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1 Interoperability and FAIRness through a novel 2 combination of Web technologies 3 4 Authors: 5 6 7 Mark D. Wilkinson - Center for Plant Biotechnology and Genomics, UPM-INIA, Madrid, 8 Spain 9 Ruben Verborgh – Ghent University – IMEC, Ghent, Belgium 10 Luiz Olavo Bonino da Silva Santos - Dutch Techcentre for Life Sciences, Utrecht, The 11 Netherlands - Vrije Universiteit Amsterdam, Amsterdam, The Netherlands 12 Tim Clark - Department of Neurology, Massachusetts General Hospital Boston MA and 13 Harvard Medical School, Boston, MA, USA 14 Morris A. Swertz - Genomics Coordination Center and Department of Genetics, University 15 Medical Center Groningen, Groningen, The Netherlands Fleur D.L. Kelpin - Genomics Coordination Center and Department of Genetics, University 16 17 Medical Center Groningen, Groningen, The Netherlands 18 Alasdair J. G. Gray - Department of Computer Science, School of Mathematical and 19 Computer Sciences, Heriot-Watt University, Edinburgh, UK 20 Erik A. Schultes - Department of Human Genetics, Leiden University Medical Center, 21 Leiden, The Netherlands 22 Erik M. van Mulligen - Department of Medical Informatics, Erasmus University Medical 23 Center Rotterdam, The Netherlands 24 Paolo Ciccarese - Perkin Elmer Innovation Lab, Cambridge MA and Harvard Medical 25 School, Boston MA, USA 26 Arnold Kuzniar, Netherlands eScience Center, Amsterdam, The Netherlands 27 Anand Gavai, Netherlands eScience Center, Amsterdam, The Netherlands 28 Mark Thompson - Leiden University Medical Center, Leiden, The Netherlands 29 Rajaram Kaliyaperumal - Leiden University Medical Center, Leiden, The Netherlands 30 Jerven T. Bolleman - Swiss-Prot group, SIB Swiss Institute of Bioinformatics, Centre 31 Medical Universitaire, Geneva, Switzerland 32 Michel Dumontier - Stanford Center for Biomedical Informatics Research, Stanford 33 University, Stanford, California 34 **Corresponding Author:** 35 36 37 Mark D. Wilkinson

- 38 markw@illuminae.com, +34 622 784 026
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42 Abstract

43 Data in the life sciences are extremely diverse and are stored in a broad spectrum of 44 repositories ranging from those designed for particular data types (such as KEGG for pathway data or UniProt for protein data) to those that are general-purpose (such as 45 FigShare, Zenodo, Dataverse or EUDAT). These data have widely different levels of 46 47 sensitivity and security considerations. For example, clinical observations about genetic 48 mutations in patients are highly sensitive, while observations of species diversity are 49 generally not. The lack of uniformity in data models from one repository to another, and in the richness and availability of metadata descriptions, makes integration and analysis of 50 51 these data a manual, time-consuming task with no scalability. Here we explore a set of 52 resource-oriented Web design patterns for data discovery, accessibility, transformation, and 53 integration that can be implemented by any general- or special-purpose repository as a 54 means to assist users in finding and reusing their data holdings. We show that by using offthe-shelf technologies, interoperability can be achieved atthe level of an individual 55 56 spreadsheet cell. We note that the behaviours of this architecture compare favourably to the 57 desiderata defined by the FAIR Data Principles, and can therefore represent an exemplar implementation of those principles. The proposed interoperability design patterns may be 58 59 used to improve discovery and integration of both new and legacy data, maximizing the 60 utility of all scholarly outputs. 61

63

64 Introduction

65 Carefully-generated data are the foundation for scientific conclusions, new hypotheses, discourse, disagreement and resolution of these disagreements, all of which drive scientific 66 67 discovery. Data must therefore be considered, and treated, as first-order scientific output, 68 upon which there may be many downstream derivative works, among these, the familiar 69 research article (Starr et al., 2015). But as the volume and complexity of data continue to 70 grow, a data publication and distribution infrastructure is beginning to emerge that is not ad 71 hoc, but rather explicitly designed to support discovery, accessibility, (re)coding to 72 standards, integration, machine-guided interpretation, and re-use.

