

NRC Publications Archive Archives des publications du CNRC

Establishing digital reference material documentation infrastructure for chemical metrology

Garrido, Bruno; Ghosh, Tanishka; Yang, Daniel; LeBlanc, Patricia; Paluch, Marcin; Roy, Sophie; McCarron, Pearse; Mester, Zoltán; Meija, Juris

This publication could be one of several versions: author's original, accepted manuscript or the publisher's version. / La version de cette publication peut être l'une des suivantes : la version prépublication de l'auteur, la version acceptée du manuscrit ou la version de l'éditeur.

For the publisher's version, please access the DOI link below. / Pour consulter la version de l'éditeur, utilisez le lien DOI ci-dessous.

Publisher's version / Version de l'éditeur:

<https://doi.org/10.1007/s00769-026-01705-w>

Accreditation and Quality Assurance, 2026-05-11

NRC Publications Archive Record / Notice des Archives des publications du CNRC :

<https://nrc-publications.canada.ca/eng/view/object/?id=d5a0aadb-6d47-485f-a0a9-dd550bb70a94>

<https://publications-cnrc.canada.ca/fra/voir/objet/?id=d5a0aadb-6d47-485f-a0a9-dd550bb70a94>

Access and use of this website and the material on it are subject to the Terms and Conditions set forth at

<https://nrc-publications.canada.ca/eng/copyright>

READ THESE TERMS AND CONDITIONS CAREFULLY BEFORE USING THIS WEBSITE.

L'accès à ce site Web et l'utilisation de son contenu sont assujettis aux conditions présentées dans le site

<https://publications-cnrc.canada.ca/fra/droits>

LISEZ CES CONDITIONS ATTENTIVEMENT AVANT D'UTILISER CE SITE WEB.

Questions? Contact the NRC Publications Archive team at

PublicationsArchive-ArchivesPublications@nrc-cnrc.gc.ca. If you wish to email the authors directly, please see the first page of the publication for their contact information.

Vous avez des questions? Nous pouvons vous aider. Pour communiquer directement avec un auteur, consultez la première page de la revue dans laquelle son article a été publié afin de trouver ses coordonnées. Si vous n'arrivez pas à les repérer, communiquez avec nous à PublicationsArchive-ArchivesPublications@nrc-cnrc.gc.ca.



Establishing digital reference material documentation infrastructure for chemical metrology

Bruno Garrido¹ · Tanishka Ghosh¹ · Daniel Yang² · Patricia LeBlanc¹ · Marcin Paluch³ · Sophie Roy⁴ · Pearse McCarron¹ · Zoltán Mester² · Juris Meija²

Received: 19 January 2026 / Accepted: 1 April 2026
© Crown 2026

Abstract

There is a significant interest by reference material producers to issue digital reference material documentation. To achieve this, a structured digital representation of the relevant data must be created and made available on the World Wide Web. The National Research Council of Canada (NRC) has accomplished this by creating unique digital identifiers and using the NRC Digital Repository which has enabled machine-readable integration with other databases. We discuss our efforts and provide applications showcasing the added value of open-access FAIR data for chemical metrology. In particular, we present two proof-of-concept applications, web and mobile versions of a Reference Material Explorer software that demonstrate how digital reference material documentation enables data retrieval, dynamic searching, visualization, and integration with external databases such as PubChem.

Keywords Digital reference material documents · Chemical metrology · Open data · Machine-readability

Introduction

Society is undergoing broad changes with the widespread adoption of digital technologies. To keep pace with this rapidly changing environment, the international measurement system must also evolve. This need has been recognized by various governments and National Metrology Institutes (NMIs) with a wide variety of ongoing efforts to enable the digital transformation of measurement infrastructure.

The paper-based documentation and certificates traditionally issued by reference material producers were augmented in recent decades by portable document format files (PDFs).

However, the PDF is not expected to remain the de facto standard for long owing to the fact that PDF is designed primarily to be human-readable, whereas digital transformation requires structured machine-readable data formats that can be understood by computers and algorithms alike [1, 2].

