

Sorption potential of Nitramines to soils

- Methodical challenges using LC-MS/MS

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Background

Based on the **precautionary principle** the impact of possible carcinogenic nitramines¹ must be assessed. Final **exposure levels** will depend on the sorption potential of nitramines to **soils**.

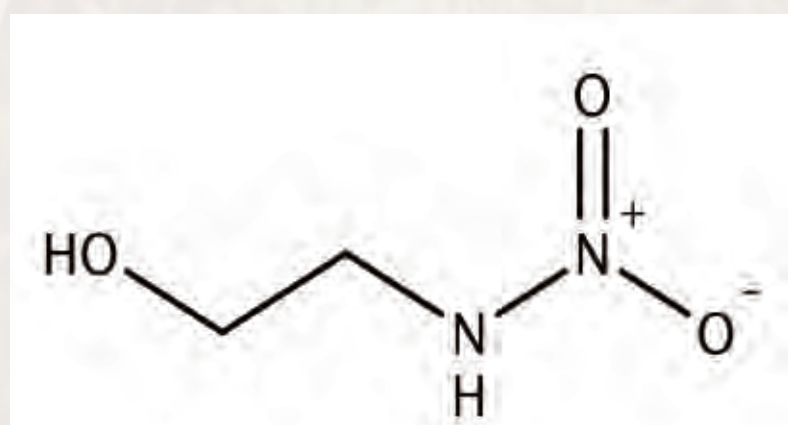
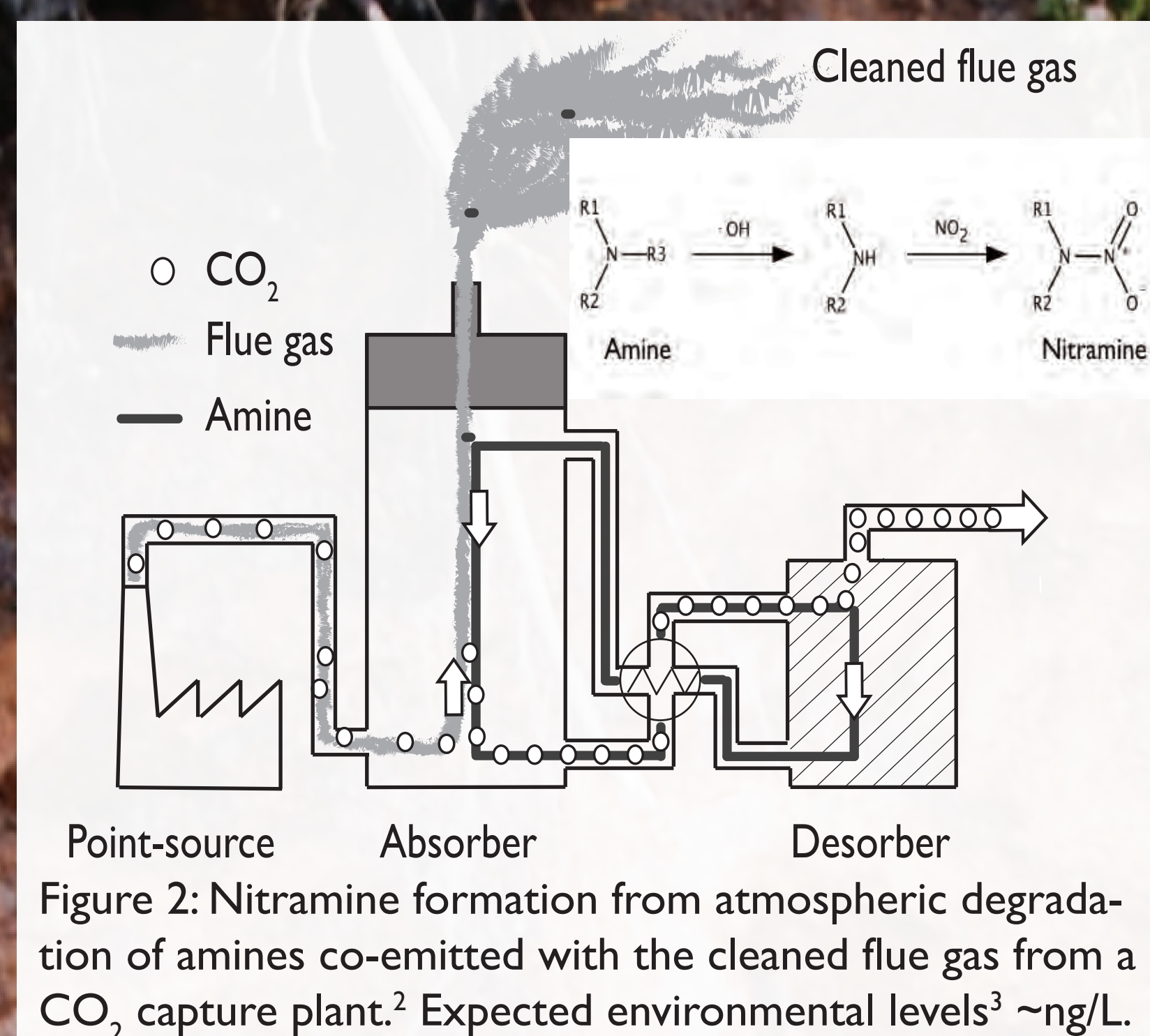


