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Embedded infrastructure for primary data in chemistry

Igor Grbavac[1*], Oliver Koepler[1], S Dohmeyer-Fischer[2], Gregor Fels[2], Irina Sens[1], J Brase[1]

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Researchers around the world produce vast amounts of experimental data each day. Primary (experimental) data are the key elements of research projects and scientific publications. During the scientific workflow from the experiment to the final scientific publication primary data is analysed, interpreted and condensed to a final quintessence. But until now the handling of primary data in chemistry contains no commonly approved standards concerning reusability and long-time accessibility. Predominantly there are no quality control, no assured long-time archival storage, no proofs and no exploitation of primary data and consequently there is no assurance of data given. The concept study "Konzeptstudie Vernetzte Primärdaten-Infrastruktur für den Wissenschaftler-Arbeitsplatz" of the TIB, the workgroup of Prof. Fels and the FIZ CHEMIE aims to identify the key factors for an embedded infrastructure of primary data in the field of chemistry. In this infrastructure, chemical primary data shall be saved persistently in a central database, linked and be citable by the use of DOI (digital object identifier), be accessible and searchable. Figure 1.

We have carried out a questionnaire among researchers to analyse the scientific workflow and the chemical life-cycle of primary data in chemistry and to identify the requirements for processes and structures in an embedded scientific infrastructure for researchers. We have furthermore defined both a general and extended metadata scheme for the storage, citation and searching primary datasets. General metadata include elements necessary for citations while chemical metadata cover specific needs of describing and searching within the data itself.

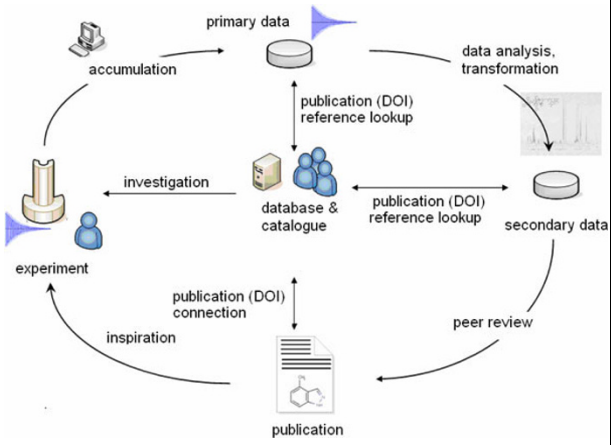

Figure 1

Author details
[1]German National Library of Science and Technology, Welfengarten 1B, 30167 Hannover, Germany. [2]Universität Paderborn, Department Chemistry, Warburgerstrasse 100, 33098 Paderborn, Germany.

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[1]German National Library of Science and Technology, Welfengarten 1B, 30167 Hannover, Germany