SafeCREW
ANALYTICAL PROTOCOL #2

ROBUST ANALYTICAL METHODS TO COMPREHENSIVELY CHARACTERISE NATURAL ORGANIC MATTER- AS THE PRECURSOR OF DISINFECTION BY-PRODUCTS IN DRINKING WATER

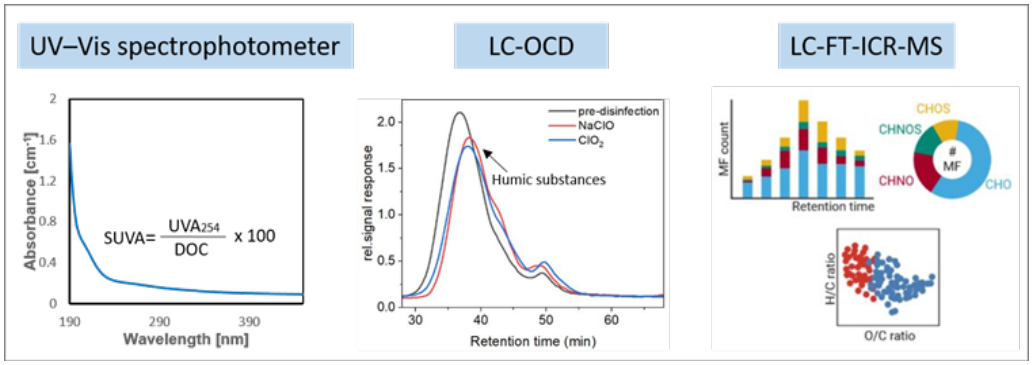

Figure 1 . Overview of analytical methods described in this guideline for characterizing natural organic matter

Introduction

Natural organic matter (NOM) is the major precursor for the formation of disinfection by-products (DBPs) during drinking water treatment and disinfection. The composition, concentration, and reactivity of NOM strongly influence both the efficiency of water treatment processes and the type and amount of DBPs formed. Comprehensive characterisation of NOM is therefore essential to understand its behaviour during treatment, to evaluate NOM removal efficiency, and to identify fractions that contribute most to DBP formation. This guideline focuses on analytical approaches that allow a comprehensive characterisation of NOM as the precursor of DBPs.

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Target Audience

This guideline targets water utilities and researchers in drinking water treatment. Water utilities can apply it to optimise treatment processes for NOM removal and DBP control, while researchers can use it to investigate DBP precursors and formation mechanisms.

Scope and Objectives

This guideline focuses on robust analytical methods for the comprehensive characterisation of NOM in drinking water, with emphasis on UV absorbance, liquid chromatography–organic carbon detection (LC-OCD), and LC coupled to Fourier transform ion cyclotron resonance mass spectrometry (LC-FT-ICR-MS). These complementary techniques enable the systematic assessment of NOM composition and reactivity and allow links to be established between specific NOM characteristics and the formation potential of regulated and emerging DBPs.

The objectives of this guideline are to support water utilities in optimising treatment processes for effective NOM removal and DBP control, and to support researchers in identifying DBP precursors and elucidating DBP formation mechanisms.

Guideline for the characterisation of NOM in drinking water

The chloro- and bromo-analogues of halomethanesulfonic acids, haloacetonitrilesulfonic acids, haloacetamidesulfonic acids, and haloacetaldehydesulfonic acids (20 compounds in total) in drinking water can be reliably characterised using the following procedures.

1) UV absorbance at 254 nm

UV absorbance at 254 nm (UVA_{254}) can be easily measured using a UV–Vis spectrophotometer and provides a rapid indication of aromatic content in NOM. The specific UV absorbance (SUVA) is calculated by dividing the UVA_{254} of a 0.45-µm filtered sample by the dissolved organic carbon concentration and multiplying by 100 to give a value reported as L/mg-m (Potter and Wimsatt, 2012). It is commonly used as an indicator of aromatic, humic-like compounds. Higher SUVA values are generally associated with higher chlorine demand and increased formation of regulated trihalomethanes (THMs) (Hua et al., 2015). UVA_{254} and SUVA therefore provide a simple screening tool for assessing DBP formation potential and treatment performance (USEPA, 2005).

2) LC-OCD analysis

LC-OCD is a powerful technique for fractionating NOM based on molecular size and character. NOM is typically grouped into biopolymers, humic substances, building blocks, low-molecular-weight acids, and neutrals. Humic substances are widely recognised as major precursors of regulated THMs. Consequently, water samples with a high proportion of humic substances often show elevated THM formation potential. LC-OCD provides valuable insight into NOM composition changes during treatment and supports targeted process optimisation.

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3) LC-FT-ICR-MS analysis

Not all DBPs follow trends observed for regulated DBPs. Results from the SafeCREW project indicate that the formation of novel sulfonated DBPs is independent of chlorine demand, SUVA, and humic substance content (Nihemaiti et al., 2026). Therefore, UV absorbance and LC-OCD alone are insufficient to predict the formation of certain emerging DBPs. LC coupled to FT-ICR-MS provides ultra-high mass resolution and accuracy, enabling molecular formula assignment for thousands of NOM components. For example, this approach proved effective in identifying sulfur- and nitrogen-containing precursors associated with novel sulfonated DBPs (Nihemaiti et al., 2026). In addition, the elemental ratio plots, i.e., hydrogen to carbon (H/C) vs. oxygen to carbon (O/C), as well as the average mass and aromaticity plots, can also allow studying the structural changes in NOM composition during drinking water treatment and disinfection.

Conclusion

The NOM characterisation methods described in this guideline were tested and evaluated at SafeCREW case study sites in Hamburg, Berlin, Milan, and Tarragona. The results demonstrate that the combined application of UV absorbance, LC-OCD, and LC-FT-ICR-MS provides complementary and robust insights into NOM composition and DBP formation potential. The effectiveness of these approaches and detailed results are documented in SafeCREW Deliverable D1.2: “Robust analytical methods to comprehensively characterise natural organic matter and related disinfection by-products formation potential”. Further details on NOM characterisation and DBP analysis are available in peer-reviewed publications (Nihemaiti et al., 2026).

References

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