Figure 1: Molecular structure of Monoethanolamine (MEA-nitramine). Slightly acidic (pKa 6.24) (Scifinder) Polar (Kow -0.5)¹ No photolysis and hydrolysis²



Aim

Focusing on the MEA-nitramine (Figure 1):

- 1. Sorption potential to soils**
Up-concentration is the likely result of soil sorption. Extent of sorption is governed by soil descriptors.
- 2. Methodical challenges (LC-MS/MS)**
Dissolved organic matter from soil influences quantification through either ion enhancement/ion suppression or by binding to the MEA-nitramine.

Results and Discussion

1. Sorption to soils

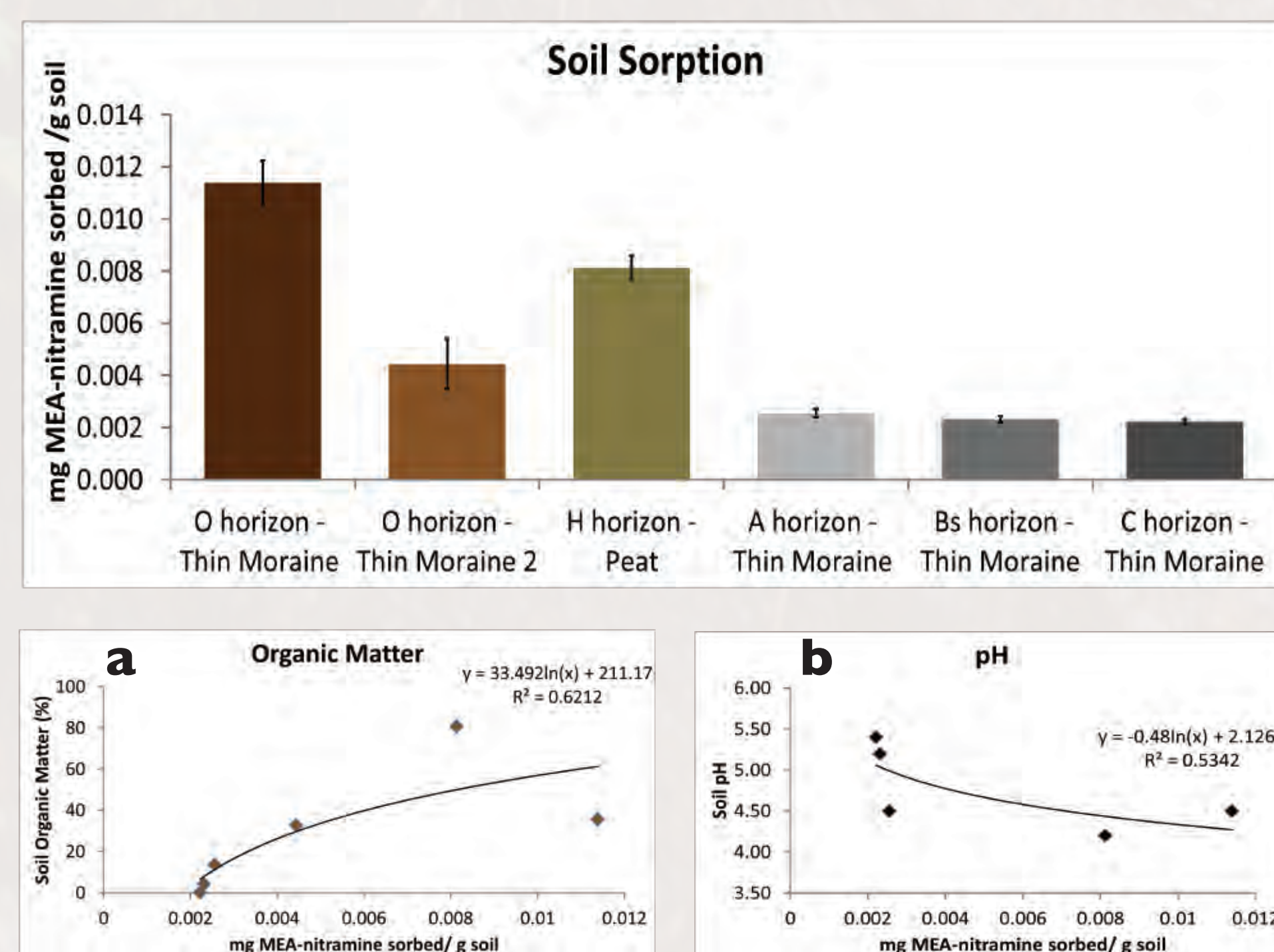


Figure 3: The magnitude of sorption is low. Higher sorption for MEA-nitramine is seen to organic rich soils (brown: H and O horizons) than to mineral soils (grey: A, Bs, and C horizons)⁴.

The majority of MEA-nitramine remain in the aqueous phase (soil-water).

