*Database*, 2016, 1–10
doi: 10.1093/database/baw033
Original article

Original article

# PGP repository: a plant phenomics and genomics data publication infrastructure

**Daniel Arend*, Astrid Junker, Uwe Scholz, Danuta Schüler, Juliane Wylie and Matthias Lange**

Leibniz Institute for Plant Genetics and Crop Plant Research (IPK), OT Gatersleben, Corrensstraße 3, Stadt Seeland, 06466, Gatersleben, Germany

*Corresponding author: Tel: +49 39482 5842, Fax: +49 39482 5407, Email: arendd@ipk-gatersleben.de

Citation details: Arend,D., Junker,A., Scholz,U. *et al.* PGP repository: a plant phenomics and genomics data publication infrastructure. *Database* (2016) Vol. 2016: article ID baw033; doi:10.1093/database/baw033

Received 5 November 2015; Revised 21 January 2016; Accepted 26 February 2016

## Abstract

Plant genomics and phenomics represents the most promising tools for accelerating yield gains and overcoming emerging crop productivity bottlenecks. However, accessing this wealth of plant diversity requires the characterization of this material using state-of-the-art genomic, phenomic and molecular technologies and the release of subsequent research data via a long-term stable, open-access portal. Although several international consortia and public resource centres offer services for plant research data management, valuable digital assets remains unpublished and thus inaccessible to the scientific community. Recently, the Leibniz Institute of Plant Genetics and Crop Plant Research and the German Plant Phenotyping Network have jointly initiated the Plant Genomics and Phenomics Research Data Repository (PGP) as infrastructure to comprehensively publish plant research data. This covers in particular cross-domain datasets that are not being published in central repositories because of its volume or unsupported data scope, like image collections from plant phenotyping and microscopy, unfinished genomes, genotyping data, visualizations of morphological plant models, data from mass spectrometry as well as software and documents.

The repository is hosted at Leibniz Institute of Plant Genetics and Crop Plant Research using e!DAL as software infrastructure and a Hierarchical Storage Management System as data archival backend. A novel developed data submission tool was made available for the consortium that features a high level of automation to lower the barriers of data publication. After an internal review process, data are published as citable digital object identifiers and a core set of technical metadata is registered at DataCite. The used e!DAL-embedded Web frontend generates for each dataset a landing page and supports an interactive exploration. PGP is registered as research data repository at BioSharing.org, re3data.org and OpenAIRE as valid EU Horizon 2020 open data archive. Above features, the programmatic interface and the support of standard metadata formats, enable PGP to fulfil the FAIR data principles—findable, accessible, interoperable, reusable.

**Database URL**: http://edal.ipk-gatersleben.de/repos/pgp/

## Introduction

The technical progress in plant genomics and phenomics enables a new quality in studying plant development and underlying mechanisms and processes (1, 2). Huge amounts of data are gathered in short time and require respective capacities for their analysis, management and storage. This development is furthermore supported by decreased costs for the use of technologies. One prominent example is the decrease of sequencing costs that result in the $1000 genome (3). In particular, metabolomics, phenomics, genotyping and next-generation sequencing are major driving forces. Discussed broadly as 'open data' policy, research data should in general be considered as a scientific asset. However, in practice, there is a big gap between the created and actual accessible data (4). Although this issue is addressed by service provider, a high number of datasets remain unpublished. Such service provider are:

-data journals (5), e.g. GigaScience (http://www.gigasciencejournal.com) or Nature Scientific Data (http://www.nature.com/sdata),
- international consortia that support public data management (6),
- primary data repositories such as figshare (7) and
- public databases (8), like Gramene (9) as comprehensive but specialized information system with a lot of embedded functionality for comparative functional genomics in crops.

a high number of datasets remain unpublished. This applies, e.g. to unprocessed raw data (especially in data domains for which no dedicated domain repository exists yet) or results confirming and/or deepening previous observations. Estimations suggest the 'odds of a dataset being extant fell by 17% per year' (10). On the other hand, a survey among authors published in the *Annals of Internal Medicine* between 2008 and 2012 found that their willingness to share their data decreased from 62% to 47% over the overserved period (11, 12). The increase in unpublished (lost and/or hidden) data contradicts the scientific self-conception, which is based on the spread and gain of knowledge among the scientific community. Potential reasons for keeping datasets unpublished might be missing archives for certain data domains, i.e. phenomics, technical barriers for researchers, unaccepted citation metrics, complex metadata schemas, laborious data documentation, privacy concerns, unsupported data volume and data exploitation priorities (13).

Publishing experimental data (even outside of scientific journal publications) has major advantages for the community and the publishing scientist him/herself. It enables to test the repeatability and reproducibility of scientific experiments and allows for drawing comparisons between datasets, given that metadata are sufficiently documented. Furthermore, it will generate a refund for the publishing scientist him/herself (14). To respond the challenge of losing 'hidden data' for the scientific value chain, international initiatives were established (15, 16). In this context, the DataCite consortium (17) was found to support data citation, providing means to increase the acceptance of research data as legitimate contributions to scholarly records. DataCite provides a free service to assign digital object identifiers (DOIs) (17) as globally proven standard for persistent identifiers, also enabling the registration of a minimal commonly accepted set of technical metadata for a scientific dataset. Since DOIs have already represent an accepted data citation standard (e.g. by publishers, journals and public databases), these identifiers are the preferred way for citation of datasets.

In this article, we introduce the Plant Phenomics and Genomics Data Publication Infrastructure (PGP) repository that implements all components of a sustainable data publication culture cycle (18) (Figure 1). The presented PGP repository contains diverse published datasets so far covering a variety of different data domains, starting with phenomics data gained in frame of high-throughput phenotyping experiments (Deutsches Pflanzen Phänotypisierungsnetzwerk (German Plant Phenotyping Network, http://www.dppn.de/dppn/en) to data gathered within Leibniz Institute of Plant Genetics and Crop Plant Research (IPK) Genome Research activities. After a brief introduction into the concept for a sustainable data publication, we describe the workflow how to publish, search and download datasets in PGP. In the last section, the current status (after 9 months of productive data publication service) and further objectives will be summarized.

## The IPK plant genomics and phenomics research data repository

Based on the universal electronic Data Archive Library (e!DAL) data publication and sharing infrastructure (19), the PGP was established in January 2015 at the IPK Gatersleben to share research data derived from studies of plant genomics and phenomics with particular emphasis

