The NanoInformatics Knowledge Commons (NIKC) Nano-Dictionary Taxonomy

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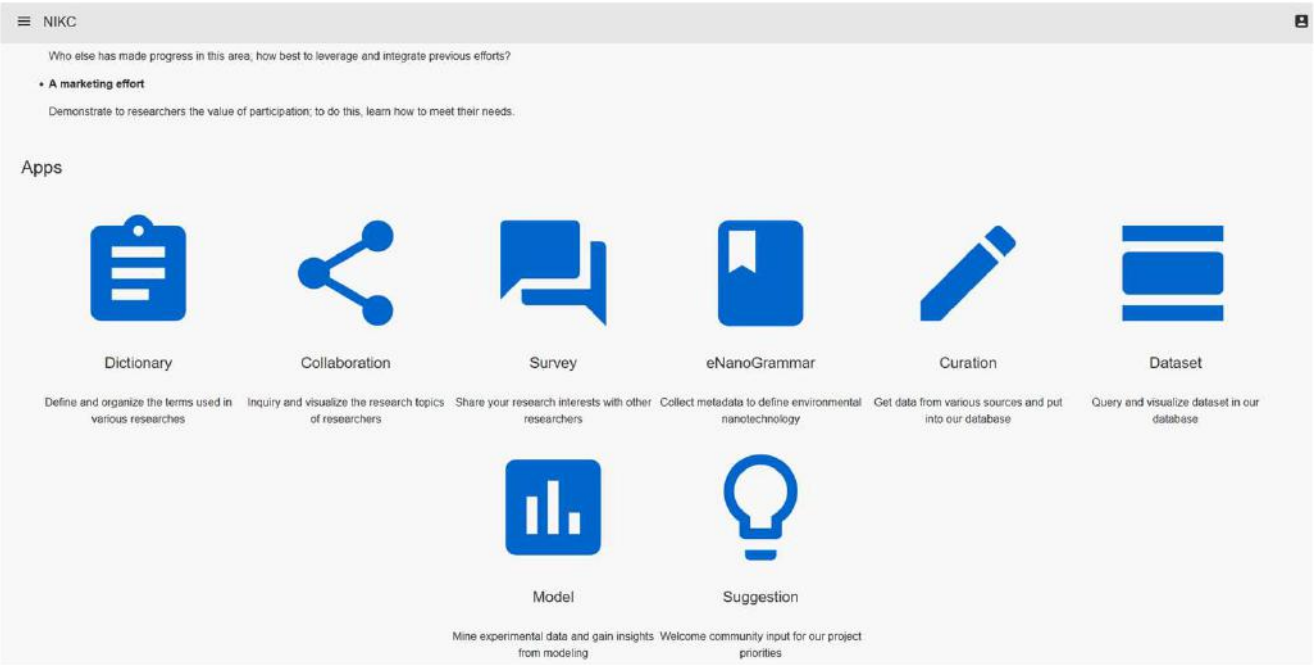
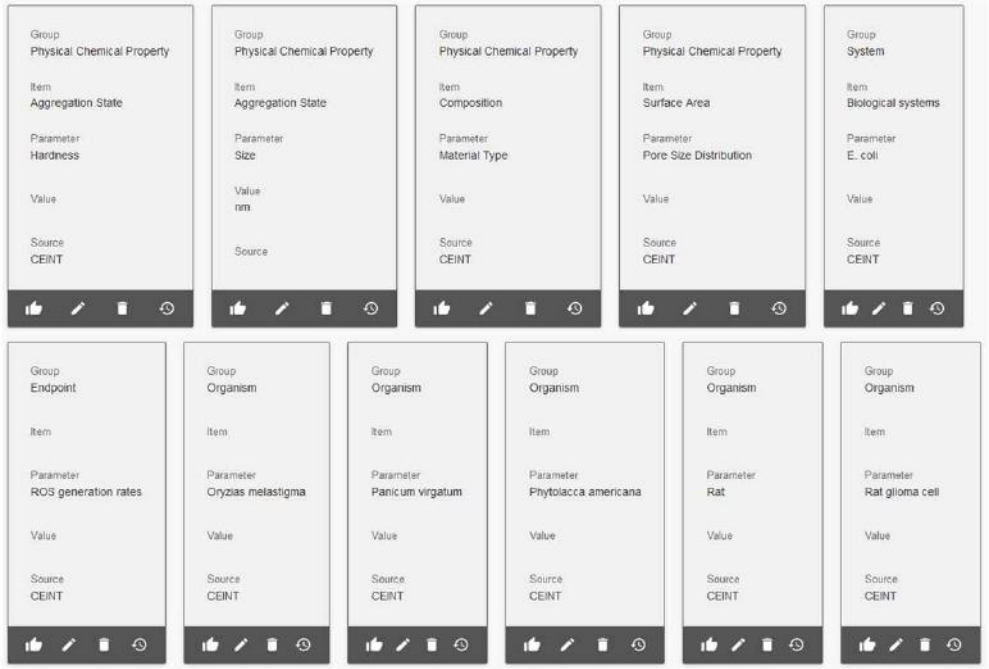
Overview & purpose