73

74 In this text, we use the word "data" to mean all digital research artefacts, whether they be 75 data (in the traditional sense), research-oriented digital objects such as workflows, or 76 combinations/packages of these (i.e. the concept of a "research object", (Bechhofer et al., 77 2013)). Effectively, all digital entities in the research data ecosystem will be considered data 78 by this manuscript. Further, we intend "data" to include both data and metadata, and 79 recognize that the distinction between the two is often user-dependent. Data, of all types, 80 are often published online, where the practice of open data publication is being encouraged 81 by the scholarly community, and increasingly adopted as a requirement of funding agencies 82 (Stein et al., 2015). Such publications utilize either a special-purpose repository (e.g. model-83 organism or molecular data repositories) or increasingly commonly will utilize general-84 purpose repositories such as FigShare, Zenodo, Dataverse, EUDAT or even institutional 85 repositories. Special-purpose repositories generally receive dedicated funding to curate and 86 organize data, and have specific query interfaces and APIs to enable exploration of their 87 content. General-purpose repositories, on the other hand, allow publication of data in 88 arbitrary formats, with little or no curation and often very little structured metadata. Both of 89 these scenarios pose a problem with respect to interoperability. While APIs allow 90 mechanized access to the data holdings of a special-purpose repository, each repository has 91 its own API, thus requiring specialized software to be created for each cross-repository 92 query. Moreover, the ontological basis of the curated annotations are not always 93 transparent (neither to humans nor machines), which hampers automated integration. 94 General purpose repositories are less likely to have rich APIs, thus often requiring manual 95 discovery and download; however, more importantly, the frequent lack of harmonization of 96 the file types/formats and coding systems in the repository, and lack of curation, results in 97 much of their content being unusable (Roche et al., 2015). 98 99 Previous projects, specifically in the bio/medical domain, that have attempted to achieve deep interoperability include caBIO (Covitz et al., 2003) and TAPIR (De Giovanni et al., 100 101 2010). The former created a rich SOAP-based API, enforcing a common interface over all

102 repositories. The latter implemented a domain-specific query language that all participating

103 repositories should respond to. These initiatives successfully enabled powerful cross-

104 resource data exploration and integration; however, this was done at the expense of broad-

scale uptake, partly due to the complexity of implementation, and/or required the

106 unavoidable participation of individual data providers, who are generally resource-strained.

107 Moreover, in both cases, the interoperability was aimed at a specific field of study (cancer,

and biodiversity respectively), rather than a more generalized interoperability goal spanningall domains.

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111 With respect to more general-purpose approaches, and where 'lightweight' interoperability 112 was considered acceptable, myGrid (Stevens et al., 2003) facilitated discovery and 113 interoperability between Web Services through rich ontologically-based annotations of the 114 service interfaces, and BioMoby (Wilkinson et al., 2008) built on these myGrid annotations 115 by further defining a novel ontology-based service request/response structure to guarantee 116 data-level compatibility and thereby assist in workflow construction (Withers et al., 2010). 117 SADI (Wilkinson et al., 2011), and SSWAP (Gessler et al., 2009) used the emergent 118 Semantic Web technologies of RDF and OWL to enrich the machine-readability of Web 119 Service interface definitions and the data being passed - SADI through defining service 120 inputs and outputs as instances of OWL Classes, and SSWAP through passing data 121 embedded in OWL 'graphs' to assist both client and server in interpreting the meaning of the 122 messages. In addition, two Web Service interoperability initiatives emerged from the World 123 Wide Web Consortium - OWL-S (Martin et al., 2005) and SAWSDL (Martin et al., 2007), both 124 of which used semantic annotations to enhance the ability of machines to understand Web 125 Service interface definitions and operations. All of these Service-oriented projects enjoyed 126 success within the community that adopted their approach; however, the size of these 127 adopting communities have, to date, been quite limited and are in some cases highly 128 domain-specific. Moreover, each of these solutions is focused on Web Service functionality, 129 which represents only a small portion of the global data archive, where most data is 130 published as static records. Service-oriented approaches additionally require data 131 publishers to have considerable coding expertise and access to a server in order to utilize 132 the standard, which further limits their utility with respect to the 'lay' data publishers that 133 make-up the majority of the scholarly community. As such, these and numerous other 134 interoperability initiatives, spanning multiple decades, have yet to convincingly achieve a 135 lightweight, broadly domain-applicable solution that works over a wide variety of static and 136 dynamic source data resources, and can be implemented with minimal technical expertise. 137 138 There are many stakeholders who would benefit from progress in this endeavour. Scientists