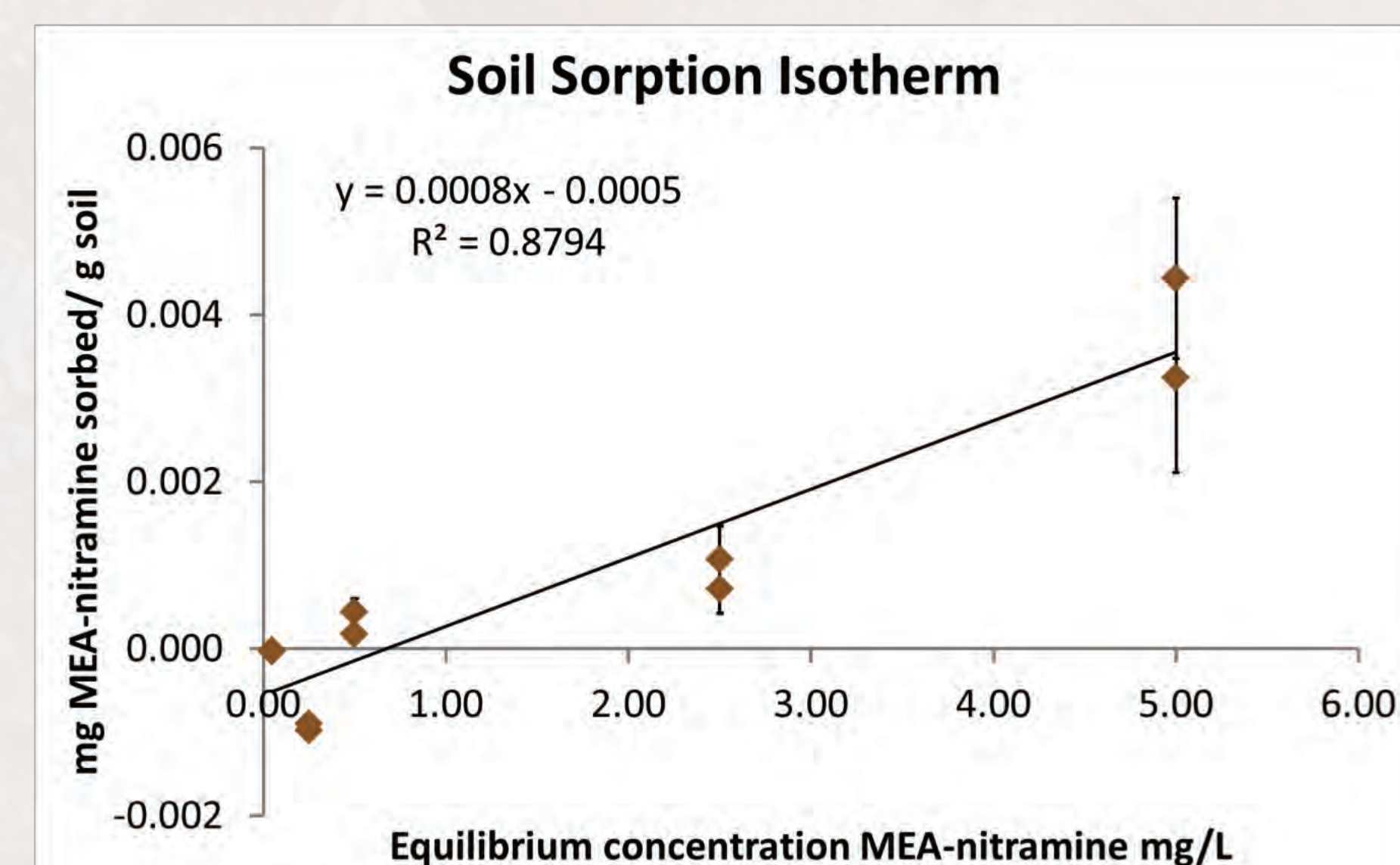


Figure 5: An organic soil (O-2) exposed to different concentrations of MEA-nitramine (0.025 - 5 mg/L, n = 2). The amount of MEA-nitramine sorbed to soil increases linearly with increasing equilibrium concentrations.

2. Effect of dissolved organic matter

MEA-nitramine is detected using LC-MS/MS with ESI in negative mode. External calibration is used for quantification.

With this method it is not possible to distinguish loss of signal caused by ion suppression from binding of MEA-nitramine to dissolved organic.

