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IBU

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Geo-ecosystems in Transition on the Tibetan Plateau (TransTiP)

Thermodynamic Indicators Decipher the Molecular Composition of Organic Matter in Phase Transition

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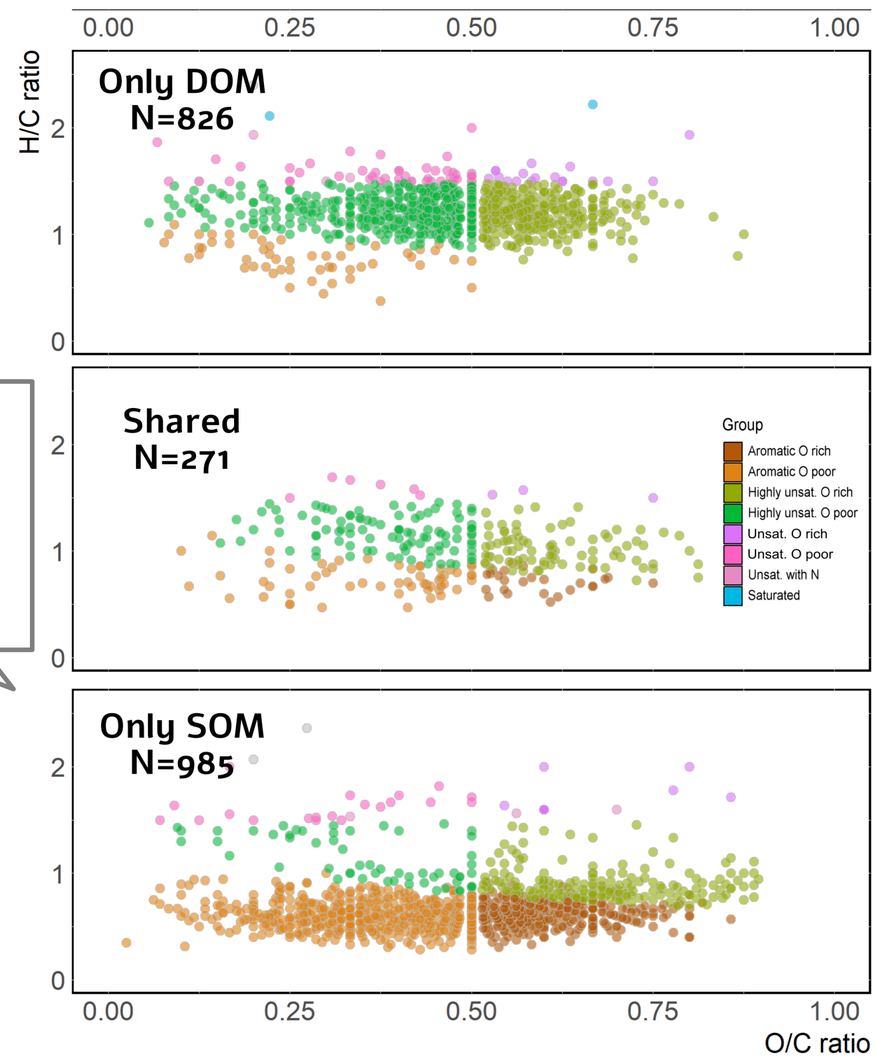
1 Towards Organic Matter Molecular Fingerprints

- **Fingerprints** are essential for identifying and characterizing organic matter. Fingerprints provide unique patterns crucial for understanding environmental impacts and behaviour. They **promise to be a tool to screen ecosystem states**
- The phase transition from soil organic matter (SOM) to dissolved organic matter (DOM) is integral to numerous biogeochemical processes that govern ecosystem functioning, nutrient cycling, soil fertility, and soil health.

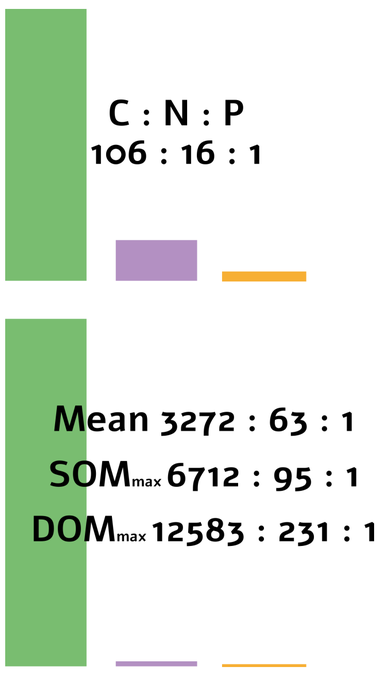
ID information is hidden in several thousand molecular formulae



- High Alpine sample set with n= 18 soil leaching extracts and n= 16 samples of adjacent stream DOM analysed with FT-ICR-MS show distinct differences for catchment endmembers (partly published [1])
- SOM and DOM share only a minority of molecular formulae → high diversity
- **Fingerprint points-of-information (POI)** are crucial and potentially well hidden, **metrics are needed** [2]