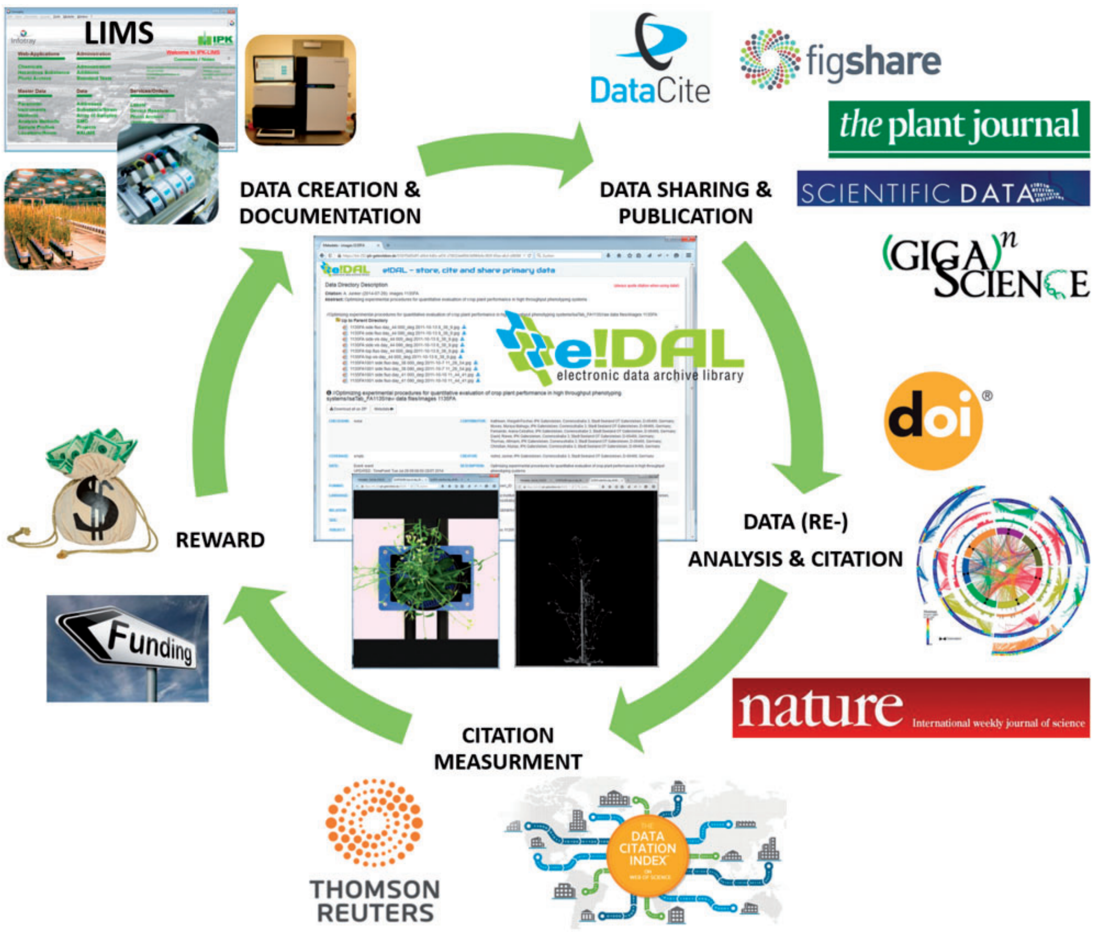


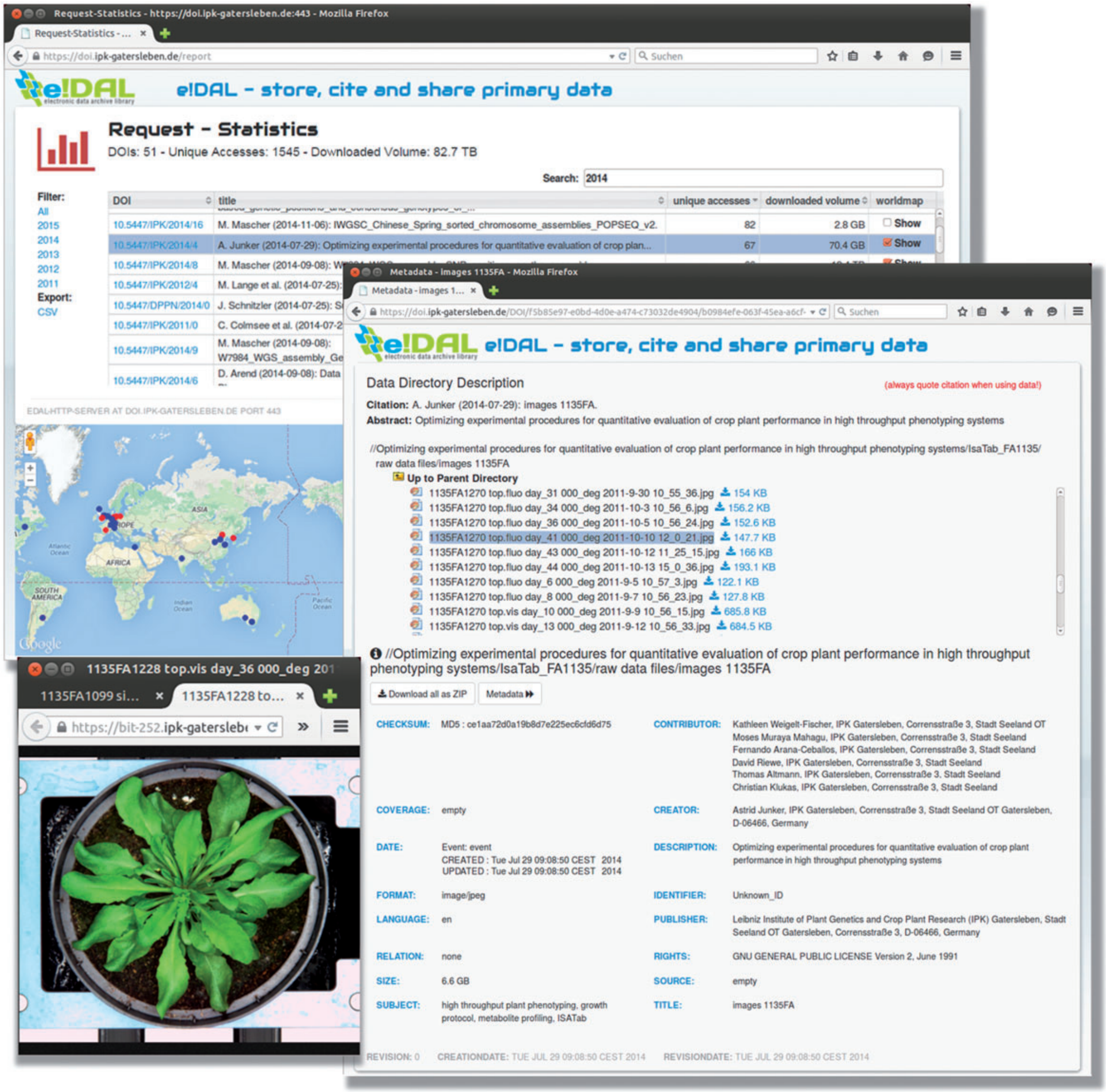
**Figure 1.** Data publication cycle. This cycle illustrates the scientific value chain for research data publication. The documentation of experimental metadata and result data represent the basis for scientific journal publications. These are the main outcomes of scientific work, representing scientific successes as the most important way of communication of research results in the community. A parallel public sharing of experimental data increase the scientific value by enabling tests for reproducibility and providing valuable resources for further downstream analysis. In turn, new findings that are reported in published datasets increase its scientific impact and boost the author's scholarly credit. Data citation indexes are increasingly accepted as measurement for scientific success which in turn represents the most important prerequisite for project proposals and the acquisition of funding for new projects.

on the support of association studies (integrating genomic and phenotypic information) as well as different kinds of supplement material, like drawings, source code and protocols. So far, published plant datasets cover different data domains ranging from phenotypic data, systems biology and molecular data to data from genome sequence analyses. The majority of data comprise collection of macroscopic and microscopic plant images, sequence assemblies, genotyping data, X-ray images and visual models of plant organs, raw data from mass spectrometry, paper supplemented spread sheets and software. As by December 2015, 54 datasets have been published as DOI and registered at the DataCite research data catalogue. Each dataset comprises a container including all records that are related to a particular experiment or scientific paper. The PGP repository currently hosts 21 157 data entities with an overall volume of 65.4 GB and is registered in the re3data registry (20) and the biosharing.org portal (21) as accepted data repositories.

## Data access

The integrated and permanently updated report frontend (Figure 2) supports the interactive exploration of stored datasets. Beside functionalities for browsing, filtering and downloading of datasets, download and access statistics are provided for each DOI.