139 themselves, acting as both producers and consumers of these public and private data; public 140 and private research-oriented agencies; journals and professional data publishers both 141 "general purpose" and "special purpose"; research funders who have paid for the underlying 142 research to be conducted; data centres (e.g. the EBI (Cook et al., 2016), and the SIB (SIB 143 Swiss Institute of Bioinformatics Members, 2016)) who curate and host these data on behalf 144 of the research community; research infrastructures such as BBMRI-ERIC (van Ommen et 145 al., 2015) and ELIXIR (Crosswell & Thornton, 2012), and diverse others. All of these 146 stakeholders have distinct needs with respect to the behaviours of the scholarly data 147 infrastructure. Scientists, for example, need to access research datasets in order to initiate 148 integrative analyses, while funding agencies and review panels may be more interested in 149 the metadata associated with a data deposition - for example, the number of views or

- 150 downloads, and the selected license. Due to the diversity of stakeholders; the size,
- 151 nature/format, and distribution of data assets; the need to support freedom-of-choice of all
- 152 stakeholders; respect for privacy; acknowledgment of data ownership; and recognition of the
- 153 limited resources available to both data producers and data hosts, we see this endeavour as
- 154 one of the *Grand Challenges of eScience*.
- 155

156 In January 2014, representatives of a range of stakeholders came together at the request of 157 the Netherlands eScience Centre and the Dutch Techcentre for Life Sciences (DTL) at the 158 Lorentz Centre in Leiden, the Netherlands, to brainstorm and debate about how to further 159 enhance infrastructures to support a data ecosystem for eScience. From these discussions 160 emerged the notion that the definition and widespread support of a minimal set of community-agreed guiding principles and practices could enable data providers and 161 162 consumers - machines and humans alike - to more easily find, access, interoperate, and 163 sensibly re-use the vast quantities of information being generated by contemporary data-164 intensive science. These principles and practices should enable a broad range of integrative 165 and exploratory behaviours, and support a wide range of technology choices and 166 implementations, just as the Internet Protocol (IP) provides a minimal layer that enables the 167 creation of a vast array of data provision, consumption, and visualisation tools on the 168 Internet. The main outcome of the workshop was the definition of the so-called FAIR guiding 169 principles aimed at publishing data in a format that is **Findable**. Accessible. Interoperable 170 and **Reusable** by both machines and human users. The FAIR Principles underwent a period 171 of public discussion and elaboration, and were recently published (Wilkinson et al., 2016). 172 Briefly, the principles state: 173 174 175 Findable - data should be identified using globally unique, resolvable, and persistent

- identifiers, and should be identified using globally unique, resolvable, and persistent
 identifiers, and should include machine-actionable contextual information that can be
 indexed to support human and machine discovery of that data.
- Accessible identified data should be accessible, optimally by both humans and
 machines, using a clearly-defined protocol and, if necessary, with clearly-defined
 rules for authorization/authentication.
- 183 Interoperable data becomes interoperable when it is machine-actionable, using
 184 shared vocabularies and/or ontologies, inside of a syntactically and semantically
 185 machine-accessible format.
- 187 Reusable Reusable data will first be compliant with the F, A, and I principles, but
 188 further, will be sufficiently well-described with, for example, contextual information, so
 189 it can be accurately linked or integrated, like-with-like, with other data sources.
 190 Moreover, there should be sufficiently rich provenance information so reused data
 191 can be properly cited.
- 192

