

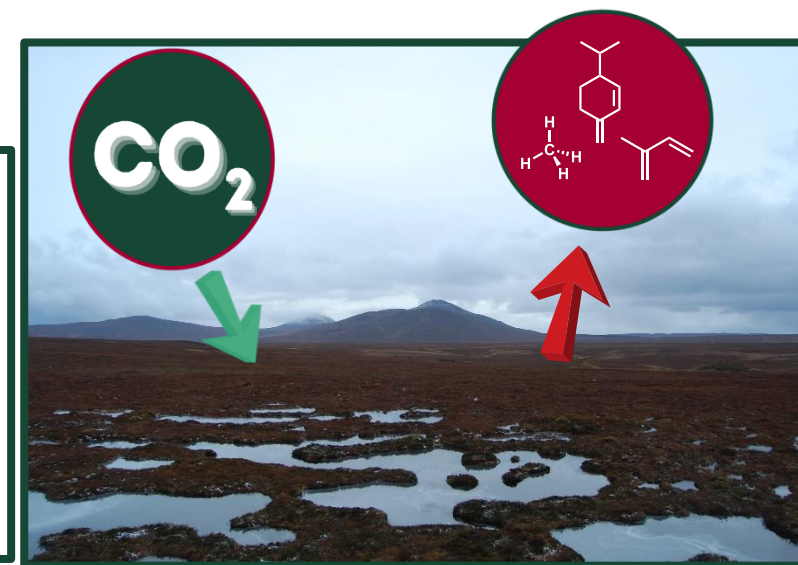
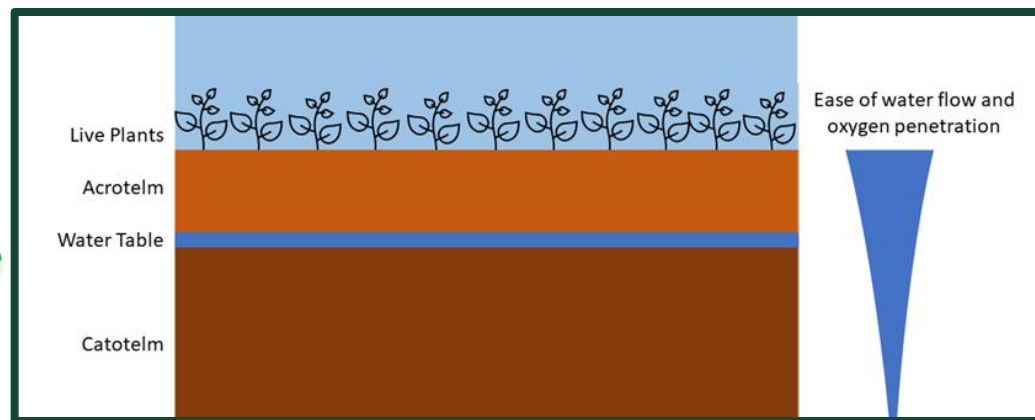
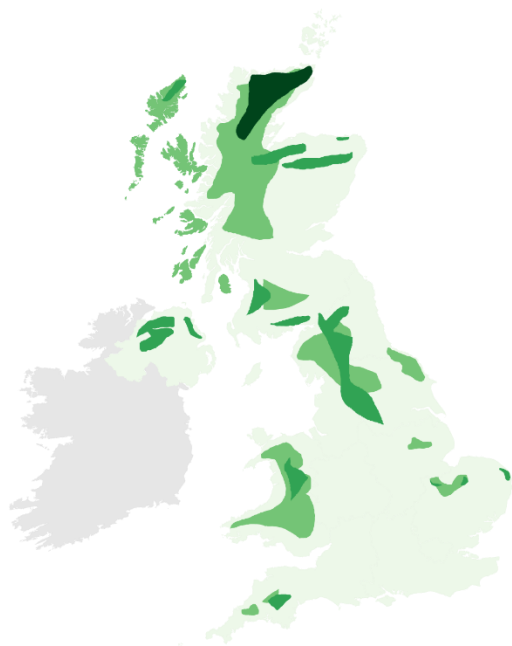
Analytical Techniques for Structural Elucidation in Peatlands and Peated Whisky

Sam Fergusson (@fergusson_sam)

Supervisor: Dr. Nicholle Bell (@nbellgroup)

Peatlands as a Carbon Store

- Peatlands are a significant global carbon store
- They also serve as a source of methane and biogenic VOCs
- Water^{table} greatest factor in balance between storage and emission



