ISA-TAB-Nano Supporting the Nanoinformatics Community*

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*adapted from
1. https://nciphub.org/resources/1615/about
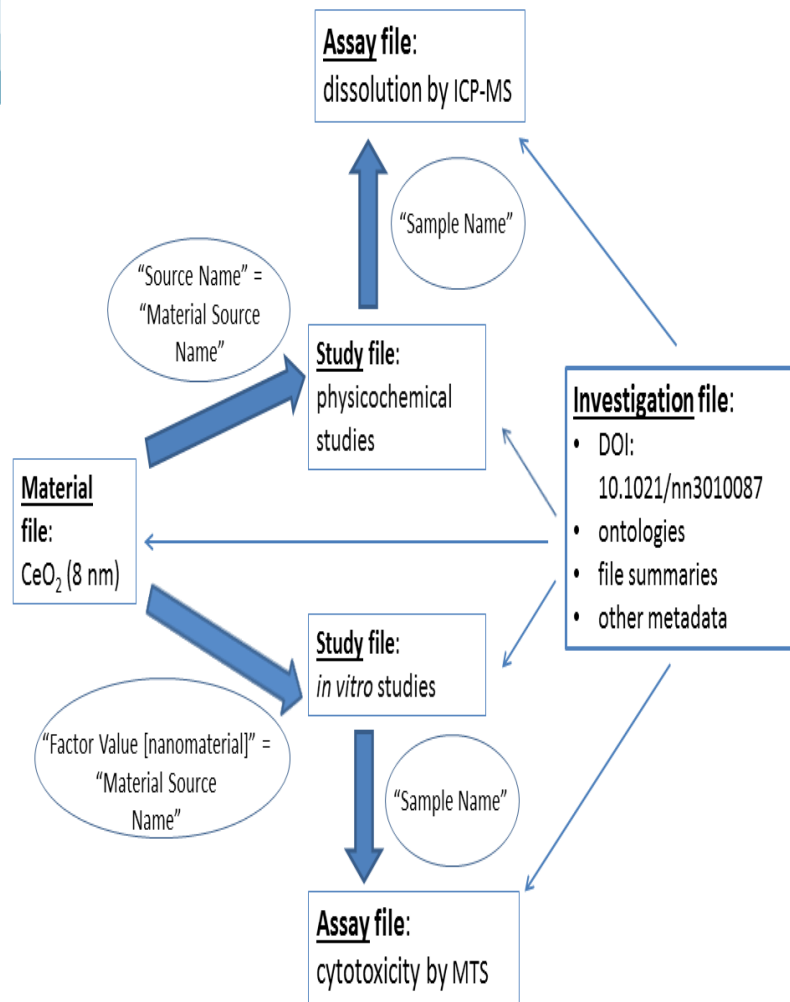2. https://dx.doi.org/10.6084/m9.figshare.1598082.v1

ISA-TAB-Nano: motivation and current status

- Proposed nanoscience community data EXCHANGE standard
  - Can record or link to data
  - Metadata standardisation PROMOTED
    - e.g. ontology links supported

- Interconnected "spreadsheet-like" file *types*
  - **I**nvestigation, **S**tudy, **A**ssay, Material – **TAB**ular files
  - Flexible – *not* fully specified fields, but field *types* e.g. factors
  - Business rules promote standardised addition of fields

- Iterative development
  - Adapted from ISA-TAB by U.S. Nano WG
  - Original publication in 2013
  - Current version: 1.2

NanoPUZZLES datasets -> MODERN database

Assay file: dissolution by ICP-MS

"Sample Name"

"Source Name" = "Material Source Name"

Study file: physicochemical studies

Material file: CeO₂ (8 nm)

Investigation file:
- DOI: 10.1021/nn3010087
- ontologies
- file summaries
- other metadata

"Factor Value [nanomaterial]" = "Material Source Name"

Study file: in vitro studies

"Sample Name"

Assay file: cytotoxicity by MTS

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nano Data Management System

Home   Browse   **Find**   Create   Upload   Logout

Find investigation ❓

Material Name	Investigation identifier	Investigation description
		NanoPUZZLES
Study identifier	**Study description**	**Measurement Type**
		cytotoxicity

Case insensitive ☐   Federated Search ☐

Find

Find results

Identifier	Title	Application	Release Date	CSV
10.1021_FS_nl0730155	Curation of carbon nanotubes experimental data reported by Zhou et al. 2008 (DOI:10.1021/nl0730155), supplemented with carbon nanotubes structure files (3D SDF) created according to the approach described by Shao et al. 2013 (DOI:10.1021/ci3005308).	current		Download ⊕
10.1021_FS_nn3010087	Toxicity and physicochemical data extracted from Zhang et al. 2012	current		Download ⊕

Outlook: Nanoinformatics community

- ISA-TAB-Nano specification under review
  - work <u>started</u> towards version 1.3
  - ongoing discussions
  - partly prompted by issues identified within NanoPUZZLES
  - will aim to harmonise with FORTHCOMING revised ISA-TAB specification

- Proposed development of community accepted templates
  - initial <u>suggestion</u>
  - to be led by ISA-TAB-Nano developers

- Resources being developed by other projects
  - e.g. tools for creating and parsing ISA-TAB-Nano files under development within eNanoMapper
  - e.g. KNIME workflows for analysing ISA-TAB-Nano datasets under development within MODERN

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NanoPUZZLES

MODern
MODELING NANOTOXICITY

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