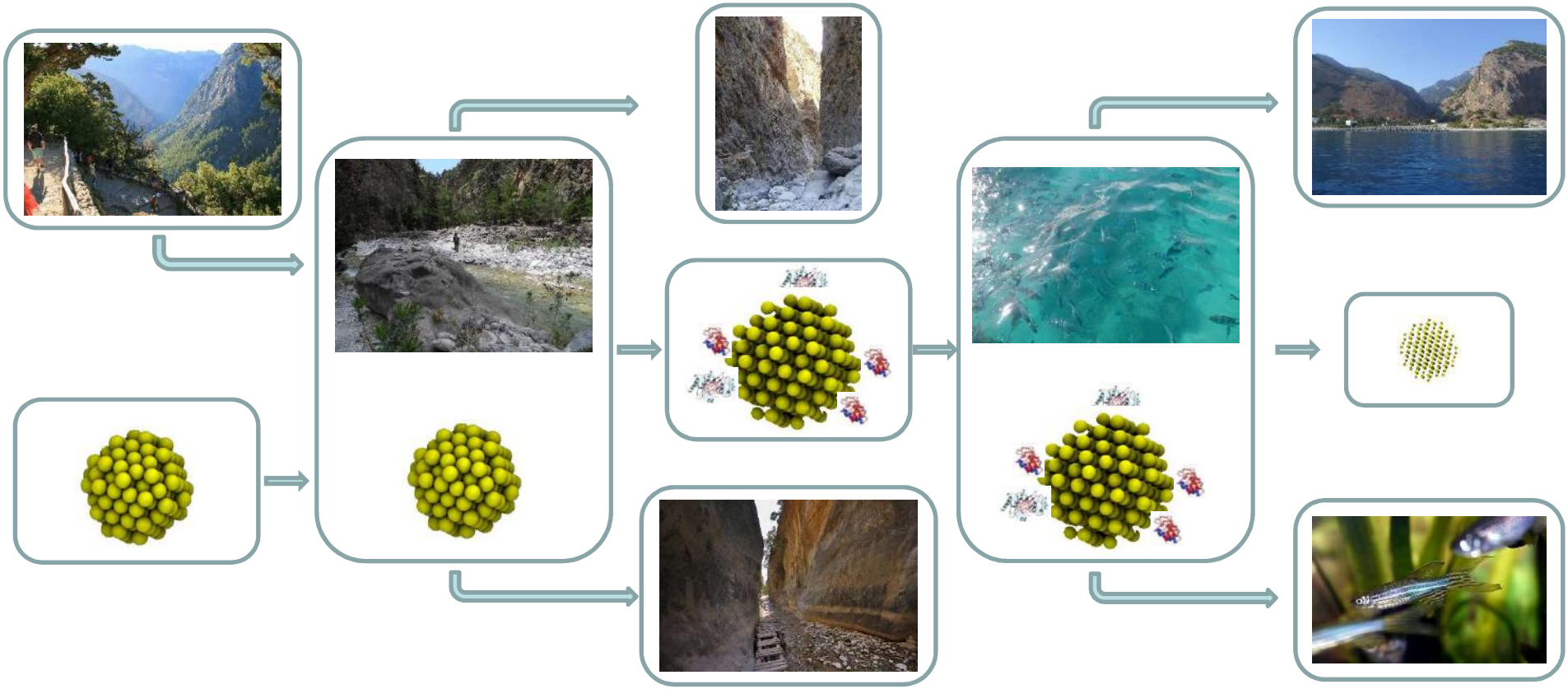
- The NIKC is an e-infrastructure consisting of a data repository and associated analytical tools developed to visualise and interrogate integrated environmental nano-datasets
- The DB is built in MySQL, and interacts with applications written in a variety of languages including R, python/django and visual basic

