Hierarchical Valuation of Bio-Products

Zahir Barahmand

University of South-Eastern Norway, Kjølnes Ring 56, 3918 Porsgrunn, Norway

E-mail address: Zahir.barahmand@usn.no
DOI: 10.23642/usn.25959250

1. Hierarchical Classification of Biochemicals

Based on the approaches discussed above, the authors introduced a two-tiered classification system for organic compounds, which aligns with the value pyramid concept used in bioproduct studies. During the primary classification tier, compounds are categorized based on their molecular weight and general structural characteristics. Subsequently, these broad categories are refined through secondary classification, in which compounds are grouped into functional groups. At this second level, specific chemical properties and reactivities of the compounds can be examined in greater detail. By employing this methodological approach, the study manages to balance a comprehensive overview with detailed analysis, thereby improving the understanding of organic chemistry in a structured and systematic manner.

The classification began with the inclusion of chemical formulas in our database, which enabled the initial level of categorization to be achieved. For example, compounds containing only hydrogen and carbon were classified as basic hydrocarbons in our classification scheme. As indicated by their nomenclature, these hydrocarbons were easily recognized, typically starting with prefixes such as "meth-", "eth-", "prop-", etc., which indicated the number of carbon atoms, and ending with suffixes such as "-ane", "-ene", or "-yne". These chemicals are further classified based on functional groups such as hydroxyl ($-OH$), carboxyl ($-COOH$), amino ($-NH_2$), nitro ($-NO_2$), halides (such as $-Cl$, $-Br$), etc. Additionally, the position of the functional group, as indicated by a number or locational prefix like 'ortho-', 'meta-', 'para-' in aromatic compounds, determined the classification. A comprehensive classification of organic chemicals and a chapter describing these classes of chemicals are available as open access supplementary materials (Barahmand, 2024a).

In spite of this, classification becomes a problem when it comes to fine chemicals that have complex structures and heavy molecules, particularly when they are classified according to different nomenclatures. To navigate this complexity, we utilized ChatGPT 4.0 (Open AI), inputting our classification framework and querying it to determine which functional group a compound belongs to or whether it is considered to be a fine chemical. Our classification system has been meticulously verified through multiple stages, ensuring its accuracy and reliability. By following this rigorous approach, we were able to strengthen the validity of our methodology and provide a strong basis for subsequent analysis of these chemicals as they relate to pyrolysis-derived products.

2. Hierarchy of value levels

Table 1 provides the proposed general classification of organic compounds and value levels assigned according to a value pyramid for bioproducts (the full list is available in open access at (Barahmand, 2024b)). A basic hydrocarbon is divided into aromatic and aliphatic hydrocarbon categories, and further subdivisions are made based on structural characteristics, such as chain type and saturation level. Compounds such as methane and ethane have a value level of 1 while unsaturated hydrocarbons such as alkenes and alkynes have a value level of 2. The highest contribution comes from functionalized hydrocarbons, which are more valuable than basic hydrocarbons. According to their functional groups, these hydrocarbons were divided into six subclasses, each with its own value level. Hydrocarbons in this class range from level 2 (alcohols, ethers, etc.) to level 4 (fatty compounds).

Hydrocarbon molecules with a higher weight were grouped into a dedicated class in which they contributed the least. Of all organic compounds, fine chemicals represent the most significant and valuable group. There are several categories in this section that reflect the complex nature of the compounds and the role they play in a variety of industries. The APIs, such as antibiotics and cardiovascular drugs, are assigned the highest value level of 5, reflecting their essential role in healthcare. Aromas and flavors, including synthetic flavors and essential oils, are rated as having a value level of 4, indicating their importance to the food and cosmetic industries. Chemical synthesis and drug design rely on heterocyclic compounds, which display diverse structures such as pyrroles, furans, and pyridines with value levels of 4. Steroids are assigned a value level of 5 due to their profound biological activities. Complex hydrocarbons, such as amino acids and complex functionalized hydrocarbons, are also highly valued. Amino acids receive the highest level of value because they are the building blocks of proteins. In food science and industry, modified carbohydrates, such as sugar alcohols and glycosides, are rated at a value level of 4. Carotenoids and hormones, which are rated at the highest level of 5, are critical for their role as pigments and regulators of physiological processes. Lastly, other byproducts such as biochar, syngas, etc. were included in the class labelled "other byproducts".