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193 While the principles describe the desired features that data publications should exhibit to 194 encourage maximal, automated discovery and reuse, they provide little guidance regarding how to achieve these goals. This poses a problem when key organizations are already 195 196 endorsing, or even requiring adherence to the FAIR principles. For example, a biological 197 research group has conducted an experiment to examine polyadenylation site usage in the 198 pathogenic fungus Magnaporthe oryzae, recording, by high-throughput 3'-end sequencing, the preference of alternative polyadenylation site selection under a variety of growth 199 200 conditions, and during infection of the host plant. The resulting data take the form of study-201 specific Excel spreadsheets, BED alignment graphs, and pie charts of protein functional 202 annotations. Unlike genome or protein sequences and microarray outputs, there is no public 203 curated repository for these types of data, yet the data are useful to other researchers, and 204 should be (at a minimum) easily discovered and interpreted by reviewers or third-party 205 research groups attempting to replicate their results. Moreover, their funding agency, and 206 their preferred scientific journal, both require that they publish their source data in an open 207 public archive according to the FAIR principles. At this time, the commonly used general-208 purpose data archival resources in this domain do not explicitly provide support for FAIR, nor 209 do they provide tooling or even guidance for how to use their archival facilities in a FAIR-210 compliant manner. As such, the biological research team, with little or no experience in 211 formal data publishing, must nevertheless self-direct their data archival in a FAIR manner. 212 We believe that this scenario will be extremely common throughout all domains of research. 213 and thus this use-case was the initial focus for this interoperability infrastructure and FAIR 214 data publication prototype.

215

216 Here we describe a novel interoperability architecture that combines three pre-existing Web 217 technologies to enhance the discovery, integration, and reuse of data in repositories that 218 lack or have incompatible APIs; data in formats that normally would not be considered 219 interoperable such as Excel spreadsheets and flat-files; or even data that would normally be 220 considered interoperable, but do not use the desired vocabulary standards. We examine the 221 extent to which the features of this architecture comply with the FAIR Principles, and suggest 222 that this might be considered a "reference implementation" for the FAIR Principles, in 223 particular as applied to non-interoperable data in any general- or special-purpose repository. 224 We provide two exemplars of usage. The first is focused on a use-case similar to that 225 presented above, where we use our proposed infrastructure to create a FAIR, self-archived 226 scholarly deposit of biological data to the general-purpose Zenodo repository. The second, 227 more complex example has two objectives - first to use the infrastructure to improve 228 transparency and FAIRness of metadata describing the inclusion criterion for a dataset. 229 representing a subset of a special-purpose, curated resource (UniProt); and second, to show 230 how even the already FAIR data within UniProt may be transformed to increase its FAIRness 231 even more by making it interoperable with alternative ontologies and vocabularies, and more 232 explicitly connecting it to citation information. Finally, we place this work in the context of 233 other initiatives and demonstrate that it is complementary to, rather than in competition with, 234 other initiatives.

235 Methods

236 Implementation

237 Overview of technical decisions and their justification

238

239 The World Wide Web Consortium's (W3C) Resource Description Framework (RDF) offers 240 the ability to describe entities, their attributes, and their relationships with explicit semantics 241 in a standardized manner compatible with widely used Web application formats such as 242 JSON and XML. The Linked Data Principles (Berners-Lee, 2006) mandate that data items and schema elements are identified by HTTP-resolvable URIs, so the HTTP protocol can be 243 244 used to obtain the data. Within an RDF description, using shared public ontology terms for 245 metadata annotations supports search and large scale integration. Given all of these 246 features, we opted to use RDF as the basis of this interoperability infrastructure, as it was 247 designed to share data on the Web.

248

249 Beyond this, there was a general feeling that any implementation that required a novel data 250 discovery/sharing "Platform", "Bus", or API, was beyond the minimal design that we had 251 committed to; it would require the invention of a technology that all participants in the data 252 ecosystem would then be required to implement, and this was considered a non-starter. 253 However, there needed to be some form of coalescence around the mechanism for finding 254 and retrieving data. Our initial target-community - that is, the biomedical sciences - have 255 embraced lightweight HTTP interfaces. We propose to continue this direction with an 256 implementation based on REST (Fielding & Taylor, 2002), as several of the FAIR principles 257 map convincingly onto the objectives of the REST architectural style for distributed 258 hypermedia systems, such as having resolvable identifiers for all entities, and a common 259 machine-accessible approach to discovering and retrieving different representations of those 260 entities. The implementation we describe here is largely based on the HTTP GET method, 261 and utilizes rich metadata and hypermedia controls. We use widely-accepted vocabularies 262 not only to describe the data in an interoperable way, but also to describe its nature (e.g. the 263 context of the experiment and how the data was processed) and how to access it. These 264 choices help maximize uptake by our initial target-community, maximize interoperability 265 between resources, and simplify construction of the wide (not pre-defined) range of client 266 behaviours we intend to support.

