Characterization of Hydrodeoxygenated Bio-oils by APPI/ESI FT-ICR Mass Spectrometry

Timo Kekäläinen[1] // Idoia Hita Del Olmo[2,3] // Tomás Cordero Lanzac[2] // Gift Ogechukwu Okafor[1] // Pedro Castaño[2,3] // Janne Jänis[1*]

[1]University of Eastern Finland, Department of Chemistry, Joensuu, Finland. [2]University of the Basque Country UPV/EHU, Department of Chemical Engineering, Bilbao, Spain. [3]King Abdullah University of Science and Technology (KAUST), Multiscale Reaction Engineering, KAUST Catalysis Center, Thuwal, Saudi Arabia

**Correspondence to: janne.janis@uef.fi*

Introduction

- Fast pyrolysis is a promising method for thermo-chemical conversion of biomass into liquid (bio-oil) and solid (charcoal) products.
- There is a need to refine bio-oils further in order to improve their combustion properties.
- The effect of three different hydrodeoxygenation (HDO) catalysts towards the chemical composition of raw poplar pyrolysis oil was studied.

Materials and methods

- Poplar pyrolysis oil (sample S1) produced at 450 °C using a lab-scale spouted bed reactor.
- Raw pyrolysis oil hydrotreating by using 1) PtPd/C, 2) NiW/C and 3) CoMo/C catalysts mixed with a HZSM-5 zeolite catalyst with a Si/Al support (corresponding samples: S2, S3 and S4, respectively).
- 12-T (+)APPI/(–)ESI FT-ICR MS (Bruker SolariX XR).
- Data interpretation with PetroOrg 16.0 software.