The proliferation of metadata is a key enabler of digital transformation because it provides the foundation for annotating, organizing, discovering, and connecting content and knowledge in the digital environment. Metadata—information that describes other data—adds essential context, structure, and meaning, allowing content to be efficiently managed, searched, and reused. As organizations move towards digital operations, the growth of information requires systems that can interpret and relate data consistently [3]. Controlled vocabularies and universally adopted identifiers play a critical role in this process: controlled vocabularies ensure that metadata terms are standardized whereas universally adopted identifiers, such as the Digital Object Identifier (DOI, doi.org) for publications, Open Researcher and Contributor ID (ORCID, orcid.org) for researchers and Research Organization Registry (ROR, ror.org) for institutions, create persistent, machine-readable links between entities, making it possible to connect content globally.

Together, metadata, controlled vocabularies, and universal identifiers transform isolated data into interconnected

✉ Juris Meija
Juris.Meija@nrc-cnrc.gc.ca

¹ Biotoxin Metrology, Metrology Research Centre, National Research Council Canada, 1411 Oxford St, Halifax, NS B3H 3Z1, Canada

² Inorganic Chemical Metrology, Metrology Research Centre, National Research Council Canada, 1200 Montreal Road, Ottawa, ON K1A 0R6, Canada

³ Chief Information Officer Branch, National Research Council Canada, 1200 Montreal Road, Ottawa, ON K1A 0R6, Canada

⁴ Secretary General Office, National Research Council Canada, 1200 Montreal Road, Ottawa, ON K1A 0R6, Canada

knowledge networks, supporting automation, semantic search, and data integration. This structured approach enhances discoverability and data governance, and turns digital assets into dynamic resources that can drive innovation. In this vein, the National Research Council of Canada has developed an infrastructure for digitally documenting its reference materials, an initiative that is built on the FAIR data principles (findable, accessible, interoperable, and reusable) [4].

To leverage and explore the benefits of digital reference material documentation (DRMD) infrastructure, two proof-of-concept applications were developed (both referred to as the *NRC Reference Material Explorer*), one web application written in R [5, 6] and a native mobile application written in Dart [7]. This contribution summarizes the main features of the NRC DRMD infrastructure that supports this activity and outlines some applications of this infrastructure.

Methods

Creating digital reference material documents

The infrastructure for the digital documents rests on the creation of a digital object for each reference material, which consists of descriptive metadata (bibliographic and quantitative), an assigned and registered identifier (DOI), a Certificate of Analysis or Information Sheet (both referred to as CoA here) PDF files in both official languages of Canada (English and French), Safety Data Sheet PDF files, and any supplementary information such as additional datafiles.

At the core of a digital document is a structured digital representation of the CoAs for (Certified) Reference Materials (CRM/RMs). This involves an explicit annotation of all pertinent information using descriptive metadata to create a structured digital twin that represents the electronic or paper-based CoA. To capture the bibliographic elements of a CoA, we use the Metadata Object Description Schema (MODS) created and maintained by the US Library of Congress [8]. This schema provides ample room for a variety of metadata, including information about the publisher, the release date, the individual authors, or the references cited (Table 1).

A primary interest in a CoA is the data associated with the quantity values. For digitalization, this information is collected with an additional XML schema developed by the NRC which captures the essential technical details such as the name of the analyte, an analyte identifier (e.g. InChiKey), the name of the quantity, the value of the quantity, the associated measurement units and the measurement uncertainty (Table 2) along with the data licencing and rights information. Our decision to represent measurement units as strings instead of resorting to available ontologies such as UCUM (ucum.org) or QUDT (qudt.org) is motivated largely by the fact that active research is still ongoing towards finding best digital representation of measurement units [9].

For digital documents to serve their intended function, they must be accessible via the World Wide Web. To accomplish this, we use the digital repository (NRC Digital Repository) of the National Science Library of Canada, where a dedicated collection ('Canadian Reference Materials and Methods') provides open digital access to NRC Reference

Table 1 Essential features for digitalizing the bibliographic information of a CRM/RM

Object	Property	Type	Example value
title	term	EN name	MESS-4: Marine sediment Certified Reference Material for total and extractable metal content
		FR name	MESS-4: Matériau de Référence Certifié pour la teneur en métaux totaux et extractibles des sédiments marins
name	part	family	Willie
		given	Scott
	identifier	ORCID	0000-0002-3376-0722
	role	Term	author
affiliation		EN name	National Research Council Canada
		FR name	Conseil national de recherches Canada
origin info	date issued		w3cdf:2014-11-01
	publisher	EN name	National Research Council Canada
FR name		Conseil national de recherches Canada	
ROR		04mte1k06	
identifier		DOI	https://doi.org/10.4224/crm.2014.mess-4
licence			Open Government Licence—Canada
record information	record identifier		8a3fd39a-c068-4ce0-820c-d08cf742a20a