267

268 Confidential and privacy-sensitive data was also an important consideration, and it was 269 recognized early on that it must be possible, within our implementation, to identify and richly 270 describe data and/or datasets without necessarily allowing direct access to them, or by 271 allowing access through existing regulatory frameworks or security infrastructures. For 272 example, many resources within the International Rare Disease Research Consortium 273 participate in the RD Connect platform (Thompson et al., 2014) which has defined the 274 "disease card" - a metadata object that gives overall information about the individual disease 275 registries, which is then incorporated into a "disease matrix". The disease matrix provides 276 aggregate data about what disease variants are in the registry, how many individuals

- 277 represent each disease, and other high-level descriptive data that allows, for example,
 278 researchers to determine if they should approach the registry to request full data access.
- 279

280 Finally, it was important that the data host/provider is not necessarily a participant in making 281 their data interoperable - rather, the interoperability solution should be capable of adapting 282 existing data with or without the source provider's participation. This ensures that the interoperability objectives can be pursued for projects with limited resourcing, that 283 284 'abandoned' datasets may still participate in the interoperability framework, but most 285 importantly, that those with the needs and the resources should adopt the responsibility for 286 making their data-of-interest interoperable, even if it is not owned by them. This distributes 287 the problem of migrating data to interoperable formats over the maximum number of 288 stakeholders, and ensures that the most crucial resources - those with the most demand for 289 interoperability - become the earliest targets for migration.

290

295

With these considerations in mind, we were inspired by three existing technologies whose
features were used in a novel combination to create an interoperability infrastructure for both
data and metadata, that is intended to also addresses the full range of FAIR requirements.
Briefly, the selected technologies are:

- 296 1) The W3C's Linked Data Platform (Speicher, Arwe & Malhotra, 2015). We generated 297 a model for hierarchical dataset containers that is inspired by the concept of a Linked 298 Data Platform (LDP) Container, and the LDP's use of the Data Catalogue Vocabulary 299 (DCAT, (Maali, Erickson & Archer, 2014)) for describing datasets, data elements, and 300 distributions of those data elements. We also adopt the DCAT's use of Simple 301 Knowledge Organization System (SKOS, (Miles & Bechhofer, 18 August, 2009)) 302 Concept Schemes as a way to ontologically describe the content of a dataset or data 303 record.
- The RDF MappingLanguage (RML, (Dimou et al., 2014). RML allows us to describe one or more possible RDF representations for any given dataset, and do so in a manner that is, itself, FAIR: every sub-component of an RML model is Findable, Accessible, Interoperable, and Reusable. Moreover, for many common semistructured data, there are generic tools that utilize RML models to dynamically drive the transformation of data from these opaque representations into interoperable representations (https://github.com/RMLio/RML-Mapper).
- 311 3) Triple Pattern Fragments (TPF - (Verborgh et al., 2016)). A TPF interface is a REST 312 Web API to retrieve RDF data from data sources in any native format. A TPF server 313 accepts URLs that represent triple patterns [Subject, Predicate, Object], where any of 314 these three elements may be constant or variable, and returns RDF triples from its 315 data source that match those patterns. Such patterns can be used to obtain entire datasets, slices through datasets, or individual data points even down to a single 316 317 triple (essentially a single cell in a spreadsheet table). Instead of relying on a 318 standardized contract between servers and clients, a TPF interface is self-describing 319 such that automated clients can discover the interface and its data.
- 320

321 We will now describe in detail how we have applied key features of these technologies, in

322 combination, to provide a novel data discoverability architecture. We will later demonstrate

323 that this combination of technologies also enables both metadata and data-level

interoperability even between opaque objects such as flat-files, allowing the data within

these objects to be queried in parallel with other data on the Semantic Web.