Overview



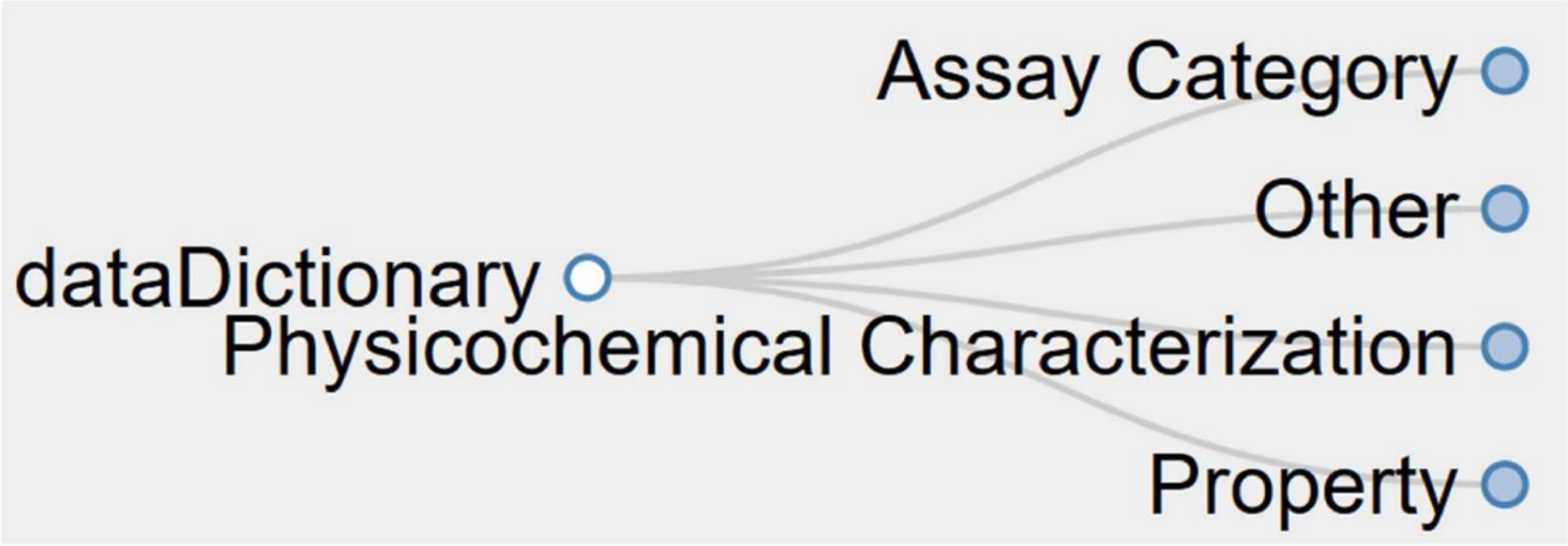
- NIKC uses the Nano-Dictionary, which is a taxonomy containing terms used in the already integrated nanomaterials fate & behaviour datasets
- The Nano-Dictionary incorporates terms from several sources (e.g. ontologies/taxonomies, other databases)
- Terms not included in other sources are defined in collaboration with relevant domain experts

