide Synthesis Handbook*, Elsevier 1996, p. 242
4. R.L. Metcalf *et al.*, “Insect Control, 2. Individual Insecticides”, in: *Ullmann’s Encyclopaedia (…)*, Wiley 2014
5. C.E. Bográn *et al.*, “Using oils as pesticides”, Texas A&M Agrilife Extension, 2011;
6. Netherlands National Government, “Compendium voor de Leefomgeving”, 2015;
7. P. Roose *et al.*, “Amines, aliphatic”, in: *Ullmann’s Encyclopaedia(…)*, Wiley 2015

# 4.2 Agrochemicals interface




- **Results**
  - 11 petrochemical agrochemicals were analysed; at least one entry point for a bio-based chemical in the value chain was identified for 91% of the agrochemicals, the majority being drop-in commodities.
  - 11 different bio-based chemicals could enter the value chains at 35 entry points that were found. Methane and methanol were the most prevalent options.
  - Only 3 of the 35 resulting value chains were simple, in general the agrochemical value chains were very complex, leading to many subsequent conversion steps for both bio-based oxygenates and hydrocarbons to the final agrochemicals.
  - The main feedstock platforms that can currently provide these bio-based chemicals are the sugar platform, the biogas platform, and the syngas platform.

# 4.3 Cosmetics map

- **Introduction**

  Cosmetics hold a wide range of different chemicals, since the applications of the different cosmetics are very distinct.

  The category cosmetics can be further divided into six main categories: skin and face, hair, body, perfume, decorative, and other. Of these six, hair products (21%) and skin care (29%) hold the largest market share.[1]

- **Value chain selection**

  In order to get an indicative sample, the pathways of the most commonly applied chemicals were described. These were supplemented by the pathways of several specific chemicals.

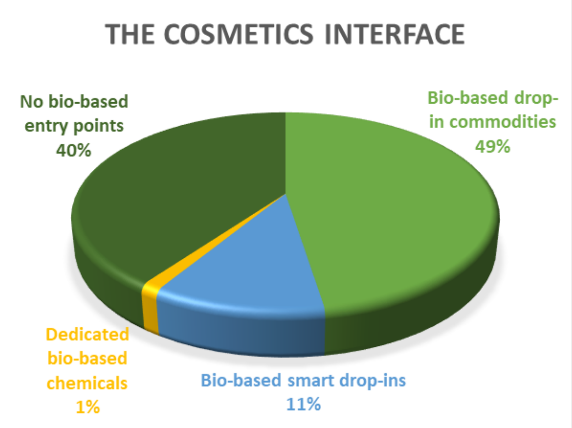
  This approach resulted in 47 pathways for the production of 35 different cosmetics: 31 pathways of chemicals commonly used in any cosmetics, such as propellants, waxes and preservatives; 7 pathways of chemicals typical for skin products (such as sun screen or anti-bacteria agent for deodorants) and 9 pathways for chemicals typically used in hair products (e.g. hair straightener, dyes and anti-dandruff agents).

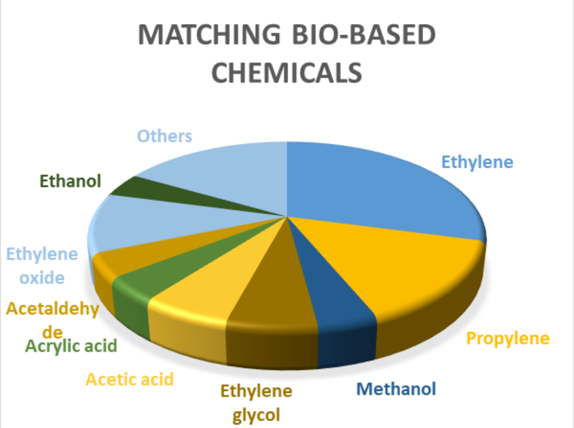
  Any bio-based chemicals, such as a number of vegetable fats and oils that are already applied within the cosmetics industry, were out of scope.

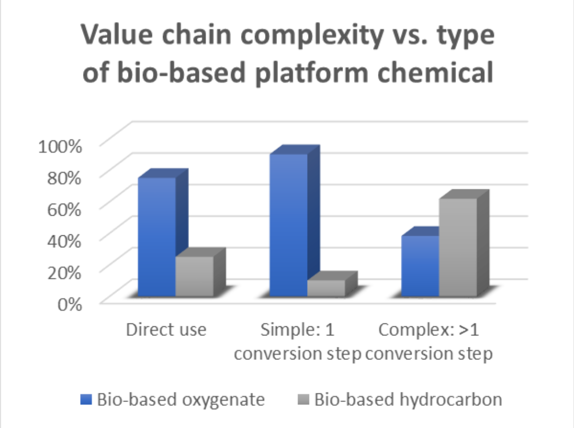
**Notes**

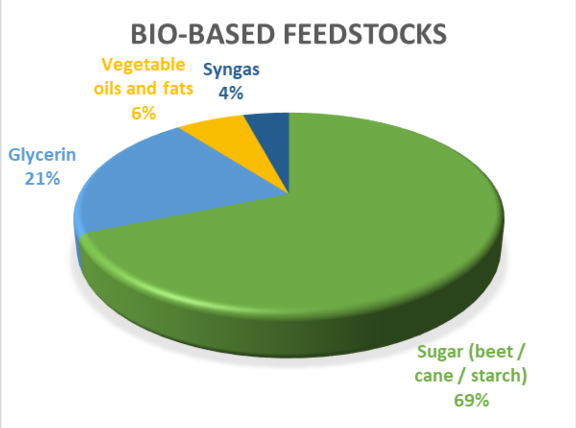
1. Main reference: Ullmann's Encyclopedia of Chemical Technology, 'Skin cosmetics', Wiley 2012

# 4.3 Cosmetics interface




- **Results**
  - 35 petrochemical cosmetics were analysed; at least one entry point for a bio-based chemical in the value chain was identified for 60% of the cosmetics, the majority being drop-in commodities.
  - 17 different bio-based chemicals could enter the value chains at 48 entry points that were found. Ethylene as well as its derivatives ethylene oxide and glycol, and propylene were common options.
  - Here also the subsequent pathways from entry point to final chemical were on average shorter for the bio-based oxygenates than for the bio-based hydrocarbons.
  - The main feedstock platforms that can currently provide these bio-based chemicals are the sugar platform and the glycerine platform.