- Peatlands historically drained and extracted for various reasons
- Drainage tips the scales of CO₂ and methane emission
- Other effects include peat erosion and surface subsidence
- Peatlands can be restored through the blocking of drains
- Impact of drainage/restoration on VOC emission poorly understood



Günther, A.; Barthelmes, A.; Huth, V.; Joosten, H.; Jurasinski, G.; Koebisch, F.; Couwenberg, J. Prompt Rewetting of Drained Peatlands Reduces Climate Warming despite Methane Emissions. *Nat. Commun.* **2020**, *11*, 1–5. <https://doi.org/10.1038/s41467-020-15499-z>.

<https://www.theguardian.com/world/2022/dec/12/like-an-oilwell-in-your-back-yard-irish-turn-to-cutting-peat-to-save-on-energy-bills>

Aerial image produced using digimaps (digimaps.edina.ac.uk)

How Peat is Used in Whisky

- Whisky is a globally recognised beverage
- Wide range of factors influence the aromas and flavours
- Peat fires impart smoky flavours upon peated whisky

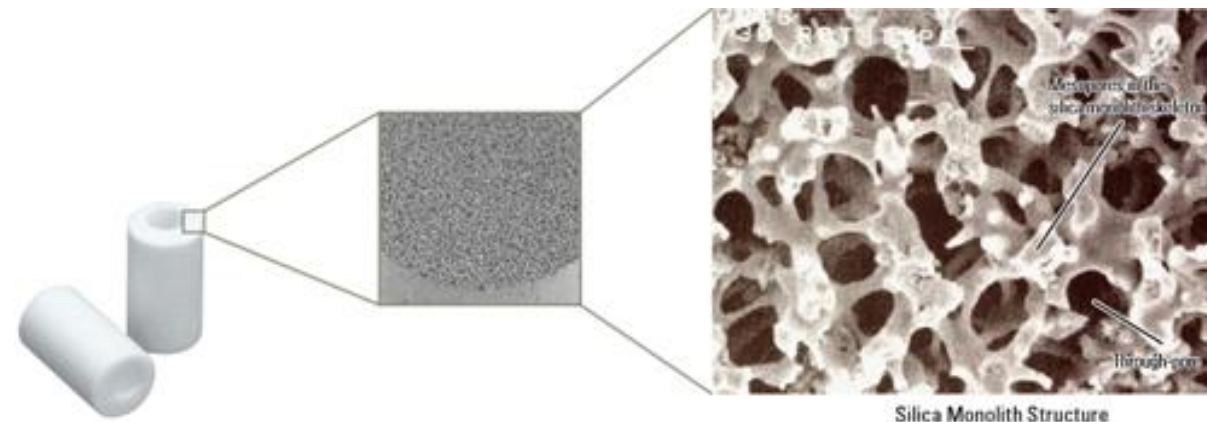
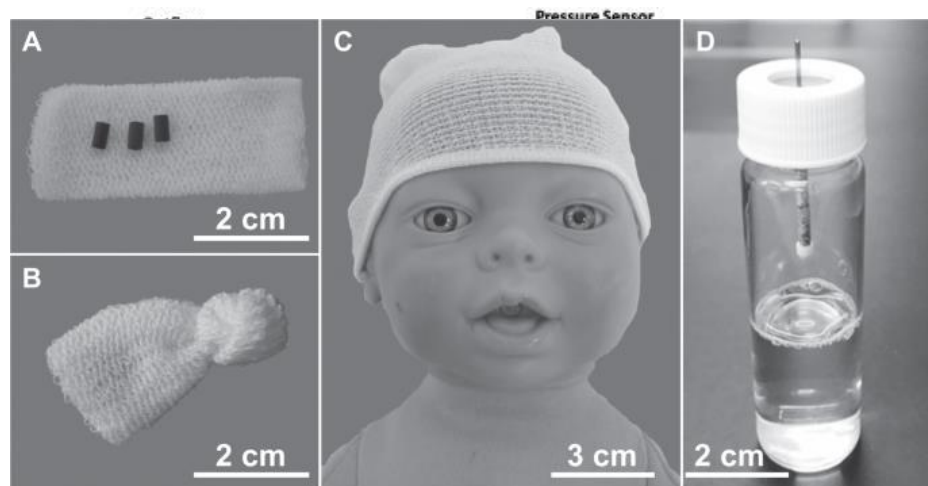


Aim: Investigate the effect of a variety of factors on the volatile organic compounds found in peatlands and peated whisky and how this relates to solid/liquid components.