NIKC world representation



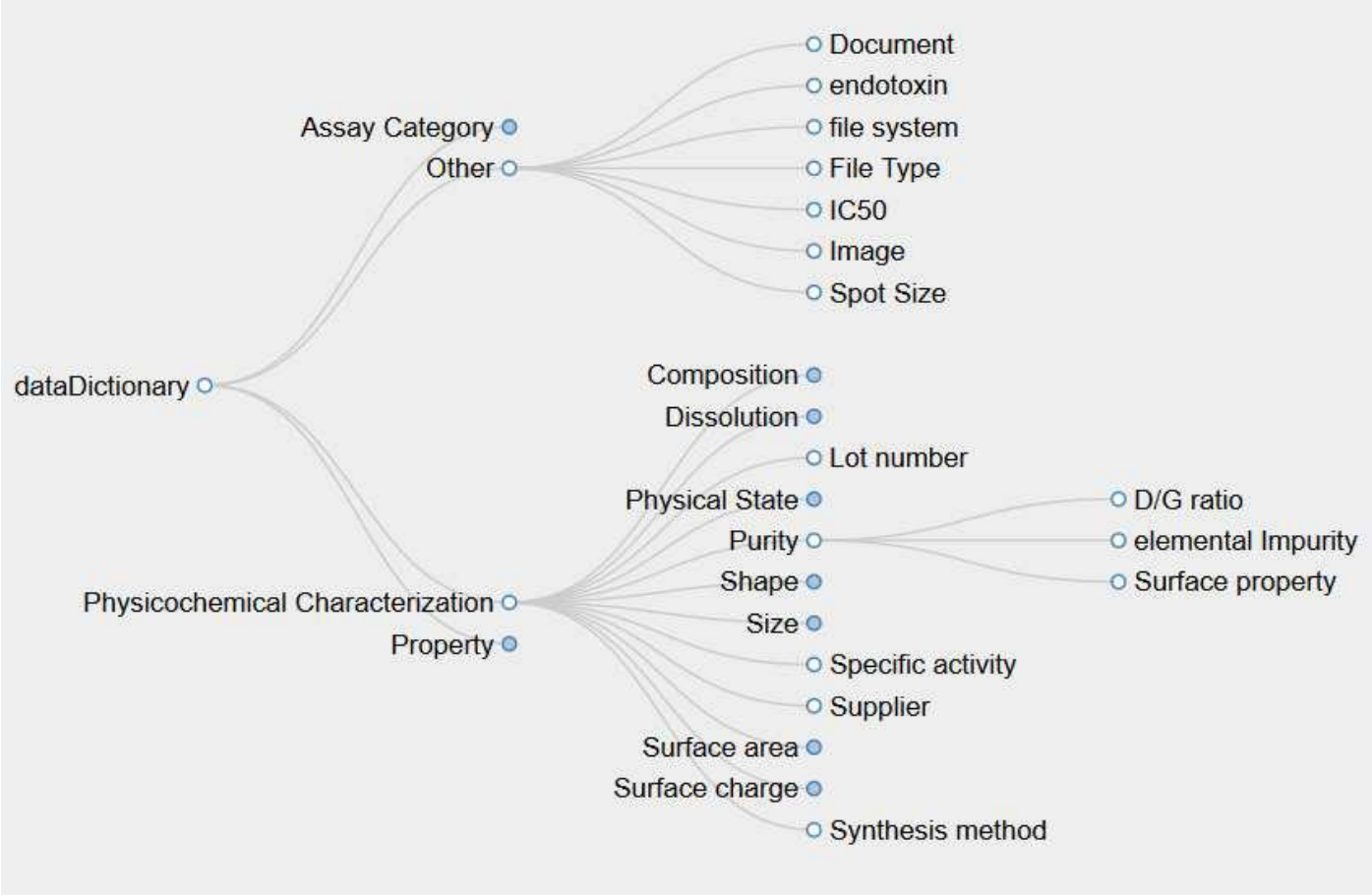
- NIKC considers ENM and surrounding environment as interconnected entities
- NIKC describes ENM, separately from the surrounding environment (which is also characterised)
- The ENM characterisation contains experimental, computational and bibliographical (i.e. atomic characteristics) descriptors

NIKC Content



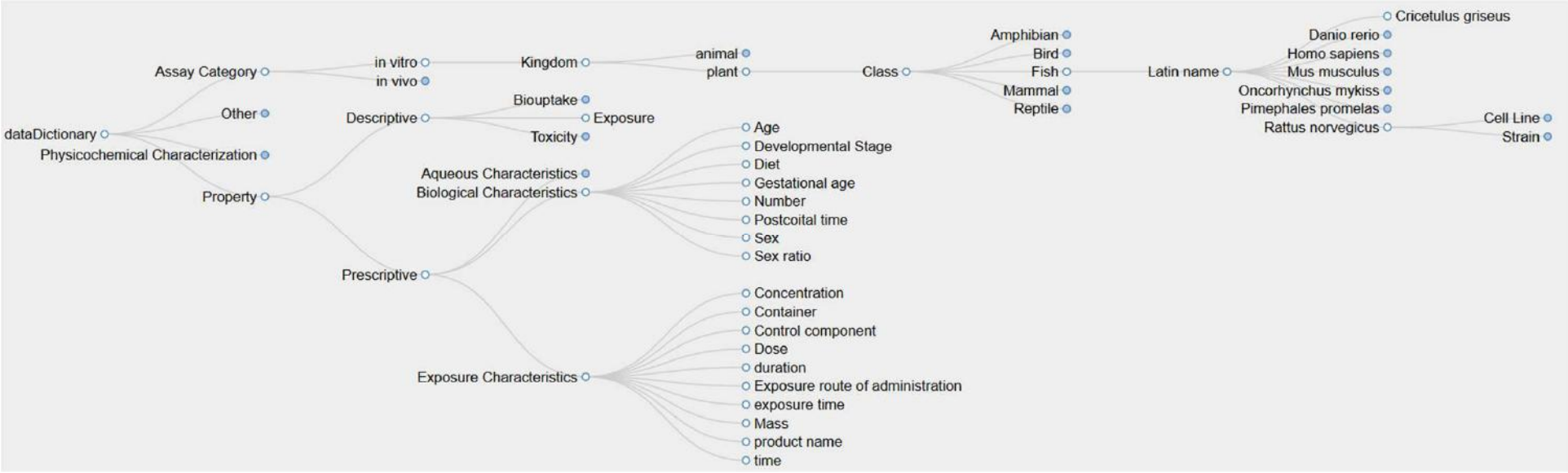
- Nanomaterials in terms of their intrinsic, extrinsic (system-dependent), and social (e.g. anticipated use scenarios, matrix, concentration in products) properties – Physicochemical characterisation
- System characteristics (environmental, biological, laboratory (methods / assays, instruments, etc.) - Property
- Exposure and Hazard measurements, calculations, and estimates - Assay
- Meta-data associated with each of these, including bibliometrics, protocols, equipment, temporal and spatial descriptors, etc. - Other