Results

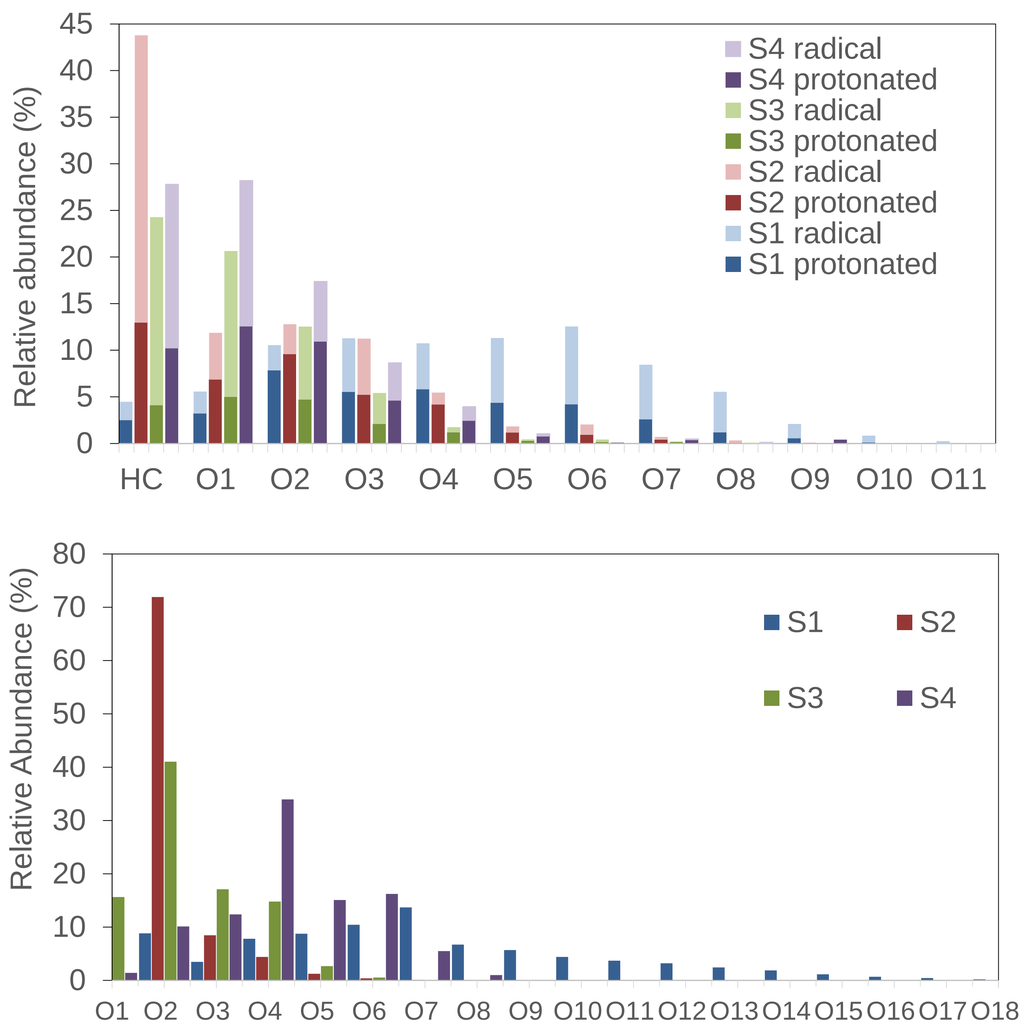

Figure 1. Heteroatom class (HC and O_y) distributions by APPI (upper) and ESI (lower) FT-ICR MS. Minor N_xO_y and S_zO_y classes are omitted.

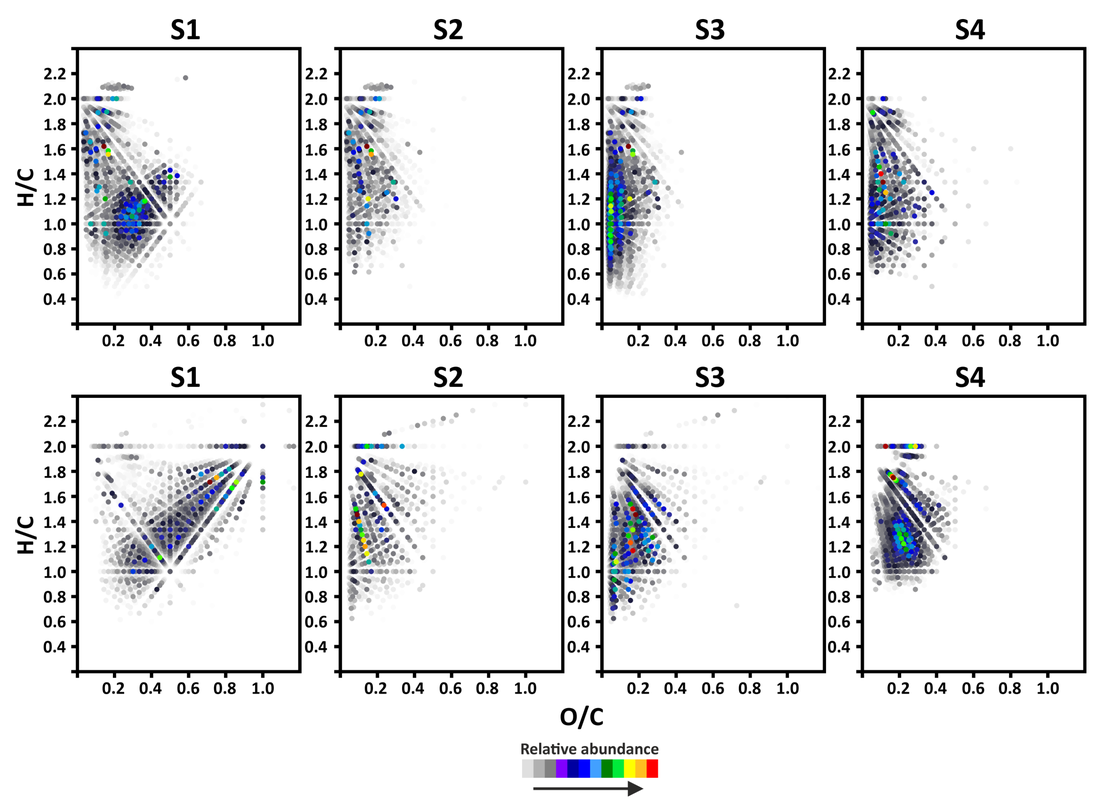

Figure 2. Colour-mapped van Krevelen diagrams for O_y compounds based on APPI (upper) and ESI (lower) FT-ICR MS data.