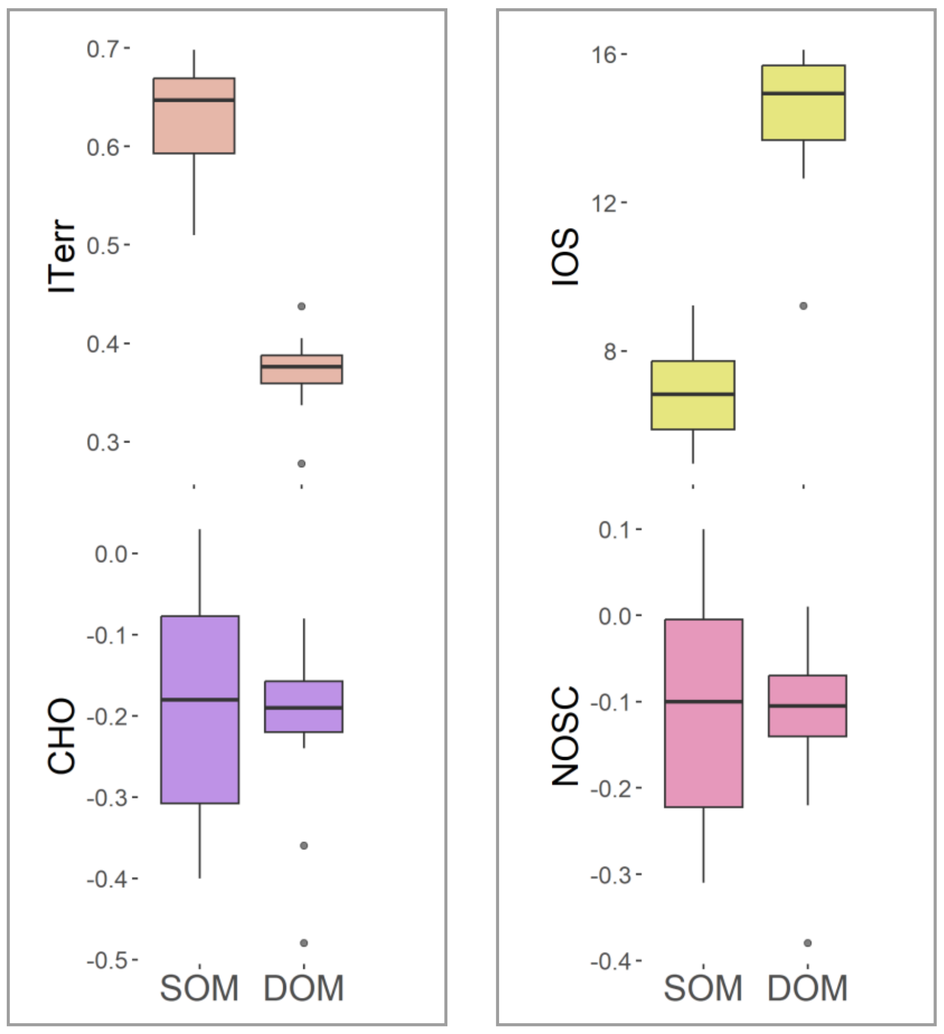
2 Problem Statement: Borrowed Metrics for Fingerprints?

- Metrics like the Redfield ratio of carbon to nitrogen to phosphorous [3]
- Determined in marine phytoplankton and confirmed by many studies beyond [4]
- Alike, many indicators and metrics used in soil science research are based on insights from other scientific fields („**Borrower attitudes**“)
- We found massive deviations from the Redfield ratio in our own dataset, even in lake and glacial DOM
- Problem: „Borrowed“ indicators can work but are they truly functional beyond empiricism? ***False positive conclusions are possible, hence trustworthy metrics are needed***



3 Multiple metrics Approach Fingerprinting

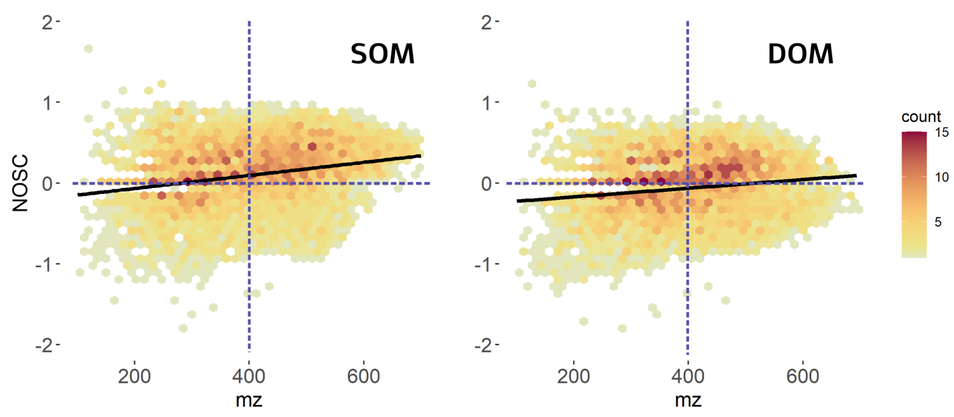
Multiple metrics join: To determine functional fingerprint POI, several metrics are needed. **Molecular differences** may be manifold and can be **scale invariant**. Molecular diversity can be found between ecosystems and also within a catchment or in a pot experiment



The terrestrial index (ITerr—[5]) distincts empirically selected riverine terrigenous formulae, while the island of stability (IOS—[6]) screens for formulae identified as refractory DOM in the deep sea. CHO determines overall compositional changes and nominal oxidation state of carbon (NOSC) tracks pot. reactivity of OM increasing with higher O/C ratio [7].

4 Bioenergetic Metrics Tell More

SOM has both, higher molecular mass and higher NOSC, with a lower overall energy content. DOM has a higher energy content visible by lower NOSC, but the availability of energy stored in DOM is lower than in SOM [8]. This can explain the higher stability of DOM proposed by IOS. **NOSC is a useful additional metric helping with understanding „borrowed“ empiricism.**



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