Analytical methods for molecular analysis of biomass and paper. Are we there yet?

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AIM OF RESEARCH

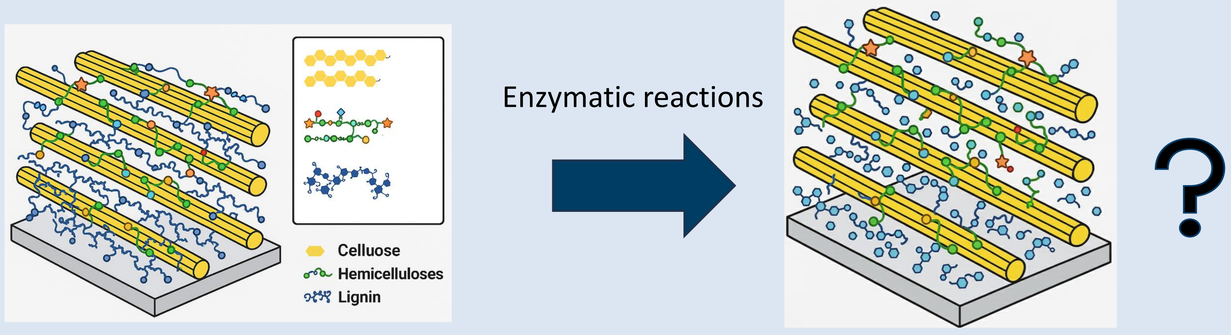
Objective:

Towards a complete chemical profile using ion chromatography (IC), linkage analysis (GC-MS) and FITDOG/OLIMP (UPLC-MS).

Why is biomass and paper molecular analysis so challenging?

- Complex composition and complex matrix
- No single universal method
- Requires a multimodal analytical strategy