Latest XML schema location: <https://www.loc.gov/standards/mods/v3/mods-3-8.xsd>

Table 2 Essential features for digitalizing the properties of a CRM/RM

Object	Property	Type	Subtype	Example value	
material	name			ORMS-6	
	identifier	DOI		https://doi.org/10.4224/crm.2025.orms-6	
validity	date	start		w3cdtf:2025-07-08	
		end		w3cdtf:2035-04-30	
storage	temperature	value		+ 20	
			unit		°C
licence				https://open.canada.ca/en/open-government-licence-canada	
rights				© His Majesty the King in Right of Canada, as represented by the National Research Council of Canada, 2025	
analyte	name			mercury	
	symbol			Hg	
	identifier	InChIKey		QSHDDOUJBYECFT-UHFFFAOYSA-N	
	amount	quantity			mass fraction
			value		26.18
	uncertainty	unit			pg/g
			expanded		1.10
standard			0.55		
type				certified	

XML schema (version 1.0, 2025) location: <https://nrc-digital-repository.canada.ca/schema/analytexml.xsd>

Materials. A feature of the NRC Digital Repository is that all entries are issued a unique DOI by DataCite, made possible owing to NRC Canada being a member of the DataCite Canada Consortium. All DOIs for NRC CRM records have a prefix '10.4224' (identifying the NRC) and descriptive suffixes that begin with 'crm' and include the CRM identifier (Table 3). These provide permanent links to a given CRM making them easily findable and citable in standards, procedures, commercial documents, or peer-reviewed publications. For example, HISN-1 CRM is assigned the <https://doi.org/10.4224/crm.2025.hisn-1> which enables direct citation in academic literature [10].

Data harvesting

All records stored in the NRC Digital Repository can be retrieved by the universally unique 32-hexadecimal digit identifiers in the standard 8-4-4-4-12 character format

(Table 4). Table 4 shows the main folder structure of the stored information.

All data available from the NRC Digital Repository are publicly accessible and can be scraped from the web after visiting the website resolved by the DOI. This type of data extraction does not require sophisticated algorithms and can be performed with the Microsoft Excel 'import data from the web' feature (Fig. 1). Once loaded, the data can be updated automatically or on demand. Programming languages such as Python and R both provide an alternative means of retrieving information from the DOI and are more suitable for large-scale data analysis.

Although web scraping provides an intuitive way to access data, collecting information through application programming interface requests (API) offers a more reliable and efficient method of data collection. The NRC Digital Repository provides this functionality using the Open Archives Initiative Protocol for Metadata Harvesting (OAI-PMH) but other approaches are possible (Table 5).

Table 3 Digital object identifiers of a select sample of NRC Reference Materials

CRM/RM	DOI	Description
MOOS-1	https://doi.org/10.4224/crm.2003.moos-1	Seawater certified reference material for nutrients
ASP-Mus-e	https://doi.org/10.4224/crm.2025.asp-mus-e.202502	Mussel tissue certified reference material for domoic acid
IRIS-1	https://doi.org/10.4224/crm.2017.iris-1	Isotopic certified reference material of natural iridium
CBIS-1	https://doi.org/10.4224/crm.2021.cbis-1	Certified reference material of dried, ground cannabis
OMIC-1	https://doi.org/10.4224/crm.2023.omic-1	Reference material for sars-cov-2 omicron ba.4/5 spike glycoprotein
NPPP-1	https://doi.org/10.4224/crm.2025.nppp-1	Nanoscale polypropylene reference material

Table 4 Data retrieval from NRC Digital Repository of CRM/RMs

URL	Description	File format
BASE/object/?id=ID	Record	HTML
BASE/ax/?id=ID	Information about the analytes	XML (Table 2 schema)
BASE/crt/?id=ID	Certificate of Analysis file	PDF
BASE/supplement/?id=ID	Safety Data Sheet file	PDF
BASE/dataset/?id=ID	Dataset	variable (CSV, TXT, PDF)
BASE/dataset/?id=ID&dp=x	Additional datasets (x=2, 3, ...)	variable (CSV, TXT, PDF)