# 4.4 Lubricants map

- **Introduction**

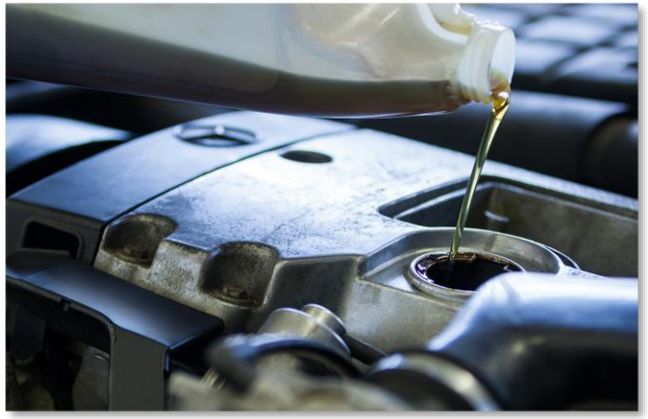
  Lubricants can generally be sorted under the following categories: synthetic lubricants, lubricant oils, grease, solid lubricants, oil additives, industrial lubricants and metal & fibre lubricants.[1]

- **Industrial lubricants**

  Within the Industrial lubricants category several chemical groups can be identified: ethoxylated alcohols, ethoxylated fatty acids, sorbitol ester & its ethoxylated derivatives, and alkyls sulfosuccinates.

- **Approach to partially bio-based lubricants**

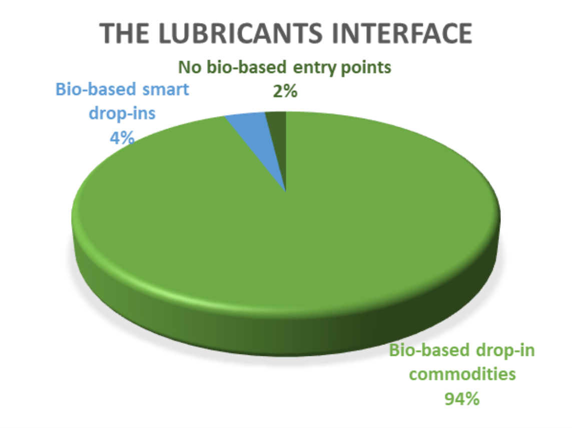
  Many lubricants are already produced with bio-based components, especially fatty acids, fatty alcohols, and glycerol. These components (all fatty acids and alcohols with a carbon chain length of eight carbon atoms or more) were excluded from the analysis. However, when a certain lubricant is made from a combination of an already bio-based component (e.g. palmitic acid) and a petrochemical component (e.g. butanol), the lubricant was included in the analysis, because then the petrochemical part of the value chain can still offer additional entry points for bio-based chemicals.

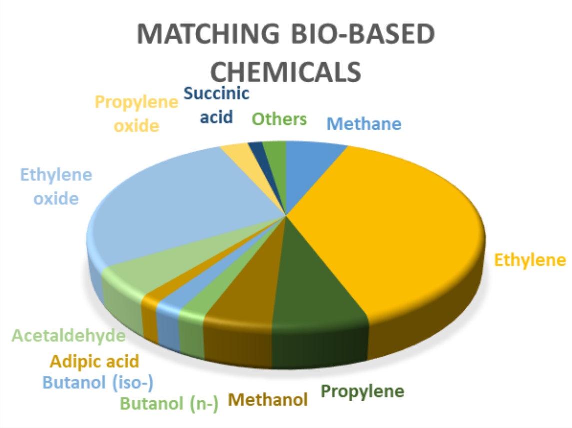


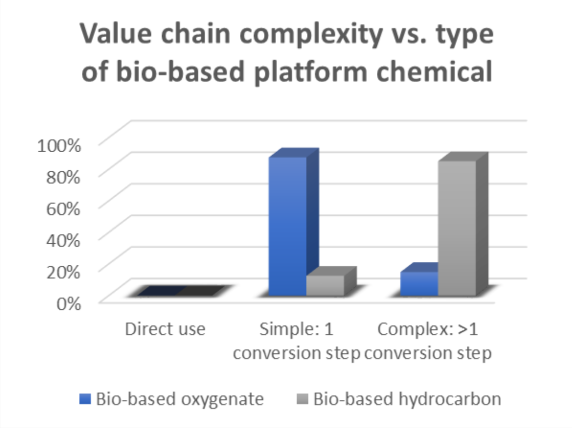
**Notes:**

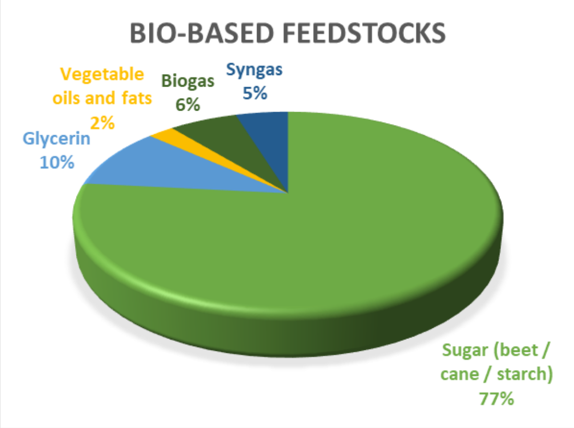
1. Main reference: Kirk-Othmer Encyclopedia of Chemical Technology, Wiley 2014

# 4.4 Lubricants interface




- **Results**
  - 103 petrochemical lubricants were analysed; at least one entry point for a bio-based chemical in the value chain was identified for 98% of them, the far majority being drop-in commodities.
  - 15 different bio-based chemicals could enter the value chains at 210 entry points that were found. Ethylene as well as its derivative ethylene oxide were the most common options in the value chains to many ethoxylated final chemicals.
  - Again the subsequent pathways from entry point to final chemical were on average shorter for the bio-based oxygenates than for the bio-based hydrocarbons.
  - The main feedstock platform that can currently provide these bio-based lubricants is the sugar platform. Important to emphasize is that already many bio-based lubricants exist on the basis of vegetable oils, which were kept out of scope.

# 4.5 Man-made fibres map

- **Introduction**

Man-made fibres can be divided into two categories: natural fibres and synthetic fibres.

