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Biomass for Swiss Energy Future
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Energy funding programme
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Commission for Technology and Innovation CTI

High-Resolution Mass Spectrometry for Biomass

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Biomass

Biomass has a high potential for energy production and can be used for the direct heat production or can be converted into biogas, biomethane, bioliquid fuels and high value chemicals.

However the high chemical and structural complexity and diversity of biomass makes the conversion quite challenging. In order to understand these processes and also develop new processes, the demand for high quality and reliable analytics is quite high.

Fig. 1: Conversion of biomass to biofuel and high value chemicals

Analysis of Lignin Depolymerization

The power of these analytical technics is shown by the analysis of hydrothermal treated lignin. The total ion chromatogram (TIC) from the sample shows the complexity of the sample. The whole mass range from 50 to 1700 m/z was measured over the separation through the column of the liquid chromatography system.

The peaks of the TIC can be separated by the software using extraction of the peaks with the same detected masses. These peaks with a specific mass belong to a compound which elutes at given time.

The High-Resolution of the MS allows to match the exact mass and isotopic pattern of a peak to a specific and unique sum formula.

Example:

RT (min)	m/z	detected ion	Sum formula	Diff (ppm)	compound
6.298	231.158961	$(M+H)^+$	$C_{12}H_{22}O_4$	0.54	1,8-diacetyloctane
	253.141028	$(M+Na)^+$		0.01	

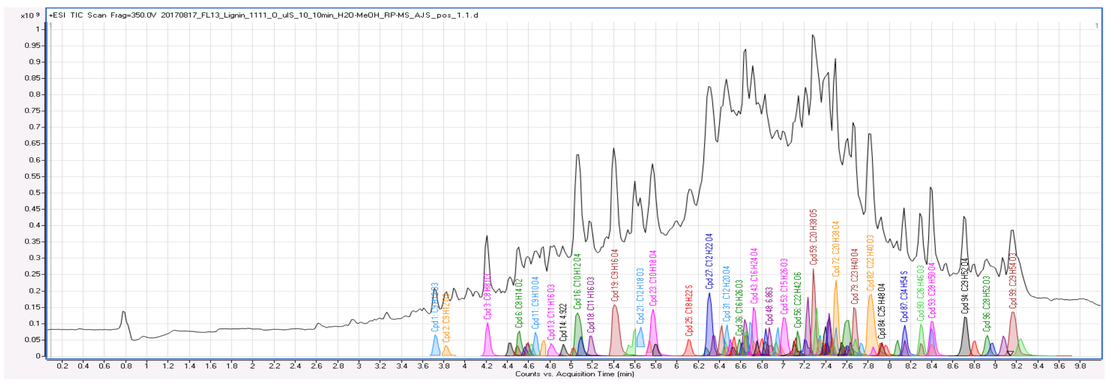

Fig. 2: TIC with extracted compounds and corresponding sum formulas

Conclusion

Elucidation of complex organic samples from biomass yielding molecular structure information and relative composition.

High-Resolution Mass Spectrometry

In our lab we use High-Resolution Mass Spectrometry (HRMS) as an experimental approach to this challenging task. With HRMS it is possible to determine the accurate mass together with the different isotopes. Therefore it is possible to identify the correct molecular formula from unknown substances.

The coupling of HRMS together with liquid chromatography and gas chromatography makes it a powerful tool for the analysis of complex mixtures, like mixtures produces by high temperature liquefaction (HTL).

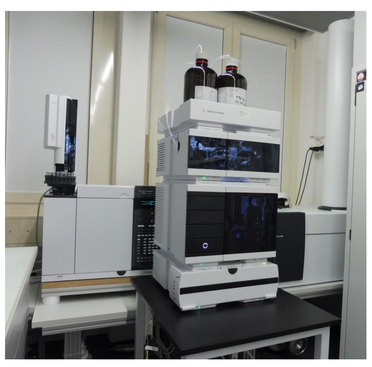

Fig. 3: Analytical Equipment

Q-Exactive + LC (Thermo)
Resolution > 70 000
- ESI
- APCI

Q-TOF + LC / GC (Agilent)
Resolution > 30 000
- ESI
- APCI (GC-APCI)
- APPI

ESI: Electrospray ionization
APCI: Atmospheric pressure chemical ionization
APPI: Atmospheric pressure photo ionization

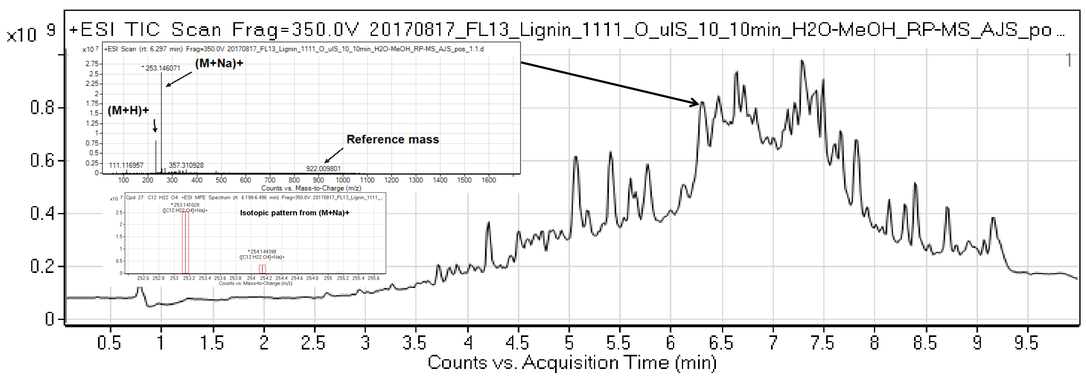

Fig. 4: Total Ion Chromatogram from hydrothermal treated lignin

Afterwards the collected data (sum formula and retention time, MS/MS spectra) can be compared with the personal and NIST 14 library to identify the structure of the compound.

If the compound cannot be identified, possible compounds with the same sum formula can be order or synthesized to measure them and compare the spectra with the unknown compound.

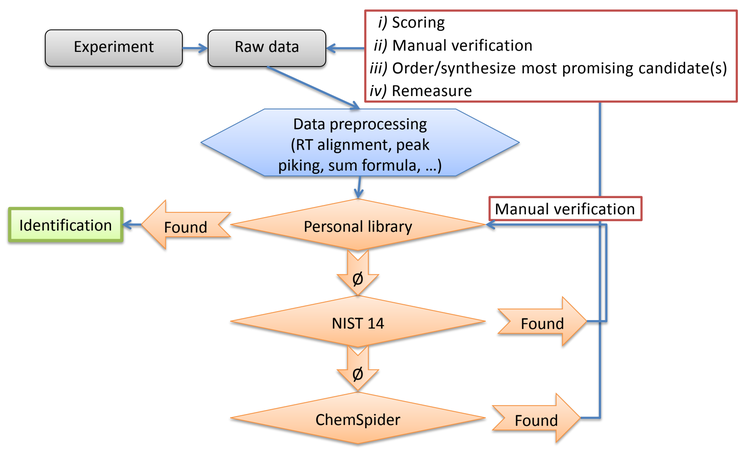

Fig. 5: Identification strategy

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FNSNF Swiss National Science Foundation