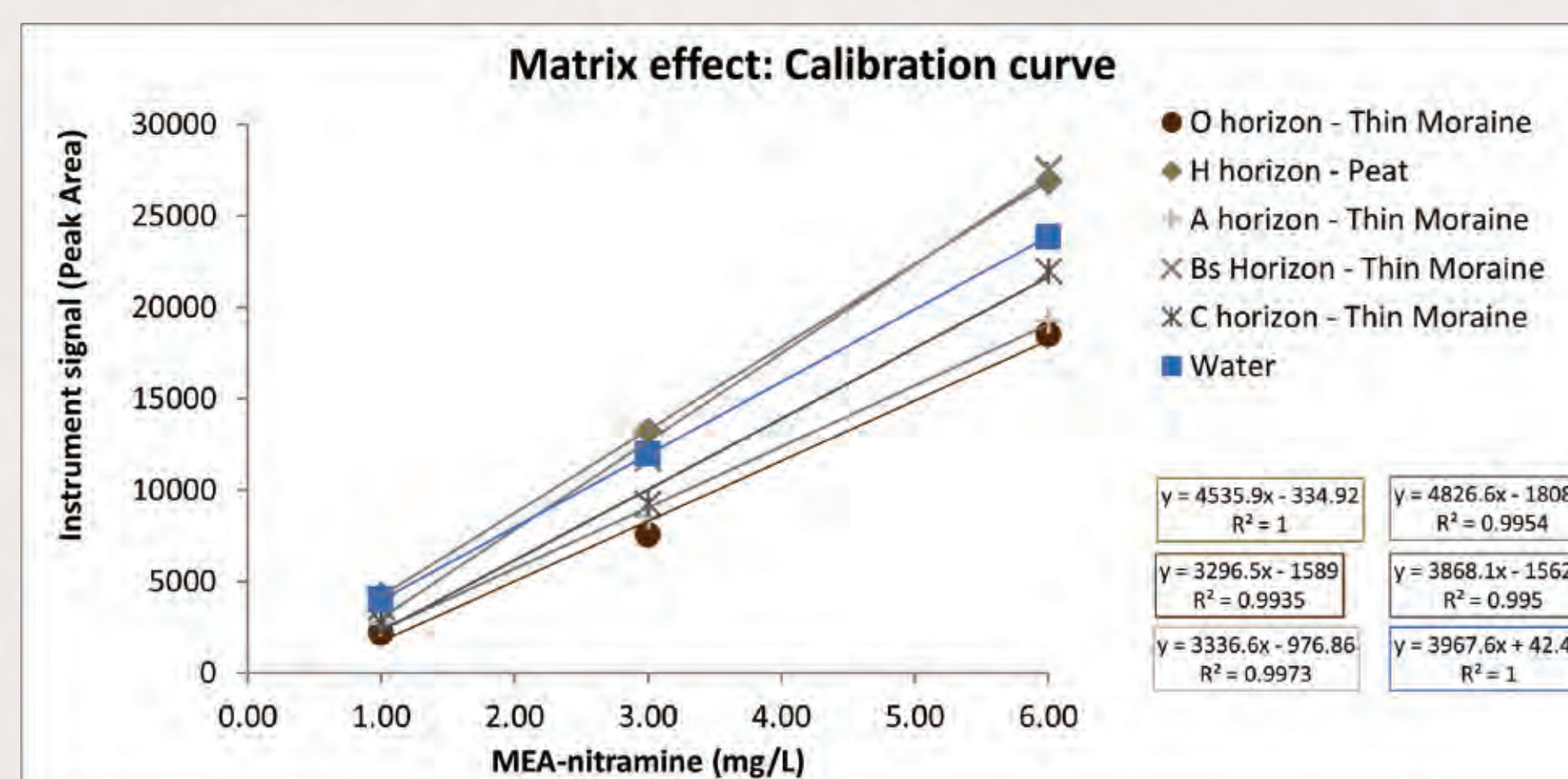


Figure 6: Matrix-matched calibration curves for each individual soil sample (brown/grey) compared with calibration curve from water-matrix (blue)⁴.

The slope values for the soil-matrix curves deviate from the water-matrix curve with -22 to 3 %.

This demonstrates matrix effects in the LC-MS/MS detection of MEA-nitramine. Disregarding this effect will lead to false calculated sorption of MEA-nitramine to soil⁴

Conclusions and Future work

MEA-nitramine is expected to be found mainly in the **aqueous phase** (e.g. lakes, rives, soil-water).

Soils rich in **organic matter** are likely to sorb MEA-nitramine but to a limited extent.

It is crucial to take **matrix effects** into account when estimating nitramine soil-sorption based on LC-MS/MS detection.

Future studies aim to reveal **mechanisms** responsible for MEA-nitramine sorption to soil, and to improve knowledge of organic matter induced **matrix effect** in MS detection.