**Natural fibres** consist of biologically produced polymers such as silk, cotton and wool which emerge from the textile manufacturing process in a relatively unaltered state. Some others, for instance rayon and cellulose acetate are based on cellulose, further modified in order to be regenerated into practical fibres.

**Synthetic fibres** are mainly made of polymers that do not occur naturally. Among these are PET (polyethylenterephthalate) and other polyesters, PVC (polyvinylchloride), PP (polypropylene), PE (polyethylene) and other polyolefins, phenol-formaldehyde based fibres, PU (polyurethane), PAN (polyacrylonitrile)…

More than 20 petrochemical pathways, starting from fossil resources (crude oil and natural gas) and yielding representative final chemicals (or families) for the manufacturing of synthetic fibres, were described. Note that these value chain descriptions overlap with those of the solvents product group.

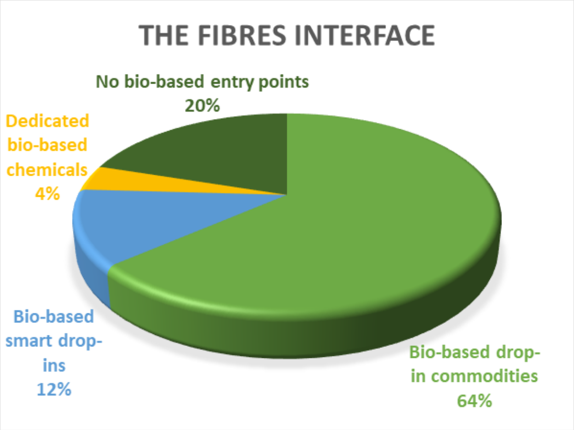
- **Special case: Polyamides**

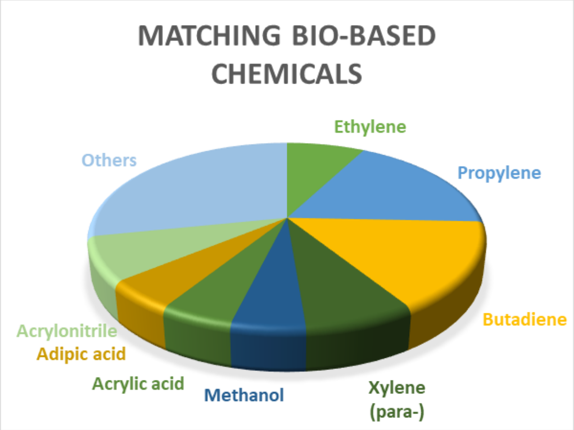
Synthetic polyamides (nylons) are formed by equal parts of an amine and a carboxylic acid (most nylons are made from the reaction of a dicarboxylic acid with a diamine).

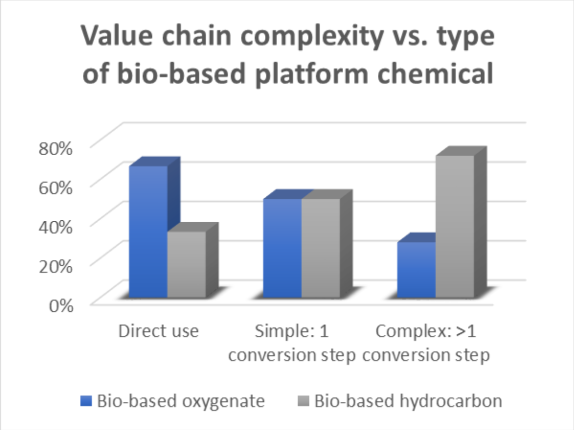
For some examples both value chains, the one for the production of the amine and the one for the production of the acid, required for the manufacturing of the polyamide were separately described.

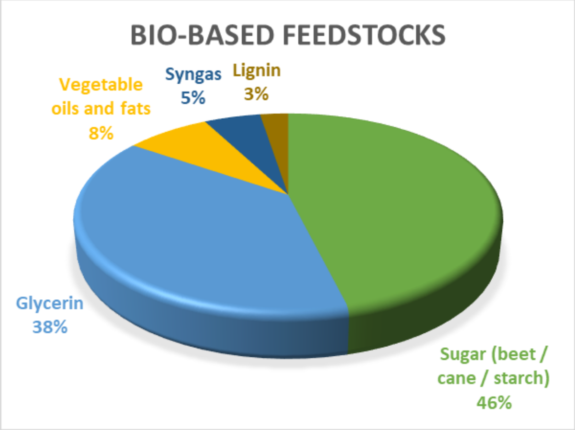
Note as well that one of the counterparts (usually the acidic component) of many synthetic polyamides are manufactured directly from natural resources (e.g. sebacic acid from castor oil).

# 4.5 Man-made fibres interface




- **Results**
  - 25 petrochemical man-made fibres were analysed; at least one entry point for a bio-based chemical in the value chain was identified for 80% of them, the majority being drop-in commodities.
  - 19 different bio-based chemicals could enter these value chains at 39 entry points that were found. No single bio-based chemical stood out as far as with other product groups; propylene and butadiene were the most common options.
  - The bio-based chemicals that could be directly used were in this case all polymers, so in this case it was difficult to compare the remaining complexity of the value chains after the bio-based chemical entry. Some specific examples such as adipic acid were able to reduce the value chain complexity.
  - The main feedstock platforms that can currently provide these fibres are the sugar platform and the glycerine platform. Again the already bio-based options (e.g. cellulosic fibres) were out of scope.

# 4.6 Paints / Coatings / Dyes map

- **Introduction**

  The paints and coatings value chains were built considering the four main constituents of paints as sub-groups: 1) solvents, 2) binders, 3) pigments and 4) additives. The petrochemical pathways starting from fossil resources to yield representative final chemicals (or families) of these subgroups were described.

- **Sub-group: Solvents**

  16 common solvents used in the manufacturing of paints and coatings were described. Keep in mind that for emulsion paints the solvent is simply water, whereas for resin-based paints a variety of organic solvents are used (isopropanol, propylene glycol ethers, methyl isobutyl ketone, toluene….). Note: this sub-group overlaps with the separately described value chains map of the solvents product group.

- **Sub-group: Binders**

  The binder exists to hold the pigment to the surface. The binder is a polymeric substance mainly belonging to the families of acrylic, alkyd and epoxy resins and polyurethanes. 12 representative value chains were described. Note: this sub-group overlaps with the deeply described value chain of plastics.