BASE (english) = <https://nrc-digital-repository.canada.ca/eng/view>. ID = Unique record id; 'd7ea832c-4dc9-4b36-83e1-946ac0bf096e' for MOOS-1, for example

Analyte	Quantity	Value	Expanded uncertainty	Unit	Type
Δ^9 -tetrahydrocannabinol (THC)	mass fraction	48.9		6.4 mg/g	certified
Δ^9 -tetrahydrocannabinolic acid (THCA)	mass fraction	124		7 mg/g	certified
total Δ^9 -tetrahydrocannabinol (THC)					
cannabidiol (CBD)					
cannabidiolic acid (CBDA)					
total cannabidiol (CBD)					
cannabivarin (CBV)					
cannabivarinic acid (CBVA)					
tetrahydrocannabivarin (THCV)					
tetrahydrocannabivarinic acid (THCVA)	mass fraction	0.446		0.034 mg/g	certified
cannabidivarin (CBDV)	mass fraction	0.0415		0.0038 mg/g	certified
cannabidivarinic acid (CBDVA)	mass fraction	0.126		0.008 mg/g	certified

Fig. 1 Microsoft Excel screenshot illustrating data retrieval for NRC cannabis reference material CBIS-1 from web (bibliographical information can be retrieved in this manner as well)

The API requests to the NRC Digital Repository return DRMDs in an XML format. This includes complete bibliographic data along with links to the additional XML files containing scientific information as well as links to the associated documents which include the PDF files for the CoAs, Safety Data Sheets, and other supplementary data.

Because all API requests are returned as structured XML files, the information needs to be parsed depending

on the required output. One generic application is to retrieve a single data table containing all reference materials from the NRC Digital Repository. This can be done by first retrieving a list of all unique record identifiers (see Table 5), followed by a retrieval of the information about the analytes for each record (see Table 4). The resulting list of XML files is then parsed into a data table.

Table 5 Example API requests for NRC CRM/RMs

API provider	Base URL	Example API call
DOI System	https://doi.org/api/handles	Retrieve URL associated with a DOI: BASE/10.4224/crm.2022.da-h.20210922
DataCite	https://api.datacite.org/doi	Retrieve bibliographic information from a DOI: BASE/10.4224/crm.2022.da-h.20210922
NRC	https://nrc-digital-repository.canada.ca/eng/search/atom	Retrieve all records from the CRM/RM catalogue: BASE/?q=* & cn=crm & av=1 Retrieve record with a unique record identifier: BASE/?q=d7ea832c-4dc9-4b36-83e1-946ac0bf096e & cn=crm & av=1 Retrieve all records matching 'domoic acid': BASE/?q=domoic+acid & cn=crm & av=1
NRC	https://oai-pmh.nrc-cnrc.gc.ca/dr-dn	Retrieve record with a unique record identifier: BASE/?verb=GetRecord&metadataPrefix=oai_openaire&identifier=oai:dr-dn.cisti-icist.nrc-cnrc.ca:d7ea832c-4dc9-4b36-83e1-946ac0bf096e Retrieve all records from the CRM/RM catalogue: BASE/?verb=ListRecords&metadataPrefix=oai_openaire&set=crm

Working with data: software development

Digitalization of NRC CRM/RM information facilitates access to the reference material catalogue and this access can be further enhanced by the web-based applications that leverage the digital reference material document infrastructure.

To demonstrate the value of web applications in searching the NRC CRM/RM catalogue, programming language R [5] and its 'shiny' package [6] were used to create an interactive graphical user interface for a web-based application. The API of the NRC Digital Repository is used as the starting point for user queries for which we employ the OAI-PMH protocol shown in Table 5. The resulting data are then parsed into a data frame which, in turn, is displayed to the end-user in a form of interactive data tables.

Unlike web applications, mobile applications do not require a host server and thus provide an alternative deployment solution. The development framework Flutter, an open-source framework [11], was chosen because of its cross-platform capabilities. Flutter enables use of a single codebase to manage the applications across various mobile platforms (IOS, Android) and most of the application was written in the open-source programming language Dart. The source codes for both applications, called *RM Explorer*, are available from Github (<https://github.com/RMExplorer/RME> and <https://github.com/RMExplorer/rme-flutter>).