Using the metadata search provided by DataCite (Figure 3) (http://search.datacite.org), users are enabled to explore and search specific PGP datasets of interest. A general keyword-based search functionality over all metadata, as well as a more advanced search, allows for filtering by parameters, such as authors, dates and file types are implemented. Besides, via the provided web interface, it is also



Request-Statistics - https://doi.ipk-gatersleben.de:443 - Mozilla Firefox

https://doi.ipk-gatersleben.de/report

e!DAL – store, cite and share primary data

**Request – Statistics**

DOIs: 51 - Unique Accesses: 1545 - Downloaded Volume: 82.7 TB

Search: 2014

Filter: All 2015 2014 2013 2012 2011

Export: CSV

| DOI | title | unique accesses | downloaded volume | worldmap |
|---|---|---|---|---|
| 10.5447/IPK/2014/16 | M. Mascher (2014-11-06): IWGSC_Chinese_Spring_sorted_chromosome_assemblies_POPSEQ_v2. | 82 | 2.8 GB | □ Show |
| 10.5447/IPK/2014/4 | A. Junker (2014-07-29): Optimizing experimental procedures for quantitative evaluation of crop plan... | 67 | 70.4 GB | ☑ Show |
| 10.5447/IPK/2014/8 | M. Mascher (2014-09-08): W | | | |
| 10.5447/IPK/2012/4 | M. Lange et al. (2014-07-25): | | | |
| 10.5447/DPPN/2014/0 | J. Schnitzler (2014-07-25): S | | | |
| 10.5447/IPK/2011/0 | C. Colmsee et al. (2014-07-2 | | | |
| 10.5447/IPK/2014/9 | M. Mascher (2014-09-08): W7984_WGS_assembly_Ge | | | |
| 10.5447/IPK/2014/6 | D. Arend (2014-09-08): Data | | | |

EDAL-HTTP-SERVER AT DOI.IPK-GATERSLEBEN.DE PORT 443

Metadata - images 1135FA - Mozilla Firefox

https://doi.ipk-gatersleben.de/DOI/f5b85e97-e0bd-4d0e-a474-c73032de4904/b0984efe-063f-45ea-a6cf-

e!DAL – store, cite and share primary data

Data Directory Description

(always quote citation when using data!)

**Citation:** A. Junker (2014-07-29): images 1135FA.

**Abstract:** Optimizing experimental procedures for quantitative evaluation of crop plant performance in high throughput phenotyping systems

//Optimizing experimental procedures for quantitative evaluation of crop plant performance in high throughput phenotyping systems/IsaTab_FA1135/raw data files/images 1135FA

**Up to Parent Directory**

- 1135FA1270 top.fluo day_31 000_deg 2011-9-30 10_55_36.jpg 154 KB
- 1135FA1270 top.fluo day_34 000_deg 2011-10-3 10_56_6.jpg 156.2 KB
- 1135FA1270 top.fluo day_36 000_deg 2011-10-5 10_56_24.jpg 152.6 KB
- 1135FA1270 top.fluo day_41 000_deg 2011-10-10 12_0_21.jpg 147.7 KB
- 1135FA1270 top.fluo day_43 000_deg 2011-10-12 11_25_15.jpg 166 KB
- 1135FA1270 top.fluo day_44 000_deg 2011-10-13 15_0_36.jpg 193.1 KB
- 1135FA1270 top.fluo day_6 000_deg 2011-9-5 10_57_3.jpg 122.1 KB
- 1135FA1270 top.fluo day_8 000_deg 2011-9-7 10_56_23.jpg 127.8 KB
- 1135FA1270 top.vis day_10 000_deg 2011-9-9 10_56_15.jpg 685.8 KB
- 1135FA1270 top.vis day_13 000_deg 2011-9-12 10_56_33.jpg 684.5 KB

//Optimizing experimental procedures for quantitative evaluation of crop plant performance in high throughput phenotyping systems/IsaTab_FA1135/raw data files/images 1135FA

| | | | |
|---|---|---|---|
| CHECKSUM: | MD5 : ce1aa72d0a19b8d7e225ec6cfd6d75 | CONTRIBUTOR: | Kathleen Weigelt-Fischer, IPK Gatersleben, Corrensstraße 3, Stadt Seeland OT<br>Moses Muraya Mahagu, IPK Gatersleben, Corrensstraße 3, Stadt Seeland<br>Fernando Arana-Ceballos, IPK Gatersleben, Corrensstraße 3, Stadt Seeland<br>David Riewe, IPK Gatersleben, Corrensstraße 3, Stadt Seeland<br>Thomas Altmann, IPK Gatersleben, Corrensstraße 3, Stadt Seeland<br>Christian Klukas, IPK Gatersleben, Corrensstraße 3, Stadt Seeland |
| COVERAGE: | empty | CREATOR: | Astrid Junker, IPK Gatersleben, Corrensstraße 3, Stadt Seeland OT Gatersleben, D-06466, Germany |
| DATE: | Event: event<br>CREATED : Tue Jul 29 09:08:50 CEST 2014<br>UPDATED : Tue Jul 29 09:08:50 CEST 2014 | DESCRIPTION: | Optimizing experimental procedures for quantitative evaluation of crop plant performance in high throughput phenotyping systems |
| FORMAT: | image/jpeg | IDENTIFIER: | Unknown_ID |
| LANGUAGE: | en | PUBLISHER: | Leibniz Institute of Plant Genetics and Crop Plant Research (IPK) Gatersleben, Stadt Seeland OT Gatersleben, Corrensstraße 3, D-06466, Germany |
| RELATION: | none | RIGHTS: | GNU GENERAL PUBLIC LICENSE Version 2, June 1991 |
| SIZE: | 6.6 GB | SOURCE: | empty |
| SUBJECT: | high throughput plant phenotyping, growth protocol, metabolite profiling, ISATab | TITLE: | images 1135FA |

REVISION: 0 CREATIONDATE: TUE JUL 29 09:08:50 CEST 2014 REVISIONDATE: TUE JUL 29 09:08:50 CEST 2014

1135FA1228 top.vis day_36 000_deg 201

**Figure 2.** Report page PGP repository. Screenshot of the report page embedded in the PGP Repository for each experiment. The report provides information on the current data stock, access frequencies and the number of downloads for the respective DOI. All datasets are linked and access statistics are mapped on a world map.

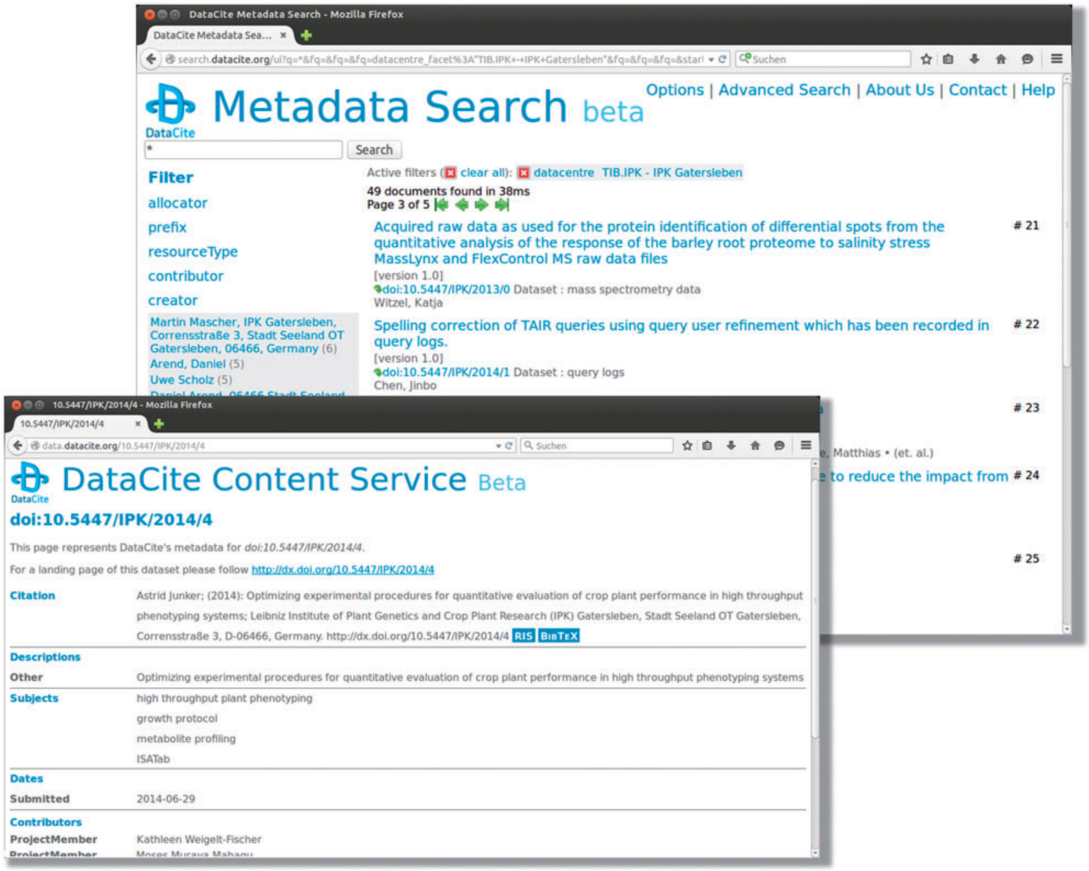
possible to use the search engine programmatically via an Apache Solr interface.