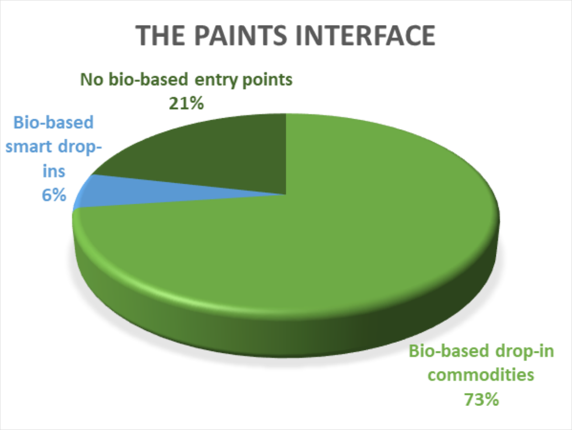
- **Sub-group: Pigments**

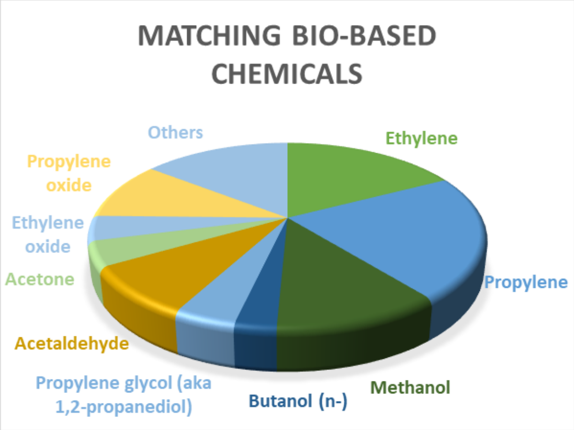
  70% of the pigments in paints are inorganic (70%). Azo-, phthalocyanine and anthaquinone derivatives dominate the organic pigments (30%) in paints. Due to the heterogeneity of these derivatives basic building blocks required for the production of these derivatives were described.

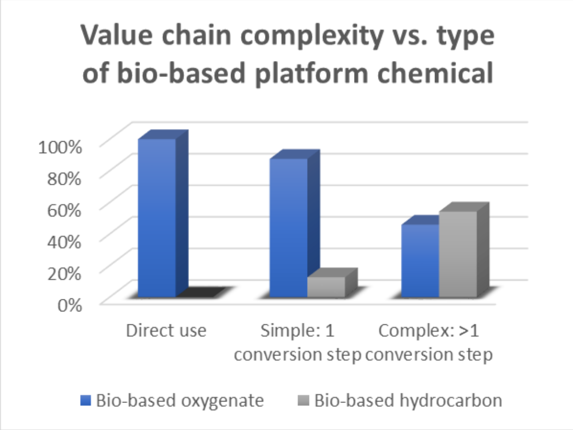
- **Sub-group: Additives**

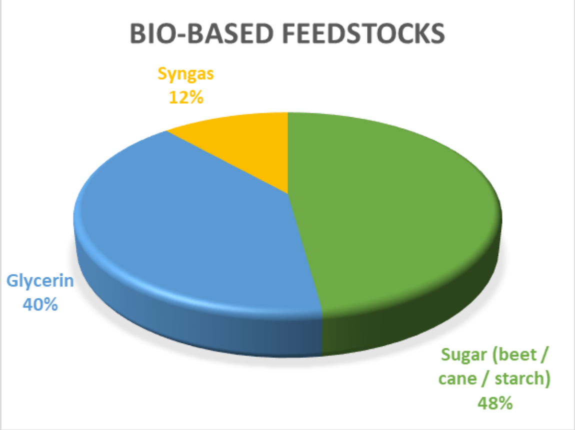
  A heterogeneus sub-group (dispersants, silicones, dry agents, bactericides…) that only contributes to approximately 5% of the final formulation. One common value chain (silicone) was described.

# 4.6 Paints / Coatings / Dyes interface




- **Results**
  - Value chains of 28 petrochemical paints & coating components were analysed; at least one entry point for a bio-based chemical was identified for 79% of them, mainly being drop-in commodities.
  - 22 different bio-based chemicals could enter these value chains at 39 entry points that were found. Ethylene, propylene and methanol together made up half of the bio-based entries.
  - As in other groups, some bio-based oxygenates can be applied directly (mainly as solvents), while on average the bio-based hydrocarbons needed more subsequent conversion steps after entering the value chains.
  - The main feedstock platforms that can currently provide these fibres are the sugar platform and the glycerine platform.

# 4.7 Plastics / Polymers map

- **Introduction**

  The value chains of plastics comprise of a whole family of polymers with different properties and applications.

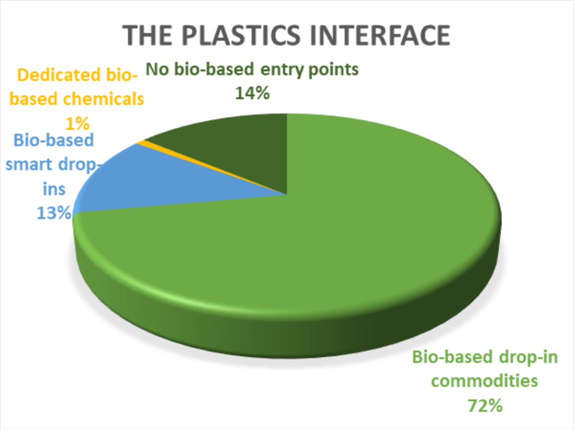
  Plastics are usually classified by the chemical structure of the polymer's backbone and side chains. Some important groups in these classifications are: the acrylic, polyester, epoxy resin, polyurethane, polyamide, silicone and fluorinated and halogenated plastics.

