IEEE Standard for Bioinformatics Analyses Generated by High-Throughput Sequencing (HTS) to Facilitate Communication

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P2791™/D4

Draft Standard for Bioinformatics Analyses Generated by High- Throughput Sequencing (HTS) to Facilitate Communication

Sponsor

Standards Committee

of the

IEEE Engineering in Medicine and Biology Society

Approved <Date Approved>

IEEE-SA Standards Board

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Abstract: A major goal of this standard is to improve communication of bioinformatics protocols and data in order to facilitate bioinformatics workflow related exchange and communication between regulatory agencies, pharmaceutical companies, bioinformatics platform providers and researchers. Detailed communication helps ensure responsibility, reproducibility, verify bioinformatics protocol, track provenance information and promote interoperability. In addition, this standard also defines the assurance program for evaluating and certifying products against those requirements.

Keywords: genomics, next generation sequencing, high throughput sequencing, massively parallel sequencing, NGS, HTS, MPS, workflow, pipeline, bioinformatics, analysis, regulatory

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43 have voted for approval, disapproval, or abstention.

44 *[To be supplied by IEEE]*

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46 Balloter2	49 Balloter5	52 Balloter8
47 Balloter3	50 Balloter6	53 Balloter9

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1 Introduction

This introduction is not part of P2791/D4, Draft Standard for Bioinformatics Analyses Generated by High-Throughput Sequencing (HTS) to Facilitate Communication.

The P2791 specification enables the description of bioinformatic genome analysis workflows in a standardized way. P2791 addresses the tremendous variability and uncertainty in communicating bioinformatics workflows and data related to analysis as a result of high throughput sequencing (HTS). The need to resolve issues in communication was felt particularly strongly between the United States Food and Drug Administration (FDA) and the entities that submit any work to the FDA for regulatory analysis that includes an HTS component¹² (<https://doi.org/10.5731/pdajpst.2016.006734> and [PMC5510742](https://doi.org/10.1093/bioinformatics/btu074)). A plan for what would become P2791 and initial goals of the project were drafted in a collaboration between the George Washington University and the FDA in 2014. The project has grown since then to include publications, workshops, applied use cases, and a large community of participants and collaborators. P2791 Objects created according to this standard are intended 1) to be both human and machine readable, 2) to be applied to genomic analysis workflows, and 3) to be able to capture details related to a workflow in such a way as to facilitate efficient communication and improve reproducibility and interoperability. Efforts were made to accommodate as many tools, platforms or scripts as possible, and to be adaptable to future developments in this field under a unified set of descriptions to standardize and streamline the representations of such complex bioinformatics processes.

P2791 is a standard and a P2791 Object is an instance of that standard. High throughput sequencing (HTS), also referred to as next-generation sequencing (NGS) or massively parallel sequencing (MPS), has increased the pace at which we generate, compute and share genomic data in biomedical sciences. As a result, scientists, clinicians and regulators are now faced with a new data paradigm that is less portable, more complex and most of all poorly standardized. The P2791 Objects are written in JSON format to encode important information on the execution of computational pipelines, or for the creation of knowledge bases. P2791 can be considered to be process oriented (for software pipelines) and/or product oriented (for knowledge bases). The goal of using a P2791 Object is to streamline communication of these otherwise difficult to elucidate details between stakeholders in academia, industry and regulatory agencies.

Standardized HTS data processing descriptions and data formats will promote interoperability and simplify the verification of the bioinformatics protocols applied against data. To do this, a schema has been developed to represent instances of computational analysis as a P2791 Object. A P2791 Object includes:

- Information about parameters and versions of the executable programs in a pipeline
- Reference to input and output test data for verification of the pipeline
- A usability domain
- Keywords
- A list of agents involved along with other important metadata, such as their specific contribution

Knowledge of input data is intended to be captured according to existing efforts, such as Minimum Information Required about a Glycomics Experiment (MIRAGE)³, Minimum Information about a

¹ Alterovitz G et al. Enabling Precision Medicine via standard communication of NGS provenance, analysis, and results. *PLoS Biol.* 2018 Dec; 16(12):e3000099 DOI: <https://doi.org/10.1371/journal.pbio.3000099>.