Objectives:

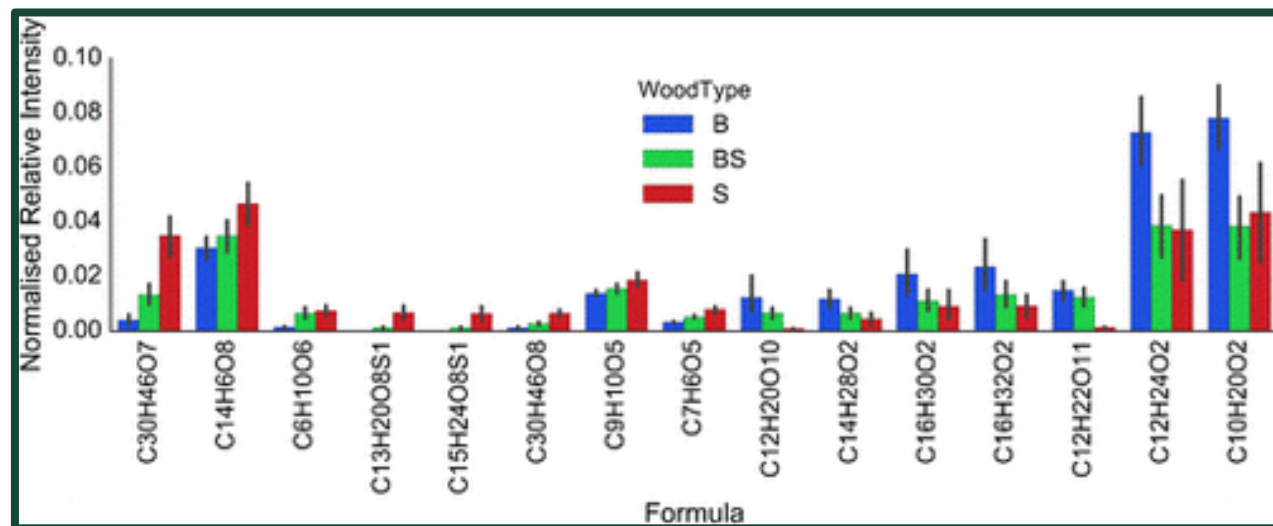
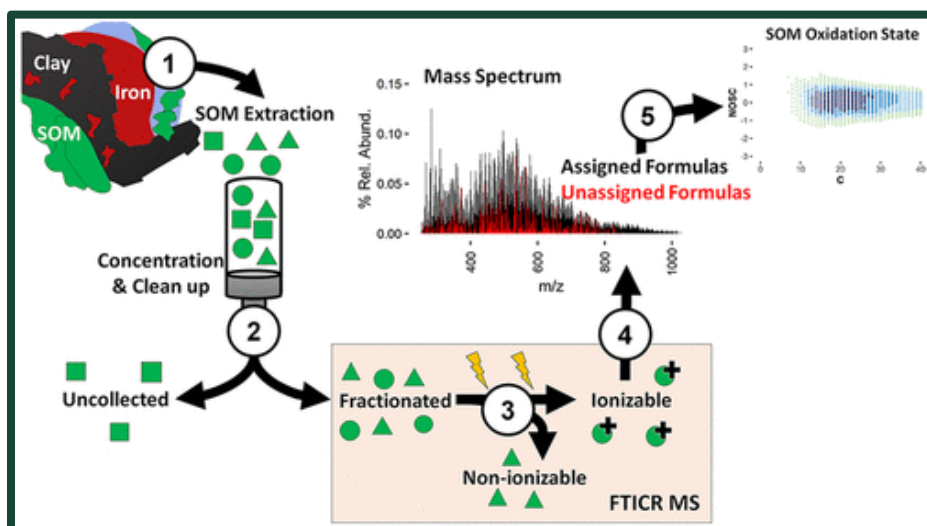
1. To develop a fingerprint of volatile organic compounds emitted by peatlands of varying health and establish links to the solid components of peatlands.
2. To identify how peat fires and maturation influences the aroma and flavour of peated whisky

- Dynamic Chamber Method
- Headspace collection of VOCs possible in whisky
- MonoTraps commonly used in collection of VOCs (MMSE)
- Make use of thermal desorption for introduction to analytical instruments (GCxGC MS)