Table 1. The classification of organic compounds and value level assigned according to the value pyramid of bioproducts.

	Categories and subcategories	Value Levels		Categories and subcategories	Value Levels
1	Basic Hydrocarbons		4	Fine Chemicals	
1.1	Aromatic Hydrocarbons		4.1	Active Pharmaceutical Ingredients (APIs)	
1.1.1	Monocyclic Aromatic Hydrocarbons	1	4.1.1	Antibiotics, Cardiovascular Drugs, etc.	5
1.1.2	Polycyclic Aromatic Hydrocarbons (PAHs)	2	4.2	Flavors and Fragrances	
1.2	Aliphatic Hydrocarbons		4.2.1	Synthetic Flavors and Essential Oils	4
1.2.1	Saturated Hydrocarbons (Alkanes)		4.3	Heterocyclic Compounds	
1.2.1.1	Straight-Chain Alkanes (n-Alkanes)	1	4.3.1	Pyrroles and Pyrrolidines	4
1.2.1.2	Branched-Chain Alkanes (Isoalkanes)	1	4.3.2	Furans and Thiophenes	4
1.2.2	Unsaturated Hydrocarbons		4.3.3	Pyridines and Pyrimidines	4
1.2.2.1	Alkenes (Olefins)	2	4.3.4	Quinolines and Isoquinolines	4
1.2.2.2	Alkynes	2	4.3.5	Triazines	4
1.2.3	Cycloalkanes, Cycloalkenes and Cycloalkynes	2	4.3.6	Purines and Pyrazines	4
2	Functionalized Hydrocarbons		4.3.7	Indoles	4
2.1	Halogenated Hydrocarbons		4.3.8	Diazabicyclo Nonanones	4
2.1.1	Alkyl Halides and Aryl Halides	2	4.3.9	Azetidines	4
2.2	Oxygen-Containing Compounds		4.3.10	Piperidines	4
2.2.1	Alcohols, Ethers, Carboxylic Acids, Acid Halides	2	4.3.11	Imidazoles	4
2.2.2	Aldehydes, Ketones, Esters, Phenols, Epoxide, Hydrazides, Anhydrides	3	4.3.12	Oxazolidines	4
2.2.3	Fatty Acids, Fatty Alcohols, Fatty Esters	4	4.3.13	Other	4
2.3	Nitrogen-Containing Compounds		4.4	Steroids	
2.3.1	Amines, Amides	2	4.4.1	Bile Acids	5
2.3.2	Nitro Compounds, Nitriles, Thiocyanates, Oximes	3	4.4.2	Unsaturated Steroids	5
2.3.3	Fatty Amides	4	4.4.3	Steroid Esters	5
2.4	Sulfur-Containing Compounds		4.4.4	Sterols	5
2.4.1	Thiols, Sulfides, Organosulfur Compound	2	4.4.5	Terpenoids	5
2.5	Silicon-Containing Compounds		4.5	Complex Hydrocarbones	
2.5.1	Silanes	2	4.5.1	Amino Acids	5
2.5.2	Silicones	3	4.5.2	Complex Functionalized Hydrocarbons	4
2.5	Carbohydrates		4.6	Modified Carbohydrates	
2.5.1	Monosaccharides, Oligosaccharides, Polysaccharides	3	4.6.1	Sugar Alcohols, Amhydro Sugars, glycosides	4
2.6	Functionalized aromatic hydrocarbons	3	4.7	Carotenoids and Hormones	5
3	High Molecular Weight Compounds		5	Other byproducts	1
3.1	Waxes and Paraffins	2			
3.2	Plastic Monomers	2			
3.3	Heavy Oil	2			

References

Barahmand, Z., 2024a. Strategic benchmarking and classification of organic chemicals. https://doi.org/10.23642/usn.25773765.v1

Barahmand, Z., 2024b. A comprehensive inventory of 1000 organic compounds reported in bio-oil: classification and economic valuation. https://doi.org/10.23642/usn.25776879