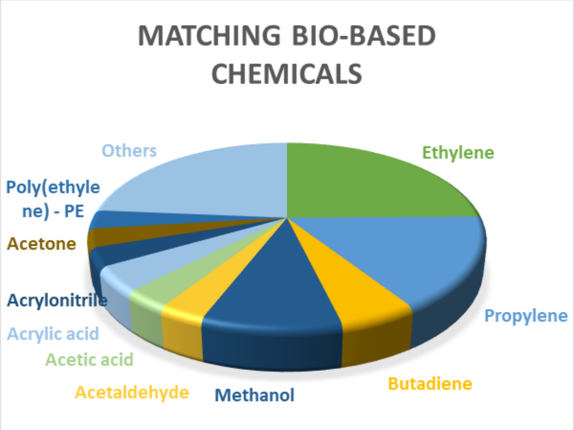
  More than 50 different classical synthetic routes (petrochemical) for the manufacturing of the main products (including co-polymers) were described.

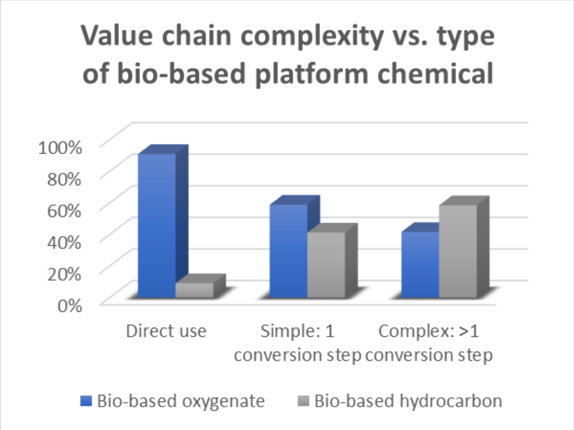
- **Examples covered:**

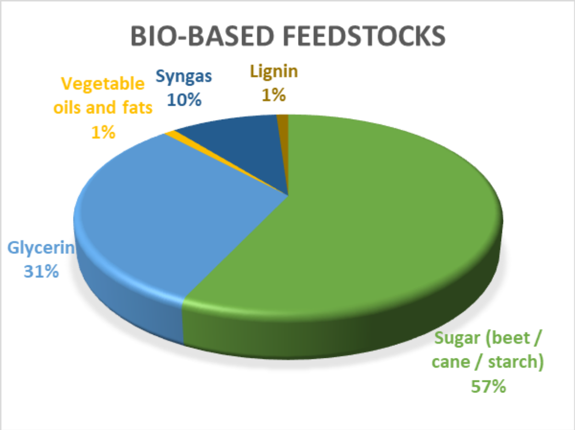
  Polyamides (PA), polycarbonate (PC), polyethylene (PE, HDPE, LDPE…), polyethylene terephthalate (PET), polypropylene (PP), polyamides (PA), polystyrene (PS), polyurethane (PU), polyvinylchloride (PVC), acrylonitrile butadiene styrene (ABS), polyepoxides, polymethyl methaacrylate (PMMA), teflon, phenol formaldehyde resins (PF), and silicone.

# 4.7 Plastics interface




- **Results**
  - 43 petrochemical plastics were analysed; at least one entry point for a bio-based chemical was identified for 86% of them, the majority being drop-in commodities, while also quite some smart drop-in options were present.
  - 28 bio-based chemicals could enter these value chains at 93 entry points that were found. Ethylene, propylene and methanol again made up half of the bio-based entries together.
  - Like with the man-made fibres, the bio-based oxygenates that can be applied directly in this product group are all polymers, of which some bio-based options had a shorter production chain, while for some there is not much difference.
  - The main feedstock platforms that can currently provide these fibres are the sugar platform and the glycerine platform.

# 4.8 Solvents map

- **Introduction**

  The value chains of three major solvents categories were mapped, in order to get a representative sample of the existing value chains. These categories are halogenated, oxygenated and hydrocarbon solvents.[1]

- **Halogenated solvents**

  This category was analysed using the following chemicals representatives: chlorinated, fluorinated, brominated and iodinated hydrocarbons.

- **Oxygenated solvents**

  This category included the following chemical groups: alcohols, aldehydes, ketones, esters, ethers, oxo acids and glycol ethers.

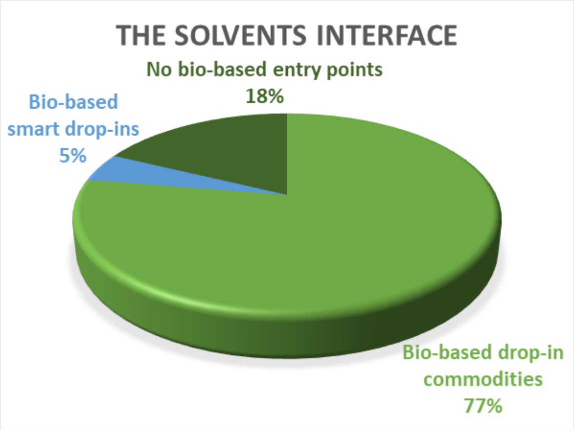
- **Hydrocarbon solvents**

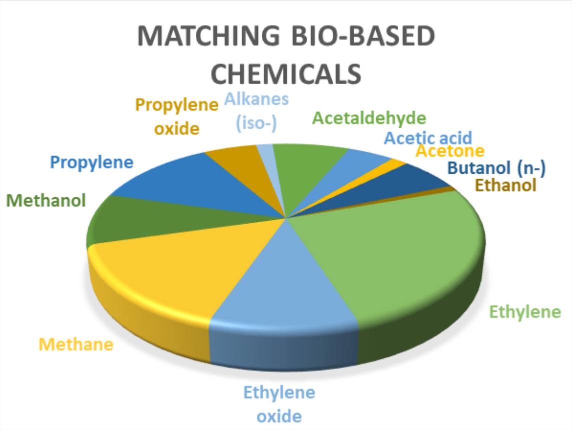
  This solvent category includes the following groups of chemicals: aliphatic solvents, aromatic and white spirits.