Taxonomy upper level



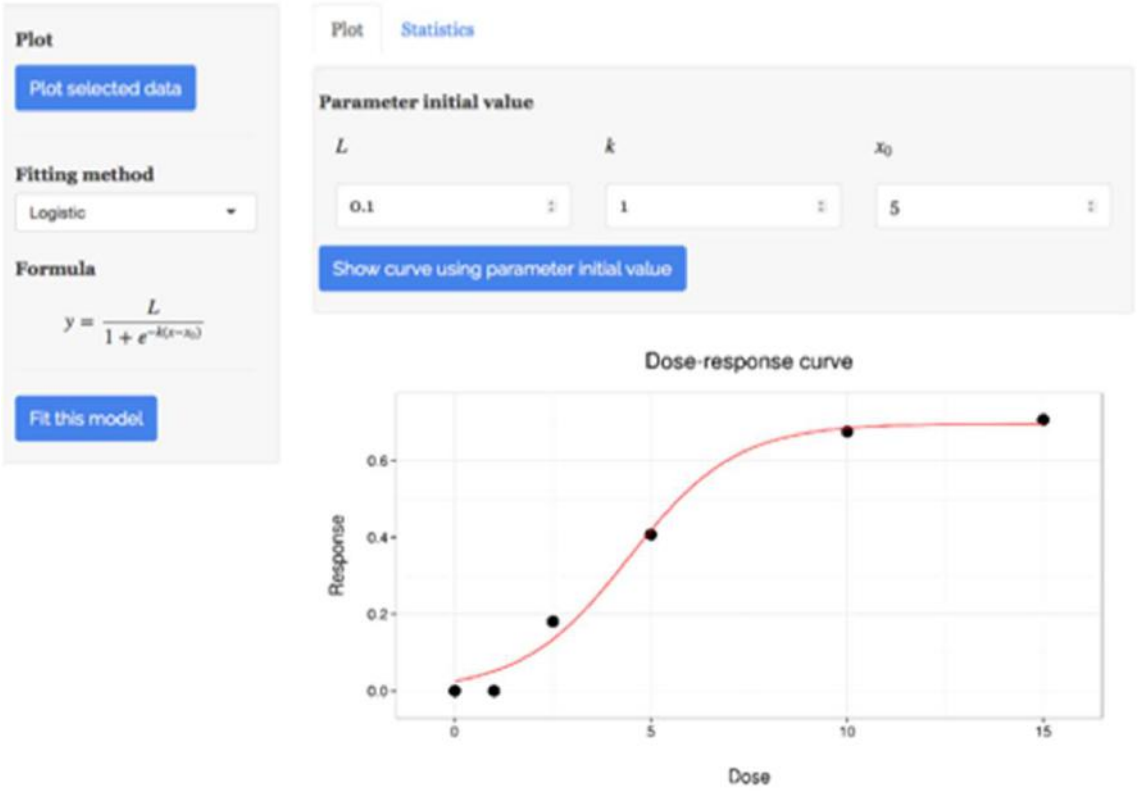
- **Phys-chem characterisation**: ENM characterisation containing all possible descriptors
- **Other**: Relevant technical metadata