326

327 Metadata Interoperability - The "FAIR Accessor" and the Linked Data Platform

328

The Linked Data Platform "*defines a set of rules for HTTP operations on Web resources... to provide an architecture for read-write Linked Data on the Web*" (https://www.w3.org/TR/ldp/). All entities and concepts are identified by URLs, with machine-readable metadata describing the function or purpose of each URL and the nature of the resource that will be returned when that URL is resolved.

334

335 Within the LDP specification is the concept of an LDP Container. A basic implementation of 336 LDP containers involves two "kinds" of resources, as diagrammed in Figure 1. The first type 337 of resource represents the container - a metadata document that describes the shared 338 features of a collection of resources, and (optionally) the membership of that collection. This 339 is analogous to, for example, a metadata document describing a data repository, where the 340 repository itself has features (ownership, curation policy, etc.) that are independent from the 341 individual data records within that repository (i.e. the members of the collection). The second 342 type of resource describes a member of the contained collection and (optionally) provides 343 ways to access the record itself.

344

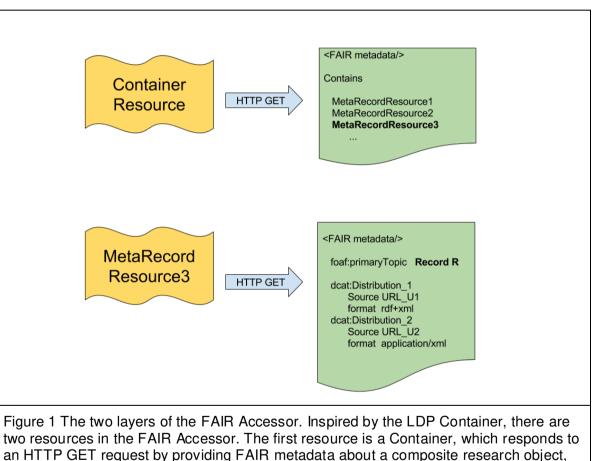
Our implementation, which we refer to as the "FAIR Accessor", utilizes the container concept described by the LDP, however, it does not require a full implementation of LDP, as we only require read functionality. In addition, other requirements of LDP would have added complexity without notable benefit. Our implementation, therefore, has two resource types based on the LDP Container described above, with the following specific features:

350

351 **Container resource:** This is a composite research object (of any kind - repository, 352 repository-record, database, dataset, data-slice, workflow, etc.). Its representation could 353 include scope or knowledge-domain covered, authorship/ownership of the object, latest 354 update, version number, curation policy, and so forth. This metadata may or may not include 355 URLs representing MetaRecord resources (described below) that comprise the individual 356 elements within the composite object. Notably, the Container URL provides a resolvable 357 identifier independent from the identifier of the dataset being described; in fact, the dataset 358 may not have an identifier, as would be the case, for example, where the container 359 represents a dynamically-generated data-slice. In addition, Containers may be published by 360 anyone - that is, the publisher of a Container may be independent from the publisher of the 361 research object it is describing. This enables one of the objectives of our interoperability 362 layer implementation - that anyone can publish metadata about any research object, thus 363 making those objects more FAIR. 364

365 **MetaRecord resource:** This is a specific element within a collection (data point, record, 366 study, service, etc.). Its representation should include information regarding licensing and 367 accessibility, access protocols, rich citation information, and other descriptive metadata. It 368 also includes a reference to the container(s) of which it is a member (the Container URL). 369 Finally, the MetaRecord may include further URLs that provide direct access to the data 370 itself, with an explicit reference to the associated data format by its MIME type (e.g. text/html, application/json, application/vnd.ms-excel, text/csv, etc.). This is achieved using 371 372 constructs from the Data Catalogue Vocabulary (DCAT: W3C, 2014), which defines the 373 concept of a data "Distribution", which includes metadata facets such as the data source 374 URL and its format. The lower part of Figure 1 diagrams how multiple DCAT Distributions may be a part of a single MetaRecord. As with Container resources, MetaRecords may be 375 376 published by anyone, and independently of the original data publisher.

377



two resources in the FAIR Accessor. The first resource is a Container, which responds to an HTTP GET request by providing FAIR metadata about a composite research object, and optionally a list of URLs representing MetaRecords that describe individual components within the collection. The MetaRecord resources resolve by HTTP GET to documents containing metadata about an individual data component and, optionally, a set of links structured as DCAT Distributions that lead to various representations of that data.