In order to harvest metadata programmatically, PGP supports the Open Archives Initiative Protocol for Metadata Harvesting (OAI-PMH) (22). Because we use the DataCite interface to register DOIs and associated metadata, all required specifications are implemented. It can be used via an application programming interface (API) integrated in DataCite (http://oai.datacite.org/oai) or the OpenAire endpoint (http://api.openaire.eu/oai_pmh) (Figure 4).

## Data submission process

In order to support the reproducibility of experimental research results, it is not sufficient to just share the produced data files and make them accessible, it is rather important to guarantee that the files are readable and reusable (23). Proprietary file formats and incomplete metadata in the worst case might even prevent opening and reading of data. A sufficient data annotation and the use of standardized file formats strongly enhance the data quality.

In general, there are two types of annotations. Technical metadata are required for data processing and managing


DataCite Metadata Search - Mozilla Firefox
DataCite Metadata Sea...
search.datacite.org/ui?q=*&fq=&fq=&fq=datacentre_facet%3A"TIB.IPK+-+IPK+Gatersleben"&fq=&fq=&fq=&start
Suchen
Metadata Search beta
DataCite
Options | Advanced Search | About Us | Contact | Help
Search
Filter
allocator
prefix
resourceType
contributor
creator

Martin Mascher, IPK Gatersleben, Corrensstraße 3, Stadt Seeland OT Gatersleben, 06466, Germany (6)
Arend, Daniel (5)
Uwe Scholz (5)

Active filters (clear all): datacentre TIB.IPK - IPK Gatersleben
49 documents found in 38ms
Page 3 of 5

Acquired raw data as used for the protein identification of differential spots from the quantitative analysis of the response of the barley root proteome to salinity stress MassLynx and FlexControl MS raw data files # 21
[version 1.0]
doi:10.5447/IPK/2013/0 Dataset : mass spectrometry data
Witzel, Katja

Spelling correction of TAIR queries using query user refinement which has been recorded in query logs. # 22
[version 1.0]
doi:10.5447/IPK/2014/1 Dataset : query logs
Chen, Jinbo

# 23
# 24
# 25
10.5447/IPK/2014/4 - Mozilla Firefox
10.5447/IPK/2014/4
data.datacite.org/10.5447/IPK/2014/4
Suchen
DataCite Content Service Beta
DataCite

doi:10.5447/IPK/2014/4

This page represents DataCite's metadata for *doi:10.5447/IPK/2014/4*.

For a landing page of this dataset please follow http://dx.doi.org/10.5447/IPK/2014/4

| | |
|---|---|
| **Citation** | Astrid Junker; (2014): Optimizing experimental procedures for quantitative evaluation of crop plant performance in high throughput phenotyping systems; Leibniz Institute of Plant Genetics and Crop Plant Research (IPK) Gatersleben, Stadt Seeland OT Gatersleben, Corrensstraße 3, D-06466, Germany. http://dx.doi.org/10.5447/IPK/2014/4 RIS BIBTEX |
| **Descriptions** | |
| **Other** | Optimizing experimental procedures for quantitative evaluation of crop plant performance in high throughput phenotyping systems |
| **Subjects** | high throughput plant phenotyping<br>growth protocol<br>metabolite profiling<br>ISATab |
| **Dates** | |
| **Submitted** | 2014-06-29 |
| **Contributors** | |
| **ProjectMember** | Kathleen Weigelt-Fischer |

**Figure 3.** DataCite metadata search interface. This screenshot shows the web interface of DataCite, where a number of filter functionalities are implemented and additional options can be defined using the advanced search functionalities.

reasons and contain information like the file type, the file size or the software environment in order to guarantee a long-term readability. The number of available technical metadata schemes is relatively small. One worldwide accepted format is the Dublin Core Metadata Element Set (DCMES) (24). In contrast, semantic metadata include a wide range of more or less complex descriptions that are strongly related to a specific research field. Semantic metadata schemas are in general dynamic and reflect ongoing discussions in the related scientific community. In consequence, homogeneous experiment documentation towards a consistent and sufficient semantic annotation of research data is a still challenging task. One interesting and promising approach is the ISA-Tab format (25), which is connected with domain-specific metadata configurations. It is a general format container for semantic annotations.

Beside a sustainable data annotation to efficiently describe the performed experiments, used parameters or the implemented source code, it is necessary that the datasets and their corresponding metadata pass through an additional, internal review process before being published. In general two reviewer groups are distinguished 'scientific' and 'administrative reviewers'.

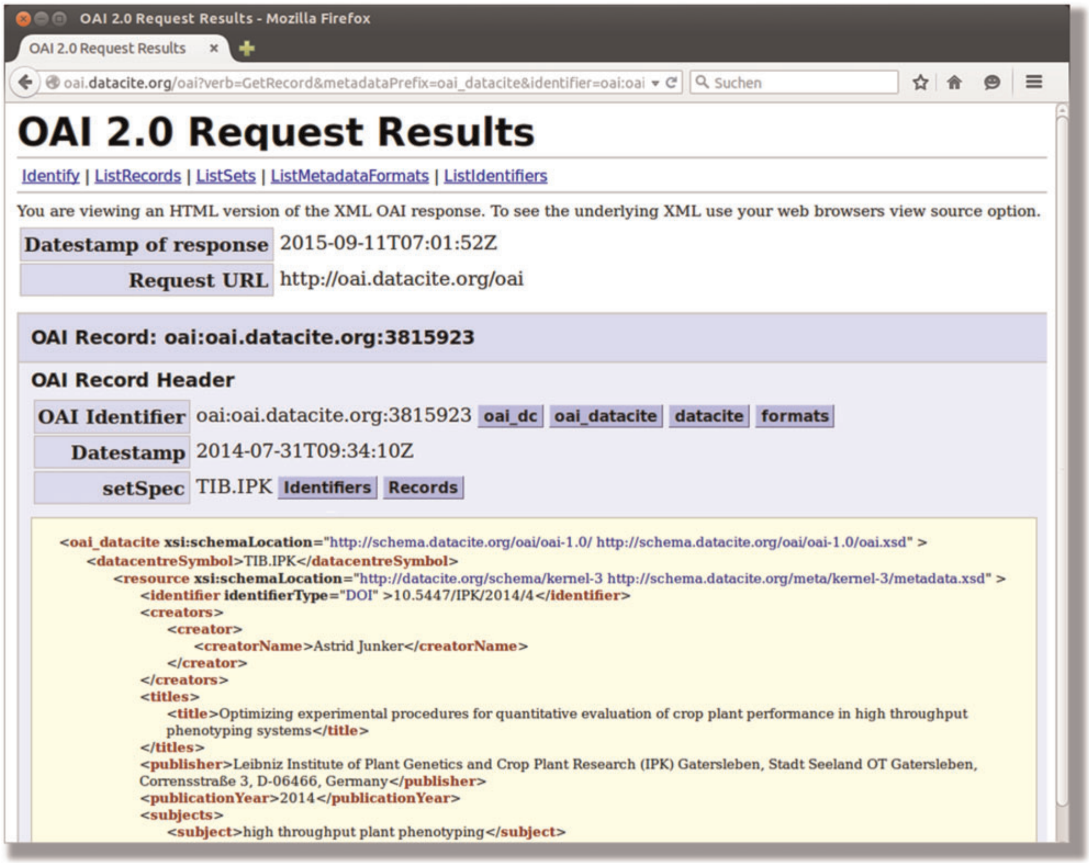
Scientific evaluation: Scientific reviewers have scientific expertise in the author's research area and are asked to evaluate the dataset for scientific quality.