Example use of web and mobile applications

Search across reference materials

One of the functions of digital repositories is to provide an access to historical records. This facilitates a variety of meta-analyses that are crucial to understanding and measuring the evolution of measurement science [12]. An

example of this is a global query across all NRC CRM/RM records to visualize the measurement capabilities for all chemical substances described (Fig. 2). This figure is generated by first fetching the unique IDs for all NRC CRM/RMs (Table 5), followed by the retrieval of the analyte information (Table 4).

Another application of the DRMD framework is to perform a search of reference materials that cover a group of specified analytes with the results being displayed in a form of fully interactive tables. A practical example of this is finding reference materials that include four toxic elements arsenic, cadmium, lead, and mercury below a certain mass fraction, w /(mg/kg) (Fig. 3).

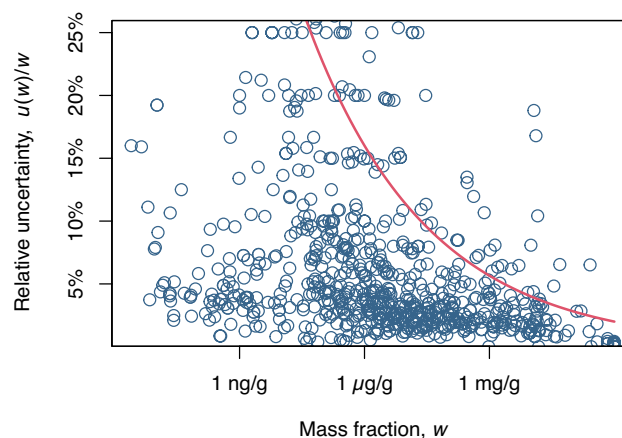


Fig. 2 Measurement results across the entire NRC CRM/RM catalogue. Each dot corresponds to a certified value and the results are compared with the classical benchmark known as the Horwitz curve (red line) that relates the relative reproducibility uncertainty ($s_R/\%$) with the mass fraction of the analytes (w) as $\log_2[s_R/\%] = 1 - 0.5 * \log_{10}[w/(g/g)]$

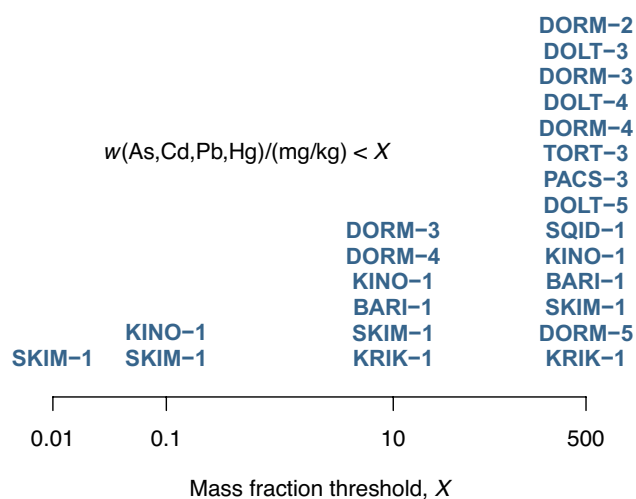


Fig. 3 Set of reference materials containing arsenic, cadmium, lead, and mercury, all below a specified level

Display of spectral data

The NRC Digital Repository can store supplementary information about each reference material which include spectral data along with the associated metadata. This information can be retrieved via API calls (see Table 5), allowing users to visualize and interact with the plots instead of displaying static images as is the case with the file formats typically used for CoAs.

Fetching additional information from metadata

The DRMD repository provides an opportunity to work with quantities that are not part of the DRMDs. In other words, new data can be obtained by computational means or by integrations with external databases. This can be made possible by leveraging chemical identifiers that are part of the DRMD, namely InChI, InChiKey or SMILES. For organic substances, one can thus retrieve structural formulas from PubChem via API:

<https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/inchikey/{inchikey}/PNG>

Other physicochemical properties can be retrieved from PubChem using its API service. For example, hydrophobicity (octanol–water partition coefficient, $\log P_{ow}$) and molar mass (M) of substances can be retrieved from InChiKey using the following API call:

<https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/inchikey/{inchikey}/property/XLogP,MolecularWeight/XML>