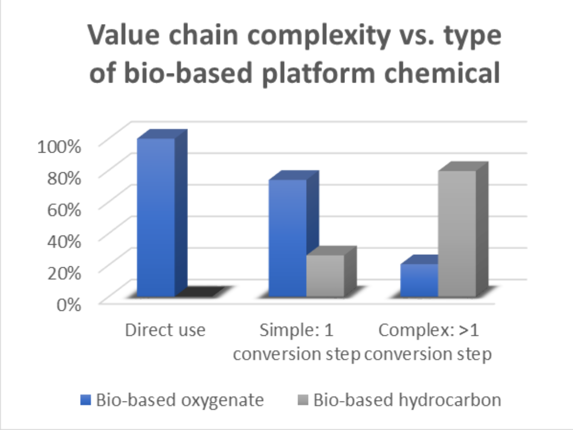
**Notes:**

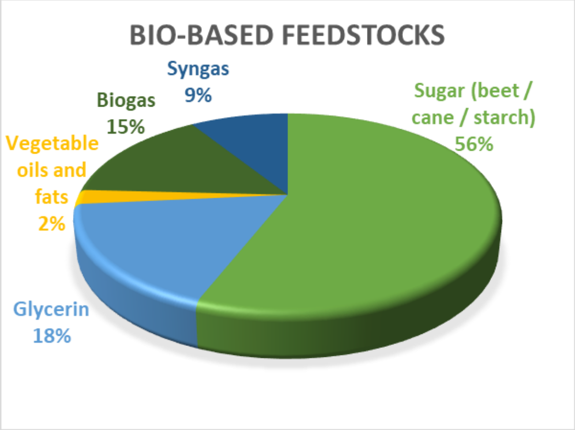
1. Main reference: Kirk-Othmer Encyclopedia of Chemical Technology, Wiley 2014

# 4.8 Solvents interface




- **Results**
  - 135 petrochemical solvents were analysed; at least one entry point for a bio-based chemical in the value chain was identified for 82% of the analysed petrochemical solvents.
  - 14 bio-based chemicals from the long-list were responsible for all the entry points in the value chains.
  - In general, bio-based oxygenates can enter the solvent value chains further downstream than bio-based hydrocarbons, while two bio-based oxygenates are direct (smart) drop-in replacements for a final product (iso- and n-butanol).
  - The main feedstock platforms that can currently provide these bio-based chemicals are the sugar platform, the glycerin platform, and the biogas platform.

# 4.9 Surfactants map

- **Introduction**

  In general all surfactants can be sorted under four categories, which are: anionic, cationic, non-ionic and amphoteric surfactants.[1] Within each of these four categories of surfactants we identified the key final chemicals and mapped all the intermediate chemicals which lead from basic building blocks to these final chemicals.

- **Anionic surfactants**

  These are typically sodium, ammonium, magnesium or fatty alcohol salts/esters of the following groups of surfactants: alkyl sulfates, sulfated ethoxylated alcohols, alkyl sulphonates, linear alkylbenzene sulphonetes, fatty acid methyl ester sulphonates , mono- and di- alkyl sulfosuccinates and soaps.

- **Cationic surfactants**

  This group includes the following chemical types: mono alkyl quaternary ammonium salts, esterquats.

- **Amphoteric surfactants**

  These surfactants include the following main groups of chemicals: alkyl betaines, alkyl amine oxides and polymeric surfactants.

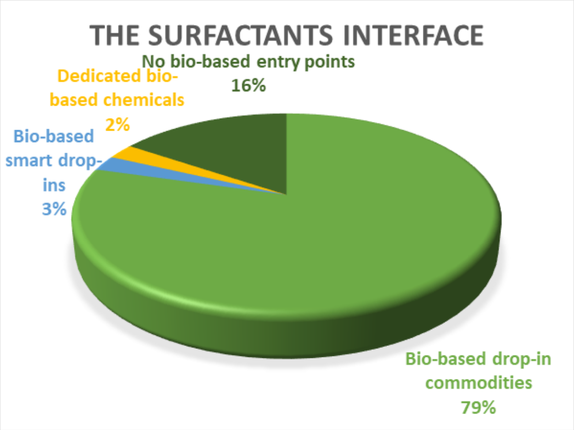
- **Non-ionic surfactants**

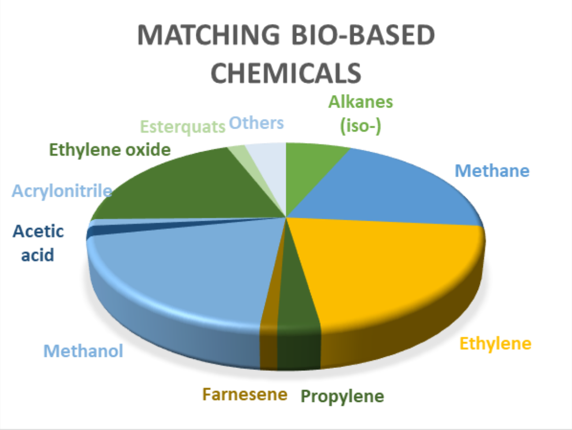
  They include the following chemicals groups: ethoxylated aliphatic alcohols, polyethylene glycol esters, sorbitol ester and its ethoxylated derivatives, alkyl polyglycosides and fatty acid alkanolamides.

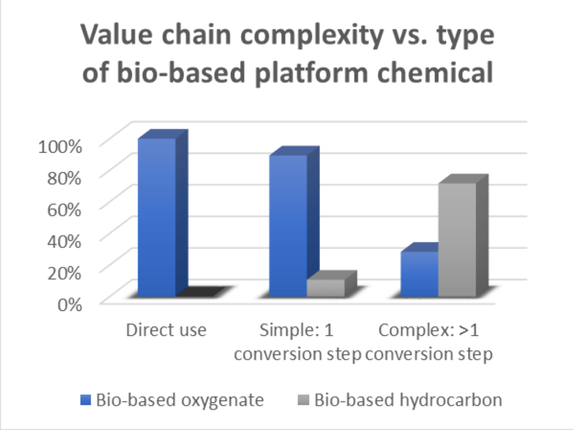
**Notes:**

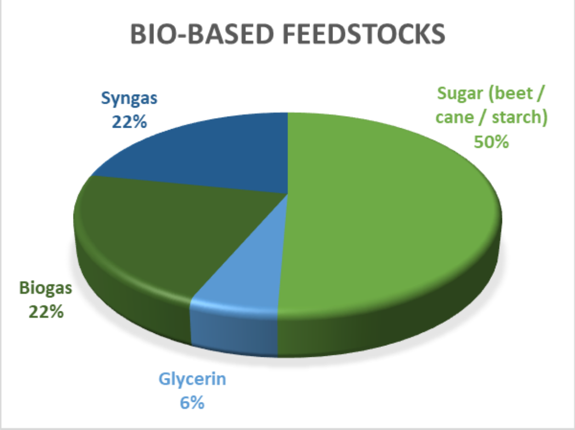
1. Main reference: Kirk-Othmer Encyclopedia of Chemical Technology, Wiley 2014