Administrative evaluation: The administrative reviewers are responsible to check for publication rights (especially open access) and potential conflicts with respect to intellectual property and patent regulations of the partners/co-authors and/affiliated institutions.

To our knowledge, no defined criteria hitherto exist for a data publication review process. Therefore, we suggest a checklist including a minimal set of quality criteria for data reviewers. This prioritized guideline is based on recommendations of the nestor working group (26) and BioSharing initiative (27). The minimal set of criteria is listed below and does not represent an obligatory catalogue or checklist, but the reviewers should rather consider these criteria as recommendations supporting their decision and should reflect commonly accepted data quality standards.

Experiment documentation: Hypothesis, materials, methods, conditions, parameters and experimental factors, results.

Authorship: Ownership, license and IP issues, patents.


OAI 2.0 Request Results - Mozilla Firefox
OAI 2.0 Request Results
oai.datacite.org/oai?verb=GetRecord&metadataPrefix=oai_datacite&identifier=oai:oai
Suchen

# OAI 2.0 Request Results

Identify | ListRecords | ListSets | ListMetadataFormats | ListIdentifiers

You are viewing an HTML version of the XML OAI response. To see the underlying XML use your web browsers view source option.

| | |
|---|---|
| Datestamp of response | 2015-09-11T07:01:52Z |
| Request URL | http://oai.datacite.org/oai |

**OAI Record: oai:oai.datacite.org:3815923**

**OAI Record Header**

| | |
|---|---|
| OAI Identifier | oai:oai.datacite.org:3815923 oai_dc oai_datacite datacite formats |
| Datestamp | 2014-07-31T09:34:10Z |
| setSpec | TIB.IPK Identifiers Records |

```
<oai_datacite xsi:schemaLocation="http://schema.datacite.org/oai/oai-1.0/ http://schema.datacite.org/oai/oai-1.0/oai.xsd" >
    <datacentreSymbol>TIB.IPK</datacentreSymbol>
        <resource xsi:schemaLocation="http://datacite.org/schema/kernel-3 http://schema.datacite.org/meta/kernel-3/metadata.xsd" >
            <identifier identifierType="DOI" >10.5447/IPK/2014/4</identifier>
            <creators>
                <creator>
                    <creatorName>Astrid Junker</creatorName>
                </creator>
            </creators>
            <titles>
                <title>Optimizing experimental procedures for quantitative evaluation of crop plant performance in high throughput
                phenotyping systems</title>
            </titles>
            <publisher>Leibniz Institute of Plant Genetics and Crop Plant Research (IPK) Gatersleben, Stadt Seeland OT Gatersleben,
            Corrensstraße 3, D-06466, Germany</publisher>
            <publicationYear>2014</publicationYear>
            <subjects>
                <subject>high throughput plant phenotyping</subject>
```

**Figure 4.** DataCite OAI-interface. This snapshot illustrates the result of an OAI request to DataCite.

Data structure: Hierarchical folder structures, consistent file naming, avoid archive files.

Semantic metadata: Representation of experimental metadata using a standardized metadata scheme.

The 'Experiment documentation' and information about 'authorships' provide metadata assigned to the submitted dataset, which provides at least a minimal experimental context and dataset description as well as technical information to ensure later data access. In contrast, 'data structure' and 'semantic metadata' are no mandatory elements, but enable long-term usability and repeatability. Further scientific criteria, such as statistical validation of the dataset, are part of the data post-processing pipeline and are not obligatory for dataset publication in PGP. Although, if available, it is very valuable to complement raw data in the repository and its publication along with these, it is kept in the reasonability of the submitting scientist.

## Submission tool

Based on the prerequisites for data publication defined in the sections above, this section describes a software tool that meets and considers all formal and technical requirements for archiving and publishing research data and comprises all necessary functionalities from data upload to DOI registration. According to the data publication workflow (Figure 5), scientists first organize and describe their experimental data, which can then be uploaded followed by a reviewing procedure as described in Data submission process section. After approval by the reviewers, a DOI is assigned as permanent reference for data sharing. In the following, the implementation of the described workflow in the frame of a data publication tool is shown.

The publication process is initiated by uploading the dataset together with a mandatory subset of technical metadata (see Data submission process section). The metadata, e.g. file size, file type or file format, will be automatically determined. Furthermore, the tool enables to reuse metadata from previous sessions. The screenshot in Figure 6 shows the graphical interface of the publication tool that was developed to submit a dataset and request for a DOI. This platform-independent Java WebStart application was designed to be user-friendly and intuitive. It supports the automatic setup of the network infrastructure, such as proxy and SMTP-server detection.

In order to facilitate the handling for the user, the graphical user interface was designed in a way that

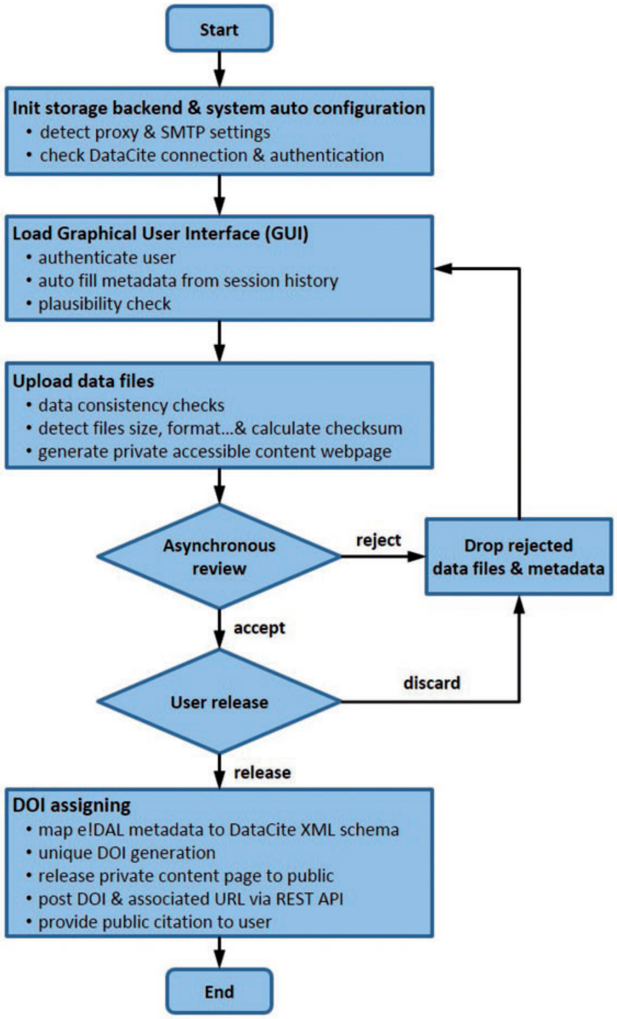

Start
Init storage backend & system auto configuration
• detect proxy & SMTP settings
• check DataCite connection & authentication
Load Graphical User Interface (GUI)
• authenticate user
• auto fill metadata from session history
• plausibility check
Upload data files
• data consistency checks
• detect files size, format…& calculate checksum
• generate private accessible content webpage
Asynchronous review
reject
Drop rejected data files & metadata
accept
User release
discard
release
DOI assigning
• map e!DAL metadata to DataCite XML schema
• unique DOI generation
• release private content page to public
• post DOI & associated URL via REST API
• provide public citation to user
End

**Figure 5.** The data publication process. This flowchart illustrates the several steps of the described data publication and approval workflow.

resembles standard submission forms of scientific journals or conferences. An optional embargo date can be defined to hide the public access to DOI landing page of a dataset up to the defined time point. After data upload to the mounted storage backend is finished, the reviewers are notified of the publication request by an email that includes a private URL with restricted access to the submitted files and metadata (Figure 7A).