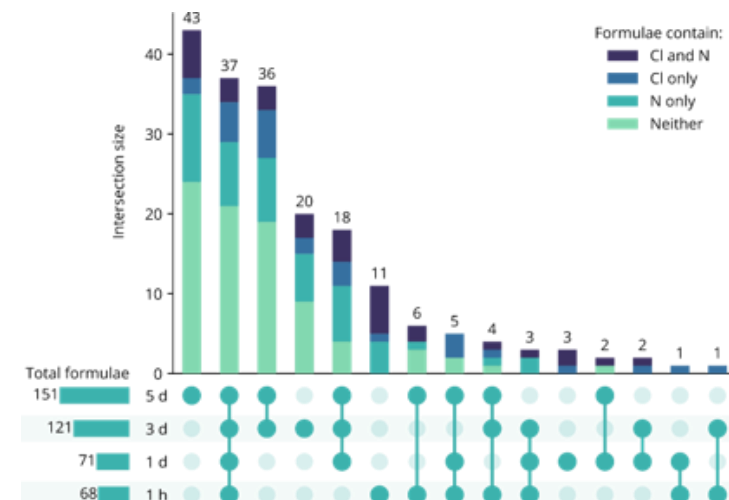
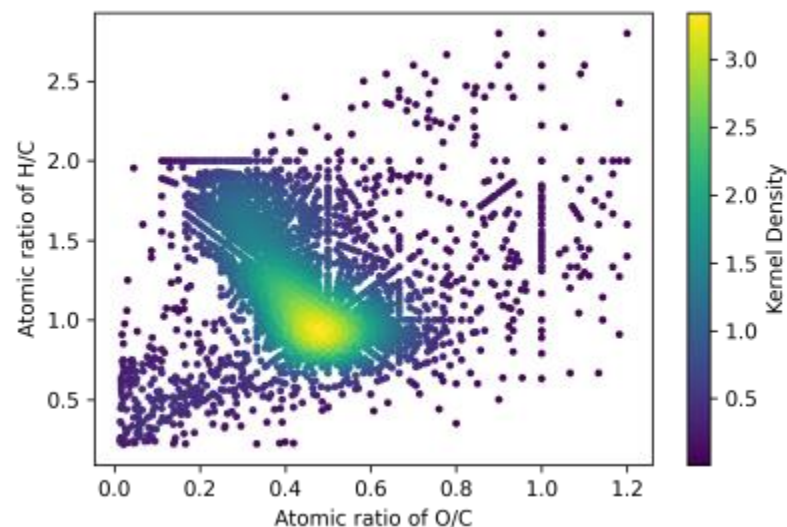
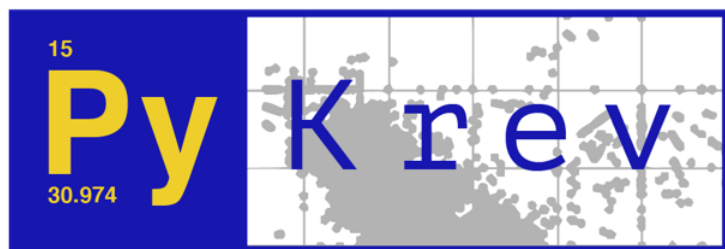


FT-ICR MS on Complex Mixtures

- Peat and whisky are two highly complex mixtures
- Thus, highly sensitive and accurate analysis is required to separate these mixtures and facilitate formula assignment
- FT-ICR MS shown to achieve this in soil organic matter and whisky



- Created by Ezra Kitson from the Bell Group
- Offers a suite of analytical and visualisation tools of FT MS data
- Requires molecular formulae, monoisotopic peak intensities and m/z
- Facilitates intersection analysis, chemical diversity calculations, PCA etc.



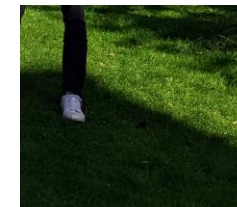
- Identify how drainage and restoration of peatlands affects their VOC fingerprint
- Develop explanations that link VOC emission to solid components of peat
- Measure how VOCs in whisky change over a period of maturation
- Identify the key compounds produced from peat fires to impart smoky flavours on peated whisky

Acknowledgements



THE UNIVERSITY of EDINBURGH
School of Chemistry

- Dr. Nicholle Bell
- Prof. Mathew Heal
- Prof. Dušan Uhrin
- Ezra Kitson
- Scotch Whisky Research Institute
- Centre for Ecology and Hydrology



Thanks for Listening