Both of these properties are computationally generated and are retrieved from PubChem API using the InChiKey

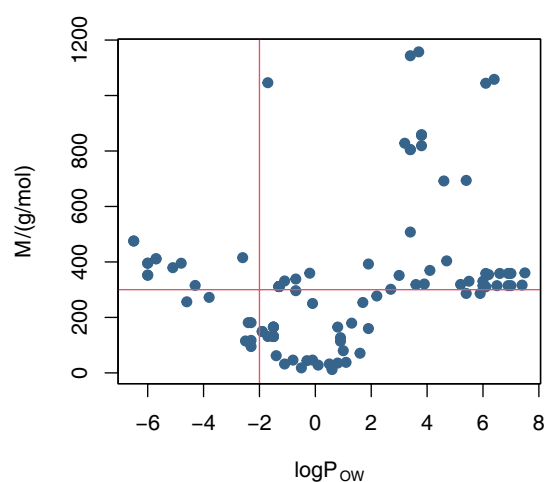


Fig. 4 Polarity–size plot of substances from the NRC CRM/RM catalogue whose quadrants mark organic substances of low and high polarity and molar mass as per Teo et al. [13]

input by the *RM Explorer*. Subsequently, one can perform such an API call for every substance in the NRC CRM/RM catalogue and generate a polarity/molar mass plot (Fig. 4). This is accomplished despite the fact that information on polarity does not actually appear in any of the reference material documents. Organic compound analysis makes frequent reference to the polarity and molecular weight of analytes as a descriptor of the complexity of the analyses.

One can rely on other facilities to generate a variety of additional properties of chemical substances. An example of such framework is the rcdk package in R which provides access to the Chemistry Development Kit (CDK) chemoinformatics library in R [14]. The use of chemical identifiers, such as InChiKey, with machine-readable formats, therefore allows users to integrate a wide variety of additional data well beyond what is provided on the CoAs.

Synonym-resolved searching

While reference material producers strive to use appropriate names for substances, those names are often not unique and even the commonly used names can be misleading. As an example, the common drug paracetamol is known as acetaminophen in North America and Japan. The use of chemical identifiers therefore provides a unique, machine-readable string to consistently identify compounds regardless of language or regional specificities.

Synonym-resolved searching circumvents the problems arising from the use of different names. We have implemented this in the *RM Explorer* by taking the user-provided search term, which is followed by a PubChem query to

What is the concentration of berberine in the NRC reference material BERB-1?

The NRC reference material BERB-1 is a **certified reference material (CRM) of berberine chloride** produced by the **National Research Council Canada (NRC)**. The official product description lists it as “Certified Reference Material of Berberine Chloride,” packaged in a **30 mg unit**. National Research Council Canada

What is the concentration of arsenobetaine in the NRC reference material ABET-1?

The NRC Certified Reference Material ABET-1 (natural arsenobetaine bromide) has **certified values for the mass fractions** of arsenobetaine species established in the material. According to the official NRC certificate documentation:

- **Arsenobetaine (as the cation) mass fraction: 0.6866 g/g ± 0.0034 g/g (certified)**

Fig. 5 ChatGPT inquiry (7 Jan 2026) about two NRC reference materials, BERB-1 and ABET-1. Whereas the PDF certificates for both BERB-1 and ABET-1 are publicly available, only ABET-1 has the associated structured metadata about its chemical composition

identify the substance, fetch its InChiKey, and then search the NRC Digital Repository for it. This ensures a robust search for organic compounds based on structure rather than name thus providing greater flexibility in finding information.

Searching by chemical properties

Chemical similarity is important in analytical chemistry, whether in the identification of impurities or potentially interfering compounds for selectivity assessment during method validation, or in the development of multi-compound screening methods. Searching for these compounds individually by name can be time-consuming and, because names are not necessarily related, can be futile (as an example, penicillin and penicillamine have very few similarities beyond their name). The chemical structure similarity search is performed by *RM Explorer* via the PubChem API call. For domoic acid, as an example, the first step is to translate the InChiKey to a PubChem compound identifier (which is cid = 5,282,253):

<https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/inchikey/VZFRNCSOCOPNDB-AOKDLOFSSA-N/cids/txt>

And then substances which have Tanimoto coefficient with domoic acid greater than 90% are retrieved:

https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/fastsimilarity_2d/cid/5282253/cids/TXT?Threshold=90

The resulting PubChem compound identifiers are converted back to InChiKeys. The top similarity search, for example, is cid = 44,568,340, whose InChiKey is:

<https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/cid/44568340/property/inchikey/txt>

Searching for this substance (epi-domoic acid) in the NRC Digital Repository provides the reference materials that contain it.