# 4.9 Surfactants interface



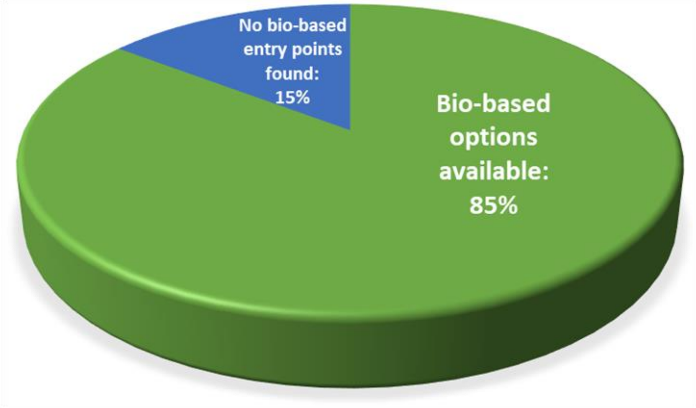




- **Results**
  - 90 different surfactants were analysed; at least one entry point for a bio-based chemical in the value chain was identified for 84% of these surfactants.
  - 17 bio-based chemicals from the long-list could enter the existing surfactant value chains. Methane, methanol, ethylene and ethylene oxide together are responsible for 80% of these bio-based options.
  - The bio-based chemicals from the long-list that could be used directly in this case were esterquats. In general, bio-based oxygenates again result in shorter subsequent value chains.
  - The main feedstock platforms that can currently provide these bio-based chemicals are the sugar platform (providing a.o. ethylene and ethylene oxide), the syngas platform (providing methanol), and the biogas platform (providing methane).

# 5 Synthesis of the results

This report summarised the analysis of a significant sample of the value chains that currently exist in the European petrochemical industry, and covers the value chains of more than 500 petrochemical final products in total, across nine different product groups. Key observations are:

- For 85%[1] of the analysed petrochemical products at least one entry point for a bio-based chemical was found in its value chain, which means that for the vast majority of the chemical products there are possibilities to fully or partially replace fossil feedstocks with bio-based ones.
- In total more than 1,000 possible bio-based entry points were identified in the value chains of these 500 petrochemical products. Extrapolating this observation leads to the conclusion that every value chain in the chemical industry on average has two entry points for bio-based chemicals.
- Another observation that applies for the majority of the analysed product groups is that bio-based oxygenates enter the petrochemical value chains further downstream, which means the subsequent value chain will be shorter. In some cases that is obvious, for example because ethylene is often oxidised to ethylene oxide before it is further used (so bio-EO from bio-ethylene is as complex as conventional EO from fossil ethylene), yet in principle it shows an opportunity for ’smart drop-ins’, that make use of oxygen functionalities that are already present in biomass.
- From the long-list of 120 bio-based chemicals, ‘only’ 49 showed entry points in these value chains. Many bio-based chemicals on our long-list that could not enter these value chains are ‘dedicated chemicals’, so they have specific (often preferential) properties and can potentially replace formulated final products on the basis of their functionality, rather than parts of the chemical value chains.
- The feedstock platforms that came out as most important in this analysis are the sugar platform and the glycerine platform. Important to note is that that is the case because those platforms are currently responsible for most relevant bio-based chemicals, yet it does not mean that the bio-based chemicals cannot be made from other feedstocks now or in the future.




**Notes:**

1. This percentage refers to the number of analysed petrochemical products, not to their production volumes.

# Discussion & Conclusions

Every analysis comes with its own bias. The methodology that was applied in this analysis of the interface between petrochemical and bio-based value chains showed a bias for drop-in chemicals. If the analysis would have been done on the basis of the functionality of formulated products rather than on the basis of existing value chains, it would probably have let to a result with more dedicated bio-based chemicals than is now the case. A clear example of this bias is that bio-based ethylene showed up at about 25% of all the entry points that were found in this analysis. That is important to keep in mind when interpreting the results of this study.

Having said that, the approach we took is a unique one in that it brings together a lot of information on how the value chains in the European chemical industry look at this moment and where the possibilities lie for relatively easy replacement of fossil feedstocks by bio-based drop-ins, and which are the most prevalent options.

Our analysis clearly shows that there are numerous possibilities for using sustainable bio-based feedstocks in the chemical industry. This analysis will also serve as part of the knowledge-base for the subsequent activities in the RoadToBio project, which include an analysis of the regulatory barriers and the public perception of bio-based chemicals, and an analysis of nine business case studies of bio-based opportunities, which will together inform a roadmap for the European chemical industry towards a goal of 30 % bio-based chemicals in 2030.

# Colophon

| | |
|---|---|
| **Project Title: Roadmap for the Chemical Industry in Europe towards a Bioeconomy** | |
| **Acronym: RoadToBio** | |
| **Grant Agreement No: 745623** | |
| **Start Date: 01 May 2017** | |
| **Duration of the Project: 24 Months** | |
| **Deliverable No.** | D1.1 |
| **Deliverable Title** | Report with opportunities for bio-based chemical feedstocks and intermediates in the chemical industry |
| **Type** | Report |
| **Due Date (first version)** | 31 October 2017 |
| **Date Delivered (final version)** | 4 September 2018 |
| **Prepared by (Lead Partner)** | BTG Biomass Technology Group B.V.<br>Contact: Spekreijse@btgworld.com |
| **Dissemination Level** | Public |

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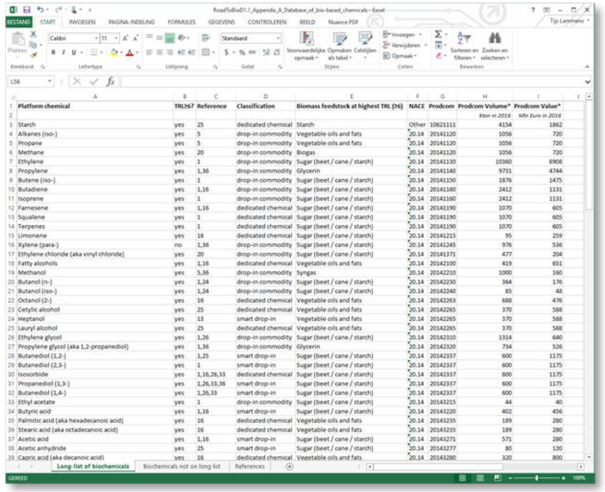
# Appendix A – Database of bio-based chemicals

