Proposals for NORMAN Joint Programme of Activities 2025

Title	**Identification Scoring System for GC-HRMS**
Type of activity	Methodological development and harmonization
Leader	Nikiforos Alygizakis (EI/NKUA), Pawel Rostkowski (NILU)
Topic / activities	***Background / Justification for the proposed activity:*** The identification of emerging contaminants using high-resolution mass spectrometry (HRMS) through non-target screening (NTS) has seen significant advancements, particularly for liquid chromatography (LC) systems. However, existing identification point (IP) scoring systems are tailored exclusively to LC workflows, limiting their applicability to gas chromatography (GC) methods. GC techniques, especially those employing hard ionization such as GC-EI-HRMS, exhibit unique characteristics that necessitate specific adaptations in IP scoring. Current scoring systems fail to account for critical parameters essential to GC-based methods, such as evidence derived from electron ionization (EI), retention index (RI), and the nuanced distribution of fragments. This gap in methodology undermines the reproducibility, automation, and harmonization of NTS approaches across analytical platforms. Drawing insights from recent methodological advancements such as those presented in Koelmel et al. (2022), this proposal seeks to adapt and refine the scoring framework for GC-specific workflows, ensuring compatibility while maintaining the rigor of LC-derived standards. ***Description of the proposed activity and expected outcomes for 2025:*** • Generation of a GC-EI-HRMS dataset by selected laboratories offering different types of GC-EI-HRMS instrumentation (in addition, utilizing raw data from ongoing activities, for example from GC-HRMS JPA that is ongoing in 2024 in 2025) • Adaptation of the IP scoring system to integrate GC-EI-HRMS-specific parameters such as isotopic patterns, retention index, and fragment ion ratios. • Development of a framework that harmonizes scoring criteria across LC- and GC-based NTS methods, emphasizing automated and transparent confidence level assignments. • Validation of the updated framework through collaboration with participating laboratories and testing on real-world datasets • Organization of an online workshop • Preparation of a manuscript for submission to a peer-reviewed journal detailing the harmonized scoring system and its application in multi-platform workflows. The manuscript will be published as gold open access. Manuscript preparation and publication may take place in 2026. ***Added value / Link with other NORMAN activities and / or other projects*** This activity bridges a critical gap in NTS methodologies by ensuring a unified scoring system applicable to both LC- and GC-based analyses, reinforcing the interoperability of data within the NORMAN network. The harmonized system will enhance the comparability of results across projects, supporting broader initiatives.
Participants	EI, NILU, participants of the GC-HRMS ongoing activity
Proposed in-kind contribution	Contribution of datasets and methodological inputs from ongoing projects in participating organizations, leveraging existing research infrastructure for framework validation, a standalone IP score script and web interface to allow efficient community uptake.
Contribution needed from NORMAN Association[1]	€5000 (EI) for analysis and modeling of the generated datasets and €3500 for covering gold open access publication costs

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[1] Please, provide here a transparent justification of the requested resources and of the in-kind contribution, thereby distinguishing between the costs associated with "person-months" for the organisation, the "travelling costs" for invited speakers and the costs for the logistics (e.g. meals, room rental etc.)