In case the submission was rejected, the requesting user is informed and asked to revise/re-format the submitted dataset. After successful review, the author is notified (Figure 7B) and can confirm the assigned DOI or alternatively discard the submission. The released DOI will be registered and sent out to the respective user within an additional email (Figure 7C). Alternatively, the author can wait with the final decision to assign a DOI and use the temporary preview link from the notification, e.g. to provide access to the reviewers of a manuscript.

After a new data submission has been recorded, the reviewers immediately receive a notification with private links to data and metadata files, including a request for evaluation (Figure 2). The scientific and administrative reviewers evaluate the dataset with regard to scientific and formal aspects and will give feedback to the author.

### Approval and DOI registration

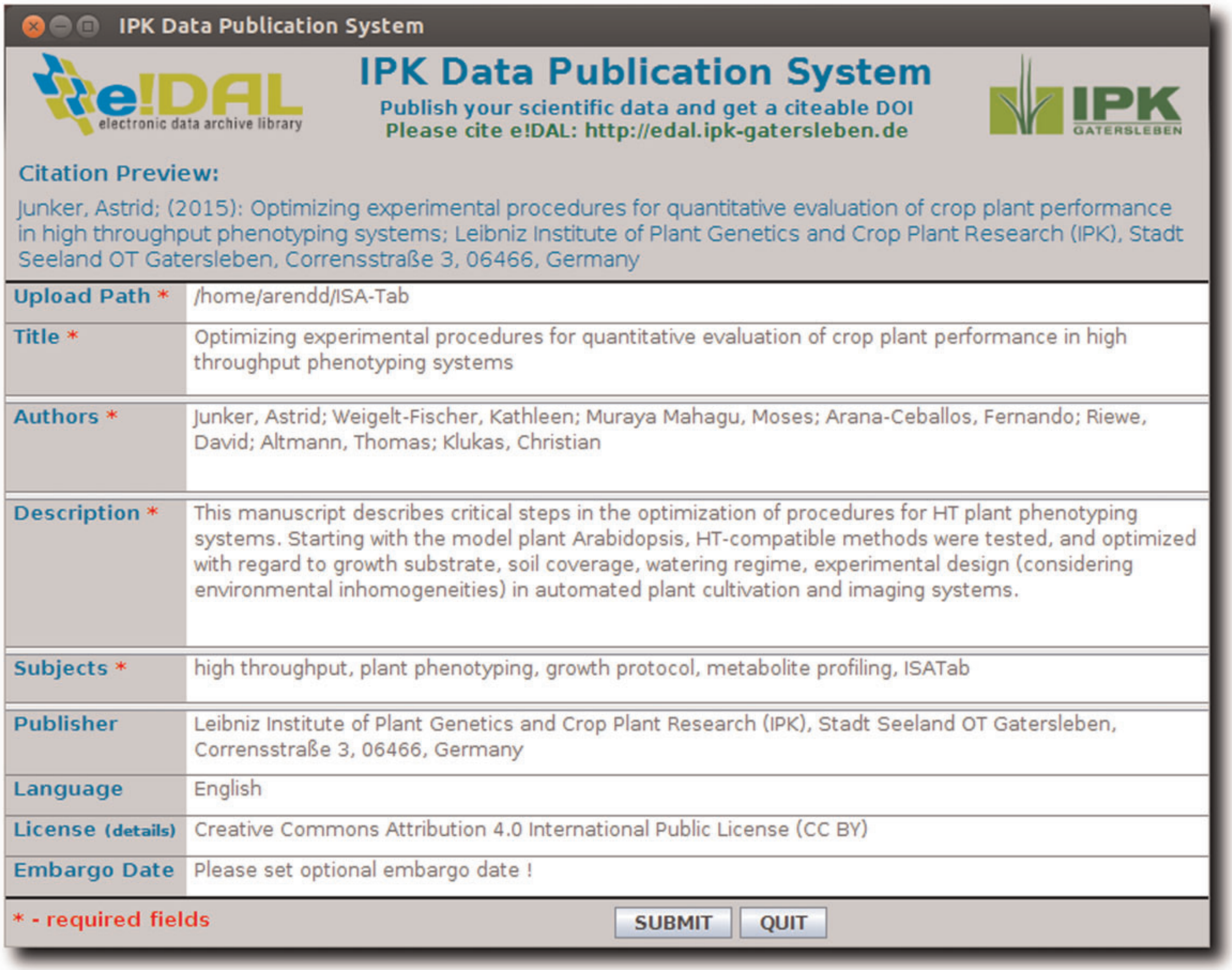
In order to approve a data publication and DOI registration, a review workflow containing two scientists and one administrative decision maker was implemented. All reviewers decide whether they accept or reject the request for publishing a dataset. The reviewer's ratings are combined by a configurable decision matrix to a final decision. The default matrix (Table 1) let a scientific reviewer or its assistant decide for reject or acceptance. The administrative reviewer may confirm their decisions or draw a veto that rejects the entire submission. As mentioned in Data submission process section, the definition of scientific and administrative reviewers increases the data quality and prevent from publishing secret information. Nevertheless, this preconfigured default review process can be customized to reflect other institutional policies.

For the final DOI registration, it is necessary to transfer the metadata and the access URL of the particular dataset to the DataCite resolving system (http://mds.datacite.org). DataCite provides a REST API to post both as XML document, which has to be conforming to the DataCite Metadata Schema (http://schema.datacite.org). The e!DAL DCMES metadata attributes are mapped to the corresponding DataCite elements. The generation of a unique DOI followed the schema illustrated in Figure 8. The Apache Solr interface of the DataCite Search API (http://search.datacite.org) allows to request the number of existing DOIs, the prefix and name of the registered data centre.

## Summary and outlook

The PGP repository provides access to plant phenomics and genomics research data, which is hitherto not supported by any existing international repository. The main focus of PGP is to publish and share primary experimental data covering a variety of data domains such as image collections from high-throughput plant phenotyping, sequence assemblies, genotyping data, visualizations of morphological plant models, data from mass spectrometry and even software. Datasets in the repository are assigned to citable DOIs that are registered at DataCite with a standardized set of technical metadata.

To lower barriers for researchers in sharing their data, the process of publishing data was made user-friendly and faster and supports best practices for data publication. Those are an online review and notification process, support of embargo and private pre-publication access,



IPK Data Publication System

Publish your scientific data and get a citeable DOI
Please cite e!DAL: http://edal.ipk-gatersleben.de

Citation Preview:

Junker, Astrid; (2015): Optimizing experimental procedures for quantitative evaluation of crop plant performance in high throughput phenotyping systems; Leibniz Institute of Plant Genetics and Crop Plant Research (IPK), Stadt Seeland OT Gatersleben, Corrensstraße 3, 06466, Germany

| | |
|---|---|
| Upload Path * | /home/arendd/ISA-Tab |
| Title * | Optimizing experimental procedures for quantitative evaluation of crop plant performance in high throughput phenotyping systems |
| Authors * | Junker, Astrid; Weigelt-Fischer, Kathleen; Muraya Mahagu, Moses; Arana-Ceballos, Fernando; Riewe, David; Altmann, Thomas; Klukas, Christian |
| Description * | This manuscript describes critical steps in the optimization of procedures for HT plant phenotyping systems. Starting with the model plant Arabidopsis, HT-compatible methods were tested, and optimized with regard to growth substrate, soil coverage, watering regime, experimental design (considering environmental inhomogeneities) in automated plant cultivation and imaging systems. |
| Subjects * | high throughput, plant phenotyping, growth protocol, metabolite profiling, ISATab |
| Publisher | Leibniz Institute of Plant Genetics and Crop Plant Research (IPK), Stadt Seeland OT Gatersleben, Corrensstraße 3, 06466, Germany |
| Language | English |
| License (details) | Creative Commons Attribution 4.0 International Public License (CC BY) |
| Embargo Date | Please set optional embargo date ! |