² Simonyan V, Goecks J and Mazumder R. Biocompute Objects—A Step towards Evaluation and Validation of Biomedical Scientific Computations. *PDA J Pharm Sci Technol.* 2017 Mar-Apr;71(2):136-146

³ Kolarich, Daniel; Rapp, Erdmann; Struwe, Weston B.; Haslam, Stuart M.; Zaia, Joseph; McBride, Ryan; Agravat, Sanjay; Campbell, Matthew P.; Kato, Masaki; Ranzinger, Rene; Kettner, Carsten; York, William S. (1 April 2013). "The Minimum Information Required for a Glycomics Experiment (MIRAGE) Project: Improving the Standards for Reporting Mass-spectrometry-based Glycoanalytic Data". *Molecular & Cellular Proteomics.* 12 (4): 991–995. doi:10.1074/mcp.O112.026492. ISSN 1535-9476. PMC 3617344. PMID 23378518

1 Proteomics Experiment (MIAPE)⁴, Standards for Reporting Enzymology Data (STREND A)⁵ and to be
2 in accordance with Minimum Information Standards⁶. In addition to all the information captured in the
3 P2791 Object, the P2791 Object itself is intended to be independent of the execution environment,
4 whether it is a local or a cloud-based infrastructure.

5

⁴ Taylor, C. F.; Paton, N. W.; Lilley, K. S.; Binz, P. A.; Julian Jr, R. K.; Jones, A. R.; Zhu, W.; Apweiler, R.; Aebersold, R.; Deutsch, E. W.; Dunn, M. J.; Heck, A. J. R.; Leitner, A.; Macht, M.; Mann, M.; Martens, L.; Neubert, T. A.; Patterson, S. D.; Ping, P.; Seymour, S. L.; Souda, P.; Tsugita, A.; Vandekerckhove, J.; Vondriska, T. M.; Whitelegge, J. P.; Wilkins, M. R.; Xenarios, I.; Yates Jr, J. R.; Hermjakob, H. (2007). "The minimum information about a proteomics experiment (MIAPE)". *Nature Biotechnology*. 25 (8): 887–893. doi:10.1038/nbt1329. PMID 17687369

⁵ Tipton, K.F., Armstrong, R.N., Bakker, B.M., Bairoch, A., Cornish-Bowden, A., Halling, P.J., Hofmeyr, J.-H., Leyh, T.S., Kettner, C., Raushel, F.M., Rohwer, J., Schomburg, D., Steinbeck, C. (2014) Standards for Reporting Enzyme Data: The STREND A Consortium: What it aims to do and why it should be helpful. *Perspect. Sci.* 1(1.6):131-137. DOI: 10.1016/j.pisc.2014.02.012

⁶ Taylor, Chris F (2008). "Promoting coherent minimum reporting guidelines for biological and biomedical investigations: the MIBBI project". *Nature Biotechnology*. 26 (8): 889–896. doi:10.1038/nbt.1411. PMC 2771753. PMID 18688244

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Draft Standard for Bioinformatics Analyses Generated by High- Throughput Sequencing (HTS) to Facilitate Communication

1. Overview

1.1 General

The P2791 standard captures relevant information from a high throughput sequencing workflow as a P2791 Object in order to enable a user to understand and interpret the workflow efficiently and with high confidence. P2791 is a standard that was initially created with a goal of improving efficiency in regulatory review. Pursuant to this, workflow steps and prerequisites to execute workflow steps are recorded in detail in a P2791 Object. Information is recorded using key/value pairs in JavaScript Object Notation (JSON), adhering to the P2791 JSON Schema.