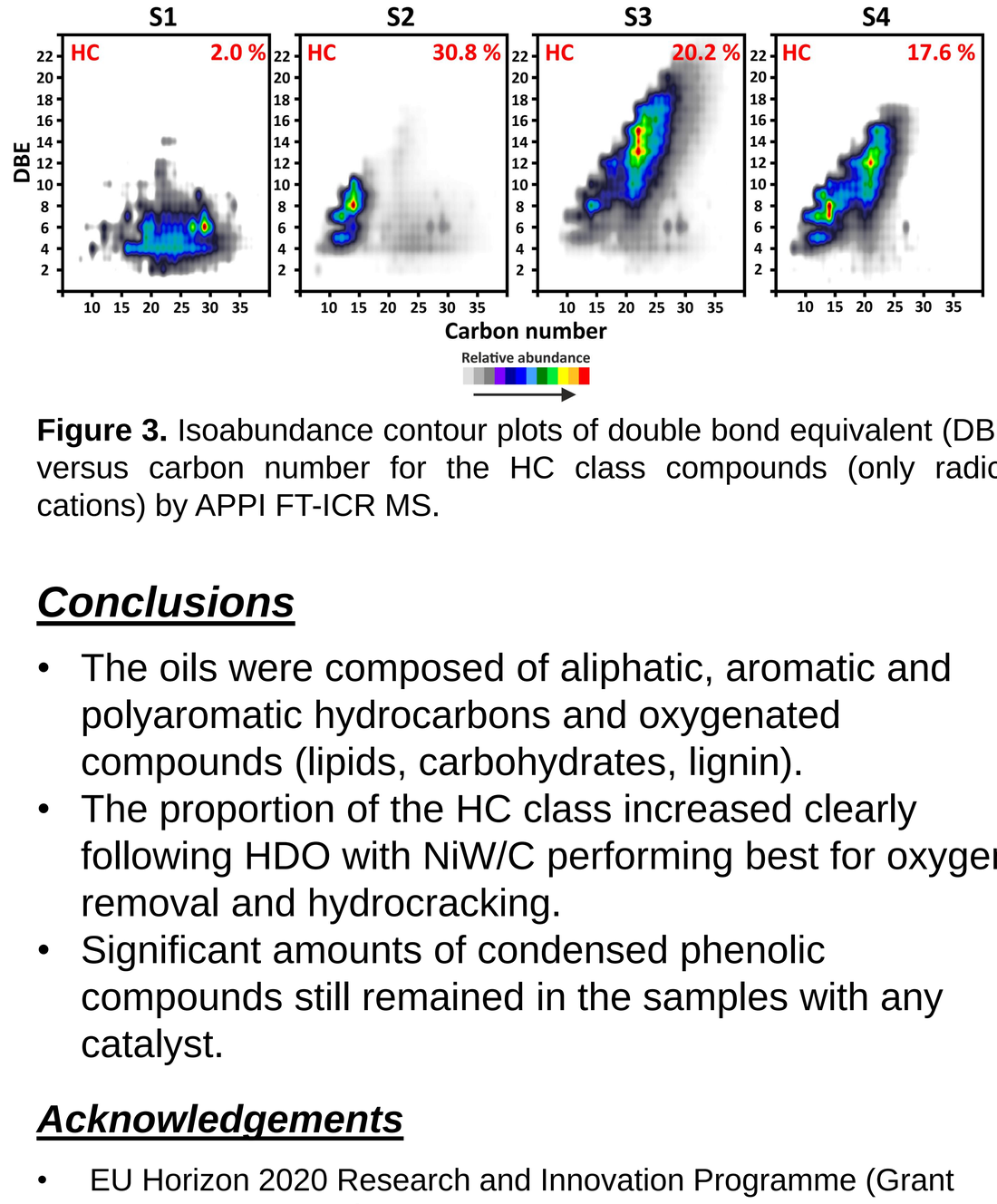

Figure 3. Isoabundance contour plots of double bond equivalent (DBE) versus carbon number for the HC class compounds (only radical cations) by APPI FT-ICR MS.

Conclusions

- The oils were composed of aliphatic, aromatic and polyaromatic hydrocarbons and oxygenated compounds (lipids, carbohydrates, lignin).
- The proportion of the HC class increased clearly following HDO with NiW/C performing best for oxygen removal and hydrocracking.
- Significant amounts of condensed phenolic compounds still remained in the samples with any catalyst.

Acknowledgements

- EU Horizon 2020 Research and Innovation Programme (Grant Agreement 731077).
- Academy of Finland/Strategic Research Council (Grant 293380).
- Biocenter Finland and Biocenter Kuopio.
- European Regional Development Fund (Grant A70135).