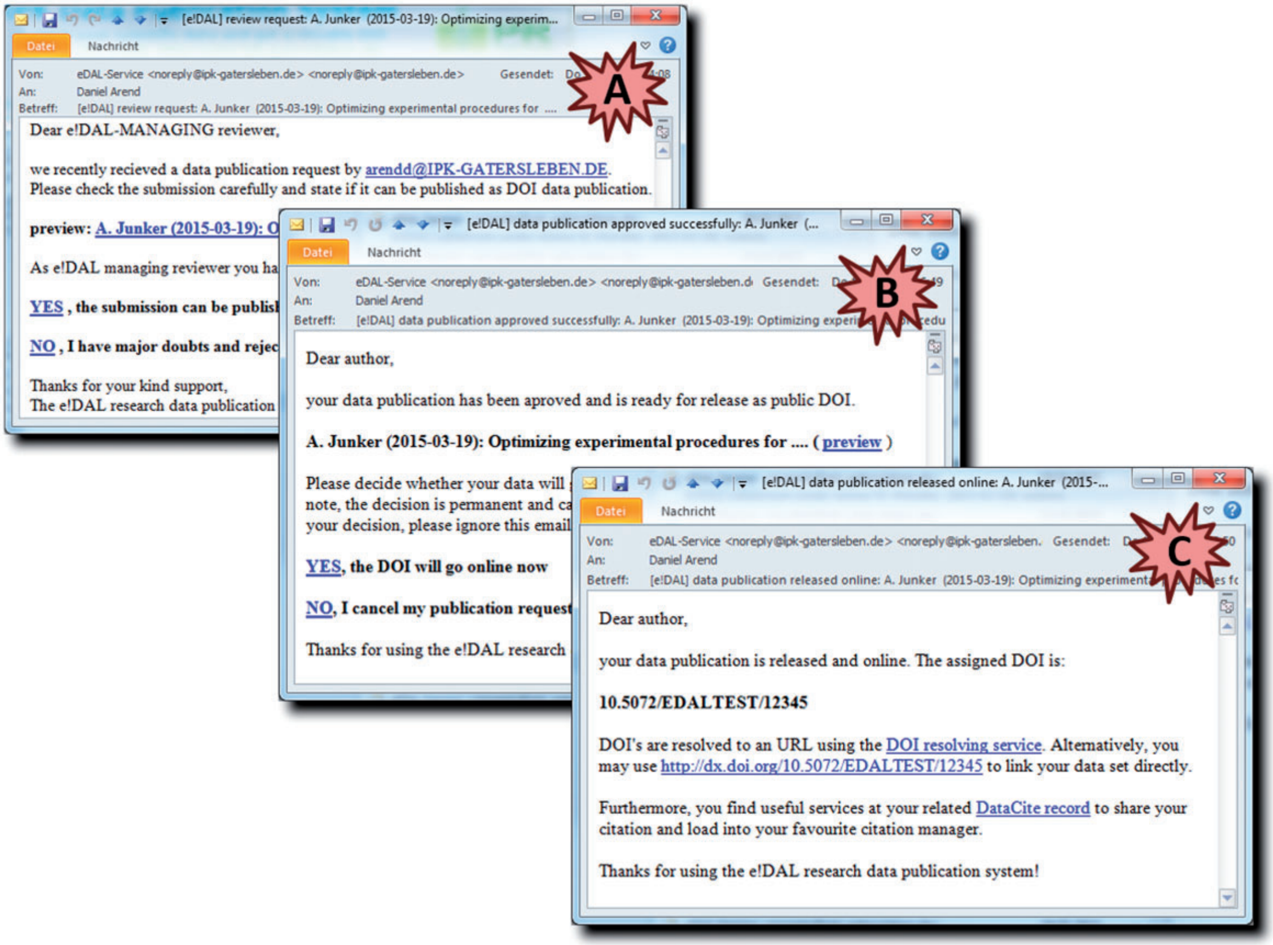
* - required fields

**Figure 6.** Data publication tool. This screenshot shows the user interface of the submission tool used for data review and publication.

bibliographically accepted data citation and the obligation to the scientist to provide a minimal set of widely accepted technical metadata. As result, the data publication has become a self-evident procedure instead of being a handicap for data producers. Currently, PGP provides access to about 22 000 files (http://edal.ipk-gatersleben.de/repos/pgp/). Since January 2015, the repository was accessed by over 1500 unique IPs addresses worldwide. Overall, PGP had in average 2500 clicks per month so far. The downloaded volume is about 82 TB and expresses the demands and interests of the scientific community in primary research data from crop plants.

The integrated Web frontend supports the interactive exploration of available datasets. Beside functionalities to search, filter and download datasets, access matrices are provided for each DOI. The comprehensive API support for programmatic access by DOI-URLs, DataCite APIs, OAI-PMH harvesting protocols and the e!DAL native programming interface enable wide range of bioinformatics tool to search, browse and access the stored datasets. Using those interfaces, we implement the FAIR data paradigm—findable, accessible, interoperable and reusable—for each published dataset. So, the PGP supports the OAI-PMH metadata harvesting protocol, it is registered at BioSharing.org, re3data and OpenAire as valid EU Horizon 2020 ‘open data’ repositories.

Beside the benefits for the public research community, the PGP repository also increases the scientific credit for publishing authors. The reports embedded in PGP for each DOI (dataset) provide statistics about total number of unique downloads of a single DOI, total downloaded data volume per DOI. These statistics are of importance for the author as a personal feedback about the use of submitted datasets and can furthermore can be used to support project proposals since funding agencies increasingly request detailed data management and publication strategies. In addition, high access to specific datasets proves scientific relevance and excellence in the respective field as well (14). More sophisticated data citation metrics, like the Thomson Reuters Data Citation Index (28), are underway to compute



[e!DAL] review request: A. Junker (2015-03-19): Optimizing experim...

Von: eDAL-Service <noreply@ipk-gatersleben.de> <noreply@ipk-gatersleben.de> Gesendet: Do
An: Daniel Arend
Betreff: [e!DAL] review request: A. Junker (2015-03-19): Optimizing experimental procedures for ....

Dear e!DAL-MANAGING reviewer,

we recently recieved a data publication request by arendd@IPK-GATERSLEBEN.DE.
Please check the submission carefully and state if it can be published as DOI data publication.

**preview: A. Junker (2015-03-19): O**

As e!DAL managing reviewer you ha

**YES , the submission can be publis**

**NO , I have major doubts and rejec**

Thanks for your kind support,
The e!DAL research data publication

[e!DAL] data publication approved successfully: A. Junker (...

Von: eDAL-Service <noreply@ipk-gatersleben.de> <noreply@ipk-gatersleben.d Gesendet: D
An: Daniel Arend
Betreff: [e!DAL] data publication approved successfully: A. Junker (2015-03-19): Optimizing experi

Dear author,

your data publication has been aproved and is ready for release as public DOI.

**A. Junker (2015-03-19): Optimizing experimental procedures for .... ( preview )**

Please decide whether your data will
note, the decision is permanent and ca
your decision, please ignore this email

**YES, the DOI will go online now**

**NO, I cancel my publication request**

Thanks for using the e!DAL research

[e!DAL] data publication released online: A. Junker (2015-...

Von: eDAL-Service <noreply@ipk-gatersleben.de> <noreply@ipk-gatersleben. Gesendet: D
An: Daniel Arend
Betreff: [e!DAL] data publication released online: A. Junker (2015-03-19): Optimizing experimenta

Dear author,

your data publication is released and online. The assigned DOI is:

**10.5072/EDALTEST/12345**

DOI's are resolved to an URL using the DOI resolving service. Altematively, you may use http://dx.doi.org/10.5072/EDALTEST/12345 to link your data set directly.

Furthermore, you find useful services at your related DataCite record to share your citation and load into your favourite citation manager.

Thanks for using the e!DAL research data publication system!

**Figure 7.** Email notification system. These screenshots show example emails that are generated for communication of the requesting user and the reviewers during the approval process. (**A**) DOI request notification to reviewer. (**B**) Accept notification to requesting user. (**C**) Notification with finally assigned DOI.