Information in P2791 Objects is organized by domains;

- The Provenance Domain - tracks metadata about the P2791 Object
- The Usability Domain - tracks what was done
- The Extension Domain - provide user-defined fields
- The Description Domain - captures a description of external resources, pipeline steps, and the relationships of I/O objects
- The Execution Domain - describes information needed for deployment, software configuration and running applications in a dependent environment
- The Parametric Domain - captures all parameters that customize a computational flow
- The Input and Output Domain - contains a list of global input and output files
- The Error Domain - describes errors, including the limits of detectability, false positives, false negatives, statistics confidence of outcomes, and description of errors (i.e. empirical or algorithmic).

This document should be read in conjunction with the open source P2791 JSON Schema files (<https://w3id.org/2791/>) which are referred to from the text, for instance “*provenance_domain.json*” refers to (https://w3id.org/2791/provenance_domain.json). Files are kept separate for organization. References in the P2791 Object schema (\$ref) to these files should be replaced with the proper domain from the appropriate file. For example, line 142 of “*p2791object.json*” (“\$ref”: “*provenance_domain.json*”) is a reference to the structure specified in the *provenance_domain.json* file. The P2791 Object Schema builds on the JSON Schema by adding domains in a way that facilitates the communication of bioinformatics workflows. A description of the domain files follows.

1.2 Scope

This standard establishes detailed and structured communication of bioinformatics protocols in order to facilitate bioinformatics workflow related exchange and communication between regulatory agencies, pharmaceutical companies, bioinformatics platform providers and researchers. Detailed communication helps ensure responsibility, verify bioinformatics protocol, track provenance information and promote interoperability.

1.3 Purpose

The standard allows for the cross platform communications of complex computation from inception to manufacturing of medical products and services. Another goal of this standard is to improve efficiency and speed of communication.

2. Normative references

The following referenced documents are indispensable for the application of this document (i.e., they must be understood and used, so each referenced document is cited in text and its relationship to this document is explained). For dated references, only the edition cited applies. For undated references, the latest edition of the referenced document (including any amendments or corrigenda) applies.

JSON (RFC8259): <https://tools.ietf.org/html/rfc8259>

JSON Schema: draft-handrews-json-schema-01

JSON Schema Validation: draft-handrews-json-schema-validation-01

3. Definitions, acronyms, and abbreviations

For the purposes of this document, the following terms and definitions apply. The *IEEE Standards Dictionary Online* should be consulted for terms not defined in this clause.¹

3.1 Acronyms and abbreviations

JSON	JavaScript Object Notation
------	----------------------------

¹IEEE Standards Dictionary Online is available at: <http://dictionary.ieee.org>.

SCM Source Control Management

4. P2791 Standard

4.1 General

This document describes the P2791 standard for describing bioinformatic workflows. A P2791 “Object” is an instance of the P2791 standard, and is a text file written in JSON data structure that shall consist of all domains required by the P2791 Schema (<https://w3id.org/2791/>). The P2791 Schema is the formal definition of the standard against which instances of the standard can be validated. JavaScript Object Notation (JSON) is a textual format used by both instances of Objects and the formal P2791 Schema, and the JSON Schema is the language used to express the P2791 Schema.

A valid Object must conform to the P2791 JSON Schema (see section 4.3), and therefore invokes all of the requirements of the JSON Schema (while a valid Object file must conform to the schema, the schema file is not technically required to create the Object file). Later versions of P2791 may be updated for conformance with future JSON Schema versions. The minimum requirement to execute the standard is the fully organized P2791 Object containing all domains in JSON Schema format. Pursuant to JSON schema, the fields required for a valid Object are listed at the top of the *2791object.json* file.

All the files in the repository are linked together (using JSON pointers as described by the JSON Schema), being referenced by the ‘*2791object.json*’ file. The *error_domain.json* is an optional domain to further describe empirical and algorithmic sources and measures of error for a bioinformatics workflow (https://w3id.org/2791/error_domain.json), and the *extension_domain.json* is an optional domain that contains user-defined fields.