- **An Excel file with the database can be downloaded [from here](from here).**



| Platform chemical | TRL≥6? | Reference | Classification | Biomass feedstock at highest TRL (≥6) | NACE | Prodcom | Prodcom Volume* | Prodcom Value* |
|---|---|---|---|---|---|---|---|---|
| | | | | | | | kton in 2016 | Mln Euro in 2016 |
| Starch | yes | 25 | dedicated chemical | Starch | Other | 10621111 | 4154 | 1862 |
| Alkanes (iso-) | yes | 5 | drop-in commodity | Vegetable oils and fats | 20.14 | 20141120 | 1056 | 720 |
| Propane | yes | 5 | drop-in commodity | Vegetable oils and fats | 20.14 | 20141120 | 1056 | 720 |
| Methane | yes | 20 | drop-in commodity | Biogas | 20.14 | 20141120 | 1056 | 720 |
| Ethylene | yes | 1 | drop-in commodity | Sugar (beet / cane / starch) | 20.14 | 20141130 | 10360 | 6908 |
| Propylene | yes | 1,36 | drop-in commodity | Glycerin | 20.14 | 20141140 | 9731 | 4744 |
| Butene (iso-) | yes | 1 | drop-in commodity | Sugar (beet / cane / starch) | 20.14 | 20141150 | 1876 | 1475 |
| Butadiene | yes | 1,16 | drop-in commodity | Sugar (beet / cane / starch) | 20.14 | 20141160 | 2412 | 1131 |
| Isoprene | yes | 1 | drop-in commodity | Sugar (beet / cane / starch) | 20.14 | 20141160 | 2412 | 1131 |
| Farnesene | yes | 1,16 | dedicated chemical | Sugar (beet / cane / starch) | 20.14 | 20141190 | 1070 | 605 |
| Squalene | yes | 1 | dedicated chemical | Sugar (beet / cane / starch) | 20.14 | 20141190 | 1070 | 605 |
| Terpenes | yes | 1 | dedicated chemical | Sugar (beet / cane / starch) | 20.14 | 20141190 | 1070 | 605 |
| Limonene | yes | 16 | dedicated chemical | Sugar (beet / cane / starch) | 20.14 | 20141215 | 95 | 259 |
| Xylene (para-) | no | 1,36 | drop-in commodity | Sugar (beet / cane / starch) | 20.14 | 20141245 | 976 | 536 |
| Ethylene chloride (aka vinyl chloride) | yes | 20 | drop-in commodity | Sugar (beet / cane / starch) | 20.14 | 20141371 | 477 | 204 |
| Fatty alcohols | yes | 1,16 | dedicated chemical | Vegetable oils and fats | 20.14 | 20142100 | 419 | 651 |
| Methanol | yes | 5,36 | drop-in commodity | Syngas | 20.14 | 20142210 | 1000 | 160 |
| Butanol (n-) | yes | 1,24 | drop-in commodity | Sugar (beet / cane / starch) | 20.14 | 20142230 | 364 | 176 |
| Butanol (iso-) | yes | 1,24 | drop-in commodity | Sugar (beet / cane / starch) | 20.14 | 20142240 | 85 | 48 |
| Octanol (2-) | yes | 16 | dedicated chemical | Vegetable oils and fats | 20.14 | 20142263 | 688 | 476 |
| Cetylic alcohol | yes | 25 | dedicated chemical | Vegetable oils and fats | 20.14 | 20142265 | 370 | 588 |
| Heptanol | yes | 13 | smart drop-in | Vegetable oils and fats | 20.14 | 20142265 | 370 | 588 |
| Lauryl alcohol | yes | 25 | dedicated chemical | Vegetable oils and fats | 20.14 | 20142265 | 370 | 588 |
| Ethylene glycol | yes | 1,26 | drop-in commodity | Sugar (beet / cane / starch) | 20.14 | 20142310 | 1314 | 640 |
| Propylene glycol (aka 1,2-propanediol) | yes | 1,36 | drop-in commodity | Glycerin | 20.14 | 20142320 | 734 | 526 |
| Butanediol (1,2-) | yes | 1,25 | smart drop-in | Sugar (beet / cane / starch) | 20.14 | 20142337 | 600 | 1175 |
| Butanediol (2,3-) | yes | 1 | smart drop-in | Sugar (beet / cane / starch) | 20.14 | 20142337 | 600 | 1175 |
| Isosorbide | yes | 1,16,26,33 | dedicated chemical | Sugar (beet / cane / starch) | 20.14 | 20142337 | 600 | 1175 |
| Propanediol (1,3-) | yes | 1,26,33,36 | smart drop-in | Sugar (beet / cane / starch) | 20.14 | 20142337 | 600 | 1175 |
| Butanediol (1,4-) | yes | 1,26,33 | smart drop-in | Sugar (beet / cane / starch) | 20.14 | 20142337 | 600 | 1175 |
| Ethyl acetate | yes | 1 | drop-in commodity | Sugar (beet / cane / starch) | 20.14 | 20143215 | 44 | 40 |
| Butyric acid | yes | 1,16 | smart drop-in | Sugar (beet / cane / starch) | 20.14 | 20143220 | 402 | 456 |
| Palmitic acid (aka hexadecanoic acid) | yes | 16 | dedicated chemical | Vegetable oils and fats | 20.14 | 20143235 | 189 | 280 |
| Stearic acid (aka octadecanoic acid) | yes | 16 | dedicated chemical | Vegetable oils and fats | 20.14 | 20143235 | 189 | 280 |
| Acetic acid | yes | 1,16 | smart drop-in | Sugar (beet / cane / starch) | 20.14 | 20143271 | 571 | 280 |
| Acetic anhydride | yes | 25 | smart drop-in | Sugar (beet / cane / starch) | 20.14 | 20143277 | 80 | 120 |
| Capric acid (aka decanoic acid) | yes | 16 | dedicated chemical | Vegetable oils and fats | 20.14 | 20143280 | 320 | 800 |

# Appendix B – Maps of the value chains

- **An Excel file with the product group maps and a table with the aggregated data results from the analysis can be downloaded [from here](#).**