CCQM Data Digitalization Task Group

Draft Terms of Reference

Purpose: The CCQM Data Digitalization Task Group (CCQM-DDTG) is established to support the implementation of digital and FAIR (Findable, Accessible, Interoperable, and Reusable) principles in chemical and biological reference measurement systems data. This task group will address challenges in unique identifiers, the digitalization of Certified Reference Material (CRM) certificates, and best practices in database development.

Scope

The Group will focus on tasks in the following key areas:

1. **Unique Identifiers for Chem/Bio Data**:
   - Develop unique interoperable identifiers for chemical and biological substances, including measurands, matrices, and sample types that can be applied to the KCDB and the JCTLM DB and potentially broader applications
   - Leverage existing standards (e.g., InChI, NPU terminology) and ontologies to ensure interoperability across databases and consistency with the SI Digital Framework

2. **Digitalization of CRM Certificates**:
   - Understand and document stakeholder needs for digital CRM certificates amongst various communities /sectors;
   - Create guidelines for developing and maintaining digital CRM certificates adhering to FAIR principles.
   - Address resource requirements, data security, and long-term maintenance of digital certificates in the guidelines.
   - Describe approaches for the audit, validation, and modification of digital certificates that are in line with ISO standards.

3. **FAIR Principles in Chem/Bio Databases**:
   - Develop guidelines and case studies on the application of FAIR principles to databases hosting chemical and biological reference data
   - Develop guidelines on infrastructure, metadata standards, and interoperability to support data stewardship for those starting to develop databases hosting

Stakeholder Engagement

In order to achieve its tasks the group will need to engage relevant stakeholders in its work, and thereby:

- Facilitate collaboration with National Metrology Institutes (NMIs), international organizations (e.g., IUPAC, ISO), and industry stakeholders to address user needs and feedback.
- Encourage engagement with instrument vendors and regulatory bodies to support the adoption of open and standardized data formats.

Structure and Membership

The Task Group will create teams to progress each of its tasks, with expert members that are required to complete the tasks to be drawn from:

1. CCQM and JCTLM WGs with relevant experience and requirements;
2. Representatives from NMIs active in chemical and biological metrology and digitalization initiatives.
3. Experts in digitalization, data management, and database development.
4. Stakeholders from relevant sectors and international organizations to ensure diverse expertise and representation and likelihood of take up of outputs.

Reporting

The Task Group will:

1. Provide regular updates to the CCQM-SPWG, CCQM and FORUM-DI on its progress.
2. Submit a comprehensive report of recommendations and outcomes at the end of its term or as requested by the CCQM President.

Duration

The CCQM-DDTG will operate for an initial term of three years, with a review of its progress and continuation at the end of the term.

Deliverables

1. A system for unique identifiers for chemical and biological reference data that can be applied in the KCDB and JCTLM DB and potentially for broader application
2. A report of stakeholder expectations and needs for digital CRM certificates across various sectors and applications
3. A framework for the digitalization of CRM certificates and guidelines for NMIs wishing to adopt this framework.
4. A set of recommendations for digitalizing CCQM products applying FAIR principles.
5. Guidelines for applying FAIR principles to databases holding chemical and biological reference data.