**Table 1.** Default decision matrix to compute the final reviewing result

| Managing reviewer | Senior scientist | Deputy scientist |
|---|---|---|
| Accept | Accept | Any |
| Accept | No response | Accept |

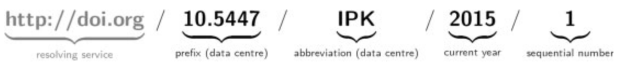


**Figure 8.** Schema of DOI assignment. This schema used to generate a unique DOI for a new dataset.

impact factors for published datasets, which offer a more consistent impact statistics and complement the common science citation indexes (29). The beforehand mentioned dedicated data journals are a further way to get credit for published experimental data. PGP is accepted as repository under the name 'IPK Gatersleben' for the *Nature Scientific Data* journal, so scientist are able to submit along their published dataset a method paper like, the publication of genotyping data from 52 highly diverse accessions of the model allopolyploid plant *Brassica napus* (30).

The e!DAL backend infrastructure is used to set-up and operate the PGP repository. As an extension, we implemented a data submission tool that uses e!DAL's client-server API and provides an intuitive user interface for data submission, review and publication. The review process was integrated into the e!DAL as novel API functions. The used server backend is a LINUX server with a 4 core CPU and 60 GB RAM. The storage backend is an Oracle Hierarchical Storage Manager with 211 TB storage capacity. As administrative prerequisite to publish DOIs, IPK as PGP hosting institute is registered as data centre.

Future developments on the technical level will comprise the support of cloud-based services, such as distributed service or peer to peer data replication to pin selected PGP datasets to the tool installation and avoid time consuming data downloads. At the level of the datasets, more emphasis will be put to the extension of the currently rather technical metadata towards semantic annotation of published experiments. It is envisaged to supplement more DOIs by ISA-Tab-formatted experiment semantics (including detailed information about experimental conditions, parameters, samples and measurements). In addition, the aim is to integrate data from IPK's Laboratory Information Management System and PGP repository into a continuous data publication workflow. Thus, an increasing number of sufficiently annotated and well-documented datasets from a variety of data domains will be stored in PGP and thereby made available to the scientific community. In the future, the presented PGP repository might also be opened to allow publication and storage of datasets provided by external users. In its function as a phenomics data repository, PGP is unique and will be further extended in order to support data management and publication in this growing community.

## Acknowledgements

We thank Thomas Münch, Jens Bauernfeind and Heiko Miehe as storage and network administrator. Furthermore, we would like to express our thanks to Anna Scholz for her great support in the spelling correction of the manuscript.

## Funding

Part of this work was performed within the German-Plant-Phenotyping Network, which is funded by the German Federal Ministry of Education and Research (project identification number: FKZ031A053). Funding for open access charge: Leibniz Association, Chausseestraße 111, 10115 Berlin, Germany.

*Conflict of interest*. None declared.

## References

1. Brooksbank,C. *et al.* (2014) The European Bioinformatics Institute's data resources 2014. *Nucleic Acids Res.*, **42**(Database issue), D18–D25.
2. Craddock,T. *et al.* (2008) e-Science: relieving bottlenecks in large-scale genome analyses. *Nat. Rev. Microbiol.*, **6**, 948–954.
3. Clarke,L. *et al.* (2012) The 1000 Genomes Project: data management and community access. *Nat. Methods*, **9**, 459–462.
4. Tellam,R. *et al.* (2015) The primary reasons behind data sharing, its wider benefits and how to cope with the realities of commercial data. *BMC Genom.*, **16**, 1–4.
5. Chavan,V. and Penev, L. (2011) The data paper: a mechanism to incentivize data publishing in biodiversity science. *BMC Bioinform.*, **12**(Suppl 15), S1–S12.
6. Kodama,Y. *et al.* (2012) The Sequence Read Archive: explosive growth of sequencing data. *Nucleic Acids Res.*, **40**(Database issue), D54–D56.
7. Singh,J. (2011) *FigShare. J. Pharmacol. Pharmacother.*, **2**, 138–139.
8. Fernandez-Suarez,X.M., Rigden,D.J. and Galperin,M.Y. (2014) The 2014 Nucleic Acids Research Database Issue and an updated NAR online Molecular Biology Database Collection. *Nucleic Acids Res.*, **42(Database issue)**, D1–D6.
9. Monaco,M.K. *et al.* (2014) Gramene 2013: comparative plant genomics resources. *Nucleic Acids Res.*, **42**(Database issue), D1193–D1199.
10. Vines,T.H. *et al.* (2014) The availability of research data declines rapidly with article age. *Curr. Biol.*, **24**, 94–97.
11. (2009) *Data's shameful neglect. Nature*, **461**, 145.
12. Gibney,E. and Van Noorden,R. (2013) Scientists losing data at a rapid rate. *Nature*, 504. (doi: 10.1038/nature.2013.14416).
13. Piwowar,H.A. (2011) Who shares? Who doesn't? Factors associated with openly archiving raw research data. *PLoS One*, **6**, e18657. 1–13.
14. Piwowar,H.A., Day,R.S. and Fridsma,D.B. (2007) Sharing detailed research data is associated with increased citation rate. *PLoS One*, **2**, e308. 1–5.
15. Crosswell,L.C. and Thornton,J.M. (2012) ELIXIR: a distributed infrastructure for European biological data. *Trends Biotechnol.*, **30**, 241–242.
16. Lagoze,C.H. and Van de Sompel (2001) The Open Archives Initiative: Building a low-barrier interoperability framework. In: *Proceedings of the 1st ACM/IEEE-CS Joint Conference on Digital Libraries, 2001*. New York, NY, USA: ACM.
17. Neumann,J. and Brase, J. (2014) DataCite and DOI names for research data. *J. Comput. Aided Mol. Des.*, **28**, 1035–1041.
18. Krajewski,P. *et al.* (2015) Towards recommendations for metadata and data handling in plant phenotyping. *J. Exp. Bot.*, **66**, 5417–5427.
19. Arend, D., *et al.* (2014) e!DAL–a framework to store, share and publish research data. *BMC Bioinform.*, **15**, 1–13.
20. Pampel,H. *et al.* (2013) Making Research Data Repositories Visible: The re3data.org Registry. *PLoS One*, **8**, e78080. 1–10.
21. Field,D. *et al.* (2009) 'Omics data sharing. *Science*, **326**, 234–236.
22. Sompel,H.V. *et al.* (2004) Resource harvesting within the OAI-PMH framework. *D-Lib Mag.*, **10**. (http://dspace.library.uu.nl/handle/1874/3163).
23. Peng,R.D. (2011) Reproducible research in computational science. *Science*, **334**, 1226–1227.
24. Weibel,S. (1997) The Dublin core: a simple content description model for electronic resources. *Bull. Am. Soc. Inform. Sci. Technol.*, **24**, 9–11.
25. Rocca-Serra,P. *et al.* (2010) ISA software suite: supporting standards-compliant experimental annotation and enabling curation at the community level. *Bioinformatics*, **26**, 2354–2356.
26. Neuroth, H. *et al.* (2010) *Nestor Handbuch: eine kleine Enzyklopädie der digitalen Langzeitarchivierung v2.3*. Niedersächsische Staats- und Universitätsbibliothek Göttingen, Platz der Göttinger Sieben 1, 37073 Göttingen, Germany.
27. Field,D. *et al.* (2010) Meeting Report: BioSharing at ISMB 2010. *Stand. Genom. Sci.*, **3**, 254–258.
28. Force,M.M. and Robinson,N.J. (2014) Encouraging data citation and discovery with the Data Citation Index. *J. Comput. Aided Mol. Des.*, **28**, 1043–1048.
29. Garfield,E. (2006) Citation indexes for science. A new dimension in documentation through association of ideas. 1955. *Int. J. Epidemiol.*, **35**, 1123–1127, discussion 1127–1128.
30. Schmutzer,T. *et al.* (2015) Species-wide genome sequence and nucleotide polymorphisms from the model allopolyploid plant *Brassica napus. Sci. Data*, **2** (doi:10.1038/sdata.2015.72)