Taxonomy upper level



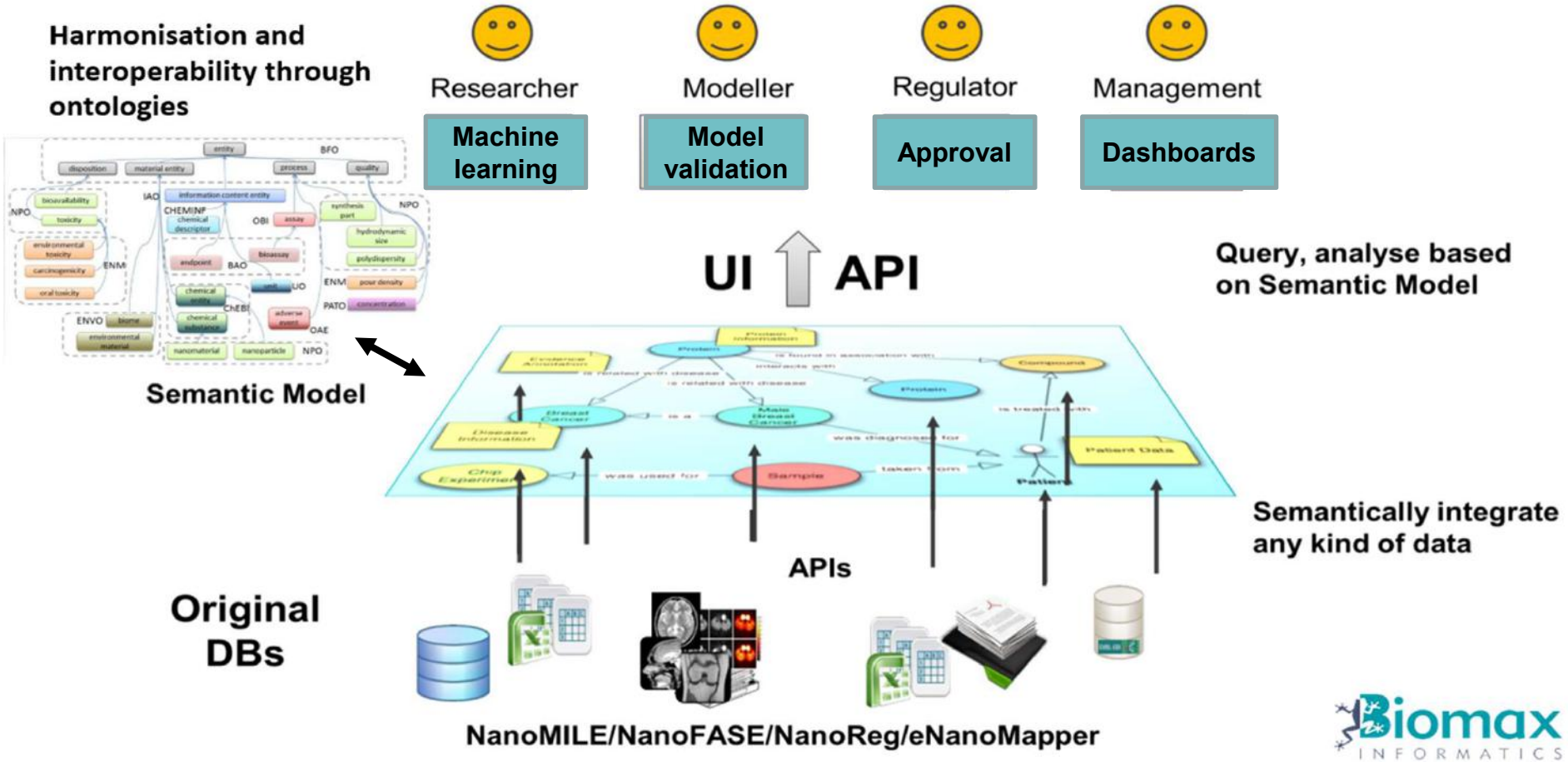
- **Assay category**: Description of the biological organisms
- **Property**: Description of the system in which the ENM is exposed

Nano Product Hazard and Exposure Assessment Tool (NanoPheat)



- NIKC will be implemented/linked with online tools allowing data harvesting, interoperability, analysis and visualisation and *in silico* modelling (through NanoCommons)
- Currently the NanoPheat tool is being developed to create dose-response curves for existing nanomaterial data

Overlap and integration



- NIKC is being integrated within the NanoCommons e-infrastructure
- To achieve maximum interoperability with other integrated databases, the nano-dictionary builds on eNanoMapper, and draws missing terms from other ontologies taxonomies (e.g. NCIT, NPO, CHEMINF, etc.)

NanoCommons

Nano-Knowledge Community

Thank you!

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