At its top-level, Objects have the following three required metadata fields: “spec_version”, “object_id”, and “etag”. These lines are external to all domains. Everything except for the etag, object_id, and spec_version shall be included in the generation of an ETag (see <https://tools.ietf.org/html/rfc7232#section-2.3>) - which can be “strong” or “weak” (see <https://tools.ietf.org/html/rfc7232#section-2.1>). It is recommended that the ETag be deleted or updated if the object file is changed (except in cases using weak ETags in which the entirety of the change comprises a simple re-writing of the JSON).

object_id is a string that follows the JSON Schema format of namespace/ref shall be a unique identifier. Users are free to number Object files in the manner of their choosing, however, in order to avoid naming conflicts, it is recommended that a domain be registered with a registration authority, such as the one at <https://www.biocomputeobject.org/registry.html>. For example, http://www.example.com/exampleproject/1.3.0/schemas/ABC_object0001.json, where “ABC” is a registered domain, and “_object0001.json” is an arbitrary identifier, chosen by the owner of that domain.

The remaining top level fields are domains that partition workflow into meaningful subunits. These are the Description domain, Error domain, Execution domain, IO domain, Parametric domain, Provenance domain, and Usability domain.

The Description Domain of an Object contains a description of external resources, pipeline steps, and the relationship of I/O objects (https://w3id.org/2791/description_domain.json).

The Error Domain contains information related to the bounds of detection (such as the minimum sequence depth and minimum sequence coverage), and statistical analyses of the pipeline (such as the false negative and false positive rates). It is recommended that the keys directly under *empirical_error* and

1 algorithmic_error use a full URI. Resolving the URI should give a JSON Schema or textual
2 definition of the field. Other keys are not allowed in error_domain.
3

4 The Execution Domain of an Object describes details of deployment, software configuration, and running
5 applications in a dependent environment (https://w3id.org/2791/execution_domain.json). This may include
6 scripts, drivers, environment variables, and other software prerequisites.
7

8 The IO Domain of an Object is a list of global input and output files that may exist on local machine or on
9 another machine (https://w3id.org/2791/io_domain.json). It does not include references to intermediate
10 files.
11

12 The Parametric Domain of a P2791 Object includes any parameters used in a workflow
13 (https://w3id.org/2791/parametric_domain.json). This is intended for use when parameters are changed
14 from default settings.
15

16 The Provenance Domain contains metadata related to the Object
17 (https://w3id.org/2791/provenance_domain.json). It is used to track the flow of data from original source to
18 final computation, and includes contributors, reviewers, and versioning. In the event that a P2791 Object
19 retrospectively references an existing Object (such as an example Object), the derived_from field
20 within the Provenance Domain shall reference the specific Object by object_id field. In the event that
21 the Object is an example Object or is created de novo without reference to existing work, this field is not
22 included. In the event that the Object is an example or template P2791 Object, best practice is to state this
23 in the Usability Domain, along with relevant details (such as completeness of data, whether data is real or
24 artificial, etc.).

25 The Usability Domain of an Object is a plain language description of what was done in the workflow
26 (https://w3id.org/2791/usability_domain.json). This should align with the actual steps described elsewhere
27 in the Object. The Usability Domain conveys the purpose of the Object.
28

29 The Extension Domain allows a user to define additional fields and is optional. The Extension Domain is
30 for the inclusion of any additional structured information. A valid JSON schema for each extension used in
31 this domain is expected to be specified. The schema should be name spaced, and it is recommended that
32 resolving the namespaced URI will provide the extension's JSON Schema. The URL should be provided in
33 the required "extension_schema" field. If execution portability is desired, then the included script
34 should be in the Common Workflow Language v1.0 (<https://w3id.org/cwl/v1.0/>) or later format. In order to
35 avoid potential naming conflicts, it is recommended that users register their domain with
36
37

1 **Annex A**

2 (informative)

3 **Bibliography**

4 Bibliographical references are resources that provide additional or helpful material but do not need to be
5 understood or used to implement this standard. Reference to these resources is made for informational use
6 only.

7 [B1] Community User Guide for Best Practices. <https://w3id.org/biocompute/1.3.1>

8 [B2] JSON Schema: A Media Type for Describing JSON Documents. [https://tools.ietf.org/html/draft-](https://tools.ietf.org/html/draft-handrews-json-schema-01)
9 handrews-json-schema-01

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