Outlook

Calibration and measurement capabilities

The Mutual Recognition Arrangement of the International Committee for Weights and Measures (CIPM-MRA) provides a framework through which NMIs demonstrate the equivalence of their measurement results. This equivalence is declared in the form of Calibration and Measurement Capabilities (CMCs) [15]. Currently, the integration of the *RM Explorer* apps with the BIPM Key Comparison database (BIPM-KCDB) enables the app to display the list of CMCs associated with the NRC. As the BIPM-KCDB evolves, the joint use of chemical identifiers and machine-readable metadata could enable further integration, allowing one to link each certified property in a reference material to a CMC that supports it. This would parallel testing and calibration laboratories' practice of clearly indicating

which services are within the scope of accreditation and which are not.

DRMD perspectives

The transition to digital documentation improves the discoverability of NRC reference materials, fosters interoperability, and machine learning applications. We have already witnessed that large language models provide more reliable information about the reference materials that are fully indexed in the NRC Digital Repository compared to those that are yet to be fully digitalized (Figure 5). Furthermore, digital documents empower researchers to conduct complex queries, such as identifying compounds with specific chemical properties or retrieving supplementary data from external databases like PubChem or the BIPM-KCDB.

Various DRMD schemas have been developed by NMIs, notably the Physikalisch-Technische Bundesanstalt (PTB, Germany) [16], The Federal Institute for Materials Research and Testing (BAM, Germany) [17], and the National Institute of Standards and Technology (NIST, USA) [18]. As more information becomes available in digital format that complies with FAIR data principles, and as user awareness about such data increases, more tools will be developed to integrate different DRMD formats into a centralized database of reference materials. Such a database would contribute to improve measurement traceability and comparability in general by enabling users to easily identify reference materials that suit their needs. As we demonstrate in this work with the *RM Explorer*, having data available in such a format enables not only simple searches and queries but also allows integrative operations, API queries and on-the-fly calculations. This enables a search based on chemical properties, synonyms, structural similarity and much more, even if reference material producers do not provide the information in their documents. General considerations surrounding harmonization and formatting of digital measurement certificates still have to be addressed, most notably a standard structured representation of measurement units, but digital access to reference material catalogues clearly demonstrates the added value to clients and reference material producers alike.

Supplementary Information The online version contains supplementary material available at <https://doi.org/10.1007/s00769-026-01705-w>.

Acknowledgements The authors wish to acknowledge Dr. Elizabeth Mudge for providing insightful comments on the manuscript.

Author contributions CRediT taxonomy: Conceptualization was performed by BG, JM, ZM, PMC; Data curation by JM, PLB, MP, SR; Formal analysis by BG, TG, DY, JM, MP, SR; Methodology by BG, JM, TG, DY, MP, SR; Project administration by JM, ZM, PMC; Software by JM, BG, TG, DY, MP, SR; Supervision by BG, JM; Writing—original draft by BG, JM; Writing—review & editing by all authors.

Funding Open access funding provided by National Research Council Canada library.

Data availability All data used in the work are publicly available via the NRC Digital Repository (<https://nrc-digital-repository.canada.ca/eng/home/>). The source codes for the *RM Explorer* applications (versions 1.0) are available from Github (<https://github.com/RMExplorer/RME>) and <https://github.com/RMExplorer/rme-flutter>). A text file containing the R code used to make Figs. 2–4 is provided in the supplementary information (figure-codes.txt).

Declarations

Conflict of interest The authors declare no conflict of interest.

Open Access This article is licensed under a Creative Commons Attribution 4.0 International License, which permits use, sharing, adaptation, distribution and reproduction in any medium or format, as long as you give appropriate credit to the original author(s) and the source, provide a link to the Creative Commons licence, and indicate if changes were made. The images or other third party material in this article are included in the article's Creative Commons licence, unless indicated otherwise in a credit line to the material. If material is not included in the article's Creative Commons licence and your intended use is not permitted by statutory regulation or exceeds the permitted use, you will need to obtain permission directly from the copyright holder. To view a copy of this licence, visit <http://creativecommons.org/licenses/by/4.0/>.