CONCEPT

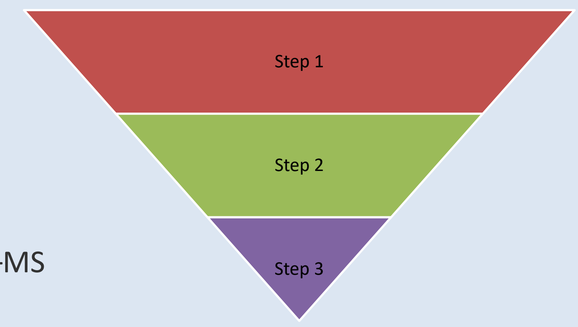


Sample of biomass

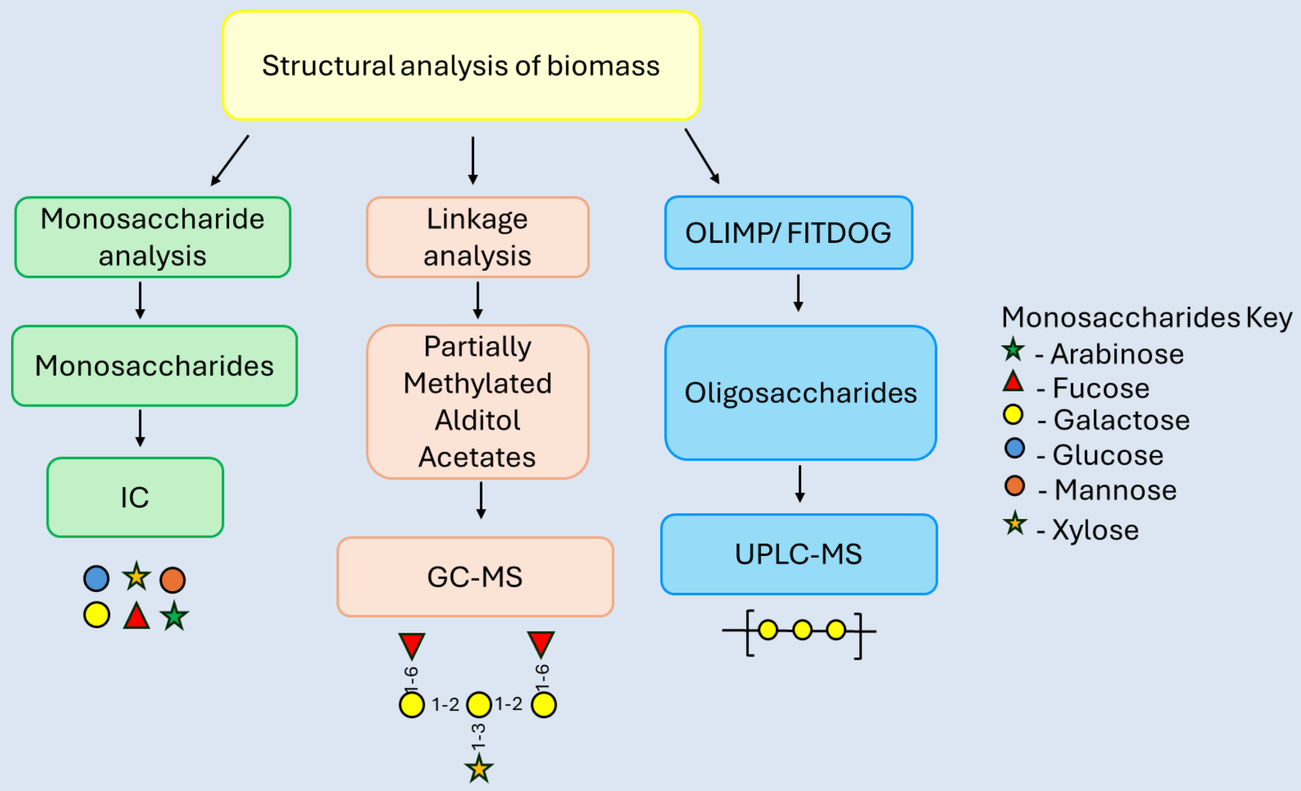
Side chains cuttings and modifications

Analytical strategy: from global to specific

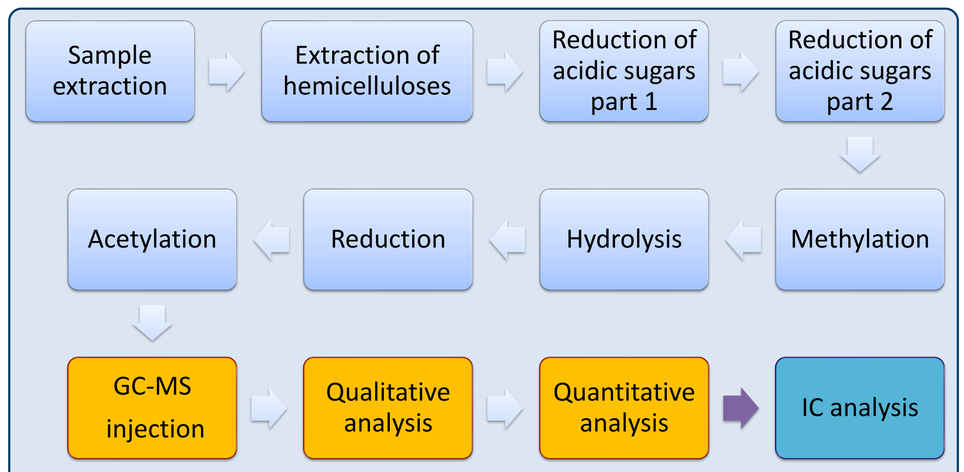
- Step 1: Global composition → Ion Chromatography (IC)
- Step 2: Structural linkages → Linkage analysis
- Step 3: Sequence & branching → OLIMP/FITDOG with UPLC–MS



ANALYTICAL METHODS



RESULTS



Scheme of linkage analysis

Table 1. Example of results of linkage analysis

Monosaccharide	Linkage residue	Biomass 1	Biomass 2
Mannose	4-mannose	✓	
	4,6-mannose	✓	
Galactose	T-galactose	✓	✓
Glucose	2-glucose	✓	✓
	4-glucose	✓	
	6-glucose		✓
	2,4-glucose	✓	
	4,6-glucose	✓	✓
	2,3,4-glucose	✓	✓
	2,4,6-glucose	✓	✓
Arabinose	2,3-arabinose	✓	✓
	2,4-arabinose	✓	
	2,3,4-arabinose	✓	✓
	2,3,5-arabinofuranose		✓
Xylose	2,3,4-xylose	✓	✓

Comparison of two UPLC methods

OLIMP	FITDOG
Enzymatic digestion specific digestion of **xyloglucanas**), xylans (xylanase) or pectins (endoPG)	**Non-enzymatic digestion** → non-specific digestion of all polysaccharides Fenton's reagent
High resolution TOF-MS	**High resolution TOF-MS**
Annotation of mass peaks with XyG calculator	Annotation of mass peaks with Python script
Characterization of specific polysaccharides like xyloglucans with regard to structure and monosac-charide composition	Relative and absolute quantitation of several types of polysaccharides

CONCLUSIONS

- The goal of establishing a complete chemical fingerprint of biomass and paper is underway.
- A combination of tools, including ion chromatography, linkage analysis, and OLIMP/FITDOG with UPLC–MS, provides a solid foundation for comprehensive characterization.
- Continued development of analytical methods for UPLC–MS remains essential to achieve greater resolution and reliability.
- While significant progress has been made, the full picture is not yet complete, and further efforts are needed to connect all analytical insights.