References

1. Stocker M, Snyder L, Anfuso M et al (2025) Rethinking the production and publication of machine-readable expressions of research findings. *Sci Data* 12:677. <https://doi.org/10.1038/s41597-025-04905-0>
2. Steffen K, Oberlies NH, Rokas A (2025) Machine-readable structural information is essential for natural products research. *J Nat Prod* 88:2815–2821. <https://doi.org/10.1021/acs.jnatprod.5C00836>
3. Amadi D, Kiwuwa-Muyingo S, Bhattacharjee T et al (2024) Making metadata machine-readable as the first step to providing findable, accessible, interoperable, and reusable population health data: framework development and implementation study. *Online J Public Health Inform* 16:e56237. <https://doi.org/10.2196/56237>
4. Wilkinton MD, Dumontier M, Aalbersberg IJJ et al (2016) The FAIR guiding principles for scientific data management and stewardship. *Sci Data* 3:160018. <https://doi.org/10.1038/sdata.2016.18>
5. R Core Team (2022) R: A language and environment for statistical computing. Vienna. <https://cran.r-project.org/>. Accessed 17 Feb 2026
6. Chang W, Cheng J, Allaire J, et al (2026) shiny: Web Application Framework for R. <https://shiny.posit.co/>. Accessed 17 Feb 2026
7. Kinari SA, Funabiki N, Aung ST et al (2024) An independent learning system for Flutter cross-platform mobile programming with code modification problems. *Information* 15:614. <https://doi.org/10.3390/info15100614>
8. Metadata Object Description Schema: MODS (Library of Congress Standards). <https://www.loc.gov/standards/mods/>. Accessed 17 Feb 2026
9. Hall BD, Kuster M (2022) Representing quantities and units in digital systems. *Meas Sensors* 23:100387. <https://doi.org/10.1016/j.measen.2022.100387>
10. Mihai O, Methven B, Brophy C et al (2025) HISN-1: High Purity Tin Certified Reference Material for Tin Mass Fraction

- and Elemental Impurities. National Res Council Canada, Ottawa. <https://doi.org/10.4224/crm.2025.hisn-1>
11. Flutter (2025) Flutter - Beautiful native apps in record time. <https://flutter.dev/>. Accessed 17 Feb 2026
 12. Duewer DL, Cecelski CE, Cleveland MH, et al (2024) NIST's engagement with CCQM studies from 1992 to 2023: History and Performance. NIST Internal Report 8524. National Institute of Standards and Technology. Gaithersburg MD. <https://doi.org/10.6028/NIST.IR.8524>
 13. Teo TL, Lippa KA, Mackay L et al (2019) Enhancing the accuracy of measurement of small molecule organic biomarkers. *Anal Bioanal Chem* 411:7341–7355. <https://doi.org/10.1007/S00216-019-02153-X>
 14. Guha R (2007) Chemical informatics functionality in R. *J Stat Softw* 18:1–16. <https://doi.org/10.18637/JSS.V018.I05>
 15. CIPM (1999) Mutual recognition of national measurement standards and of calibration and measurement certificates issued by national metrology institutes. International Bureau of Weights and Measures, Paris. <https://www.bipm.org/en/cipm-mra/cipm-mra-documents/>. Accessed 17 Feb 2026
 16. Hackel S, Härtig F, Schrader T et al (2021) The fundamental architecture of the DCC. *Meas Sensors* 18:100354. <https://doi.org/10.1016/j.measen.2021.100354>
 17. Prellwitz M, Koch C, Silke R, et al (2025) The Digital Reference Material Document: From Paper Certificates to Interoperable Data Objects in Digital Quality Infrastructure. *Proceedings of the IMEKO TC6 Conference on Digitalization - M4DConf 2025*. <https://doi.org/https://doi.org/10.21014/tc6-2025.067>
 18. Camara WD, Choquette S, Delak K et al (2023) Digital NIST: an examination of the obstacles and opportunities in the digital transformation of NIST's reference materials. *Acta IMEKO* 12:1–4. <https://doi.org/10.21014/actaimeko.v12i1.1403>

Publisher's Note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.