378

In summary, the FAIR Accessor shares commonalities with the Linked Data Platform, but
 additionally recommends the inclusion of rich contextual metadata, based on the FAIR

381 Principles, that facilitate discovery and interoperability of repository and record-level

382 information. The FAIR Accessor is read-only, utilizing only HTTP GET together with widely-

used semantic frameworks to guide both human and machine exploration. Importantly, the 383

384 lack of a novel API means that the information is accessible to generic Web-crawling agents,

- 385 and may also be processed if that agent "understands" the vocabularies used. Thus, in 386 simplistic terms, the Accessor can be envisioned as a series of Web pages, each containing
- metadata, and hyperlinks to more detailed metadata and/or data, where the metadata 387

388 elements and relationships between the pages are explicitly explained to Web crawlers. 389 390 To help clarify this component prior to presenting the more complex components of our interoperability proposal, we will now explore our first use case - data self-archival. A simple 391

392 FAIR Accessor has been published online (Rodriguez Iglesias et al., 2016) in the Zenodo

393 general-purpose repository. The data self-archival in this citation represents a scenario

394 similar to the polyadenylation use-case described in the Introduction section. In this case,

395 the data describes the evolutionary conservation of components of the RNA Metabolism

396 pathway in fungi as a series of heatmap images. The data deposit, includes a file

- 397 'RNAME Accessor.rdf' which acts as the Container Resource. This document includes 398 metadata about the deposit (authorship, topic, etc.), together with a series of 'contains'
- 399 relationships, referring to MetaRecords inside of the file

400 'RNAME Accessor Metarecords.rdf'. Each MetaRecord is about one of the heatmaps, and 401 in addition to metadata about the image, includes a link to the associated image (datatype 402 image/png) and a link to an RDF representation of the same information represented by that 403 image (datatype application/rdf+xml). It should be noted that much of the content of those 404 Accessor files was created using a text editor, based on template RDF documents. The 405 structure of these two documents are described in more detail in the Results section, which

- 406 includes a full walk-through of a more complex exemplar Accessor.
- 407

408 At the metadata level, therefore, this portion of the interoperability architecture provides a 409 high degree of FAIRness by allowing machines to discover and interpret useful metadata. 410 and link it with the associated data deposits, even in the case of a repository that provides 411 no FAIR-support. Nevertheless, these components do not significantly enhance the 412 FAIRness and interoperability of the data itself, which was a key goal for this project. We will 413 now describe the application of two recently-published Web technologies - Triple Pattern 414 Fragments and RML - to the problem of data-level interoperability. We will show that these 415 two technologies can be combined to provide an API-free common interface that may be 416 used to serve, in a machine-readable way, FAIR data transformations (either from non-FAIR 417 data, or transformations of FAIR data into novel ontological frameworks). We will also 418 demonstrate how this FAIR data republishing layer can be integrated into the FAIR Accessor 419 to provide a machine-traversable path for incremental drill-down from high-level repository 420 metadata all the way through to individual data points within a record, and back. 421

Data Interoperability: Discovery of compatible data through RML-based FAIR Profiles
In our approach to data-level interoperability, we first identified a number of desiderata that the solution should exhibit:
 View-harmonization over dissimilar datatypes, allowing discovery of <i>potentially</i> integrable data within non-integrable formats. Support for a multitude of source data formats (XML, Excel, CSV, JSON, binary,
 etc.) 3. "Cell-level" discovery and interoperability (referring to a "cell" in a spreadsheet) 4. Modularity, such that a user can make interoperable only the data component of- interest to them
 Reusability, avoiding "one-solution-per-record" and minimizing effort/waste Must use standard technologies, and reuse existing vocabularies Should not require the participation of the data host (for public data)
The approach we selected was based on the premise that data, in any format, could be metamodelled as a first step towards interoperability; i.e., the salient data-types and relationships within an opaque data "blob" could be described in a machine-readable manner. The metamodels of two data sources could then be compared to determine if their
contained data was, in principle, integrable. We referred to these metamodels as "FAIR Profiles", and we further noted that we should support multiple metamodels of the same data, differing in structure or ontological/semantic
framework, within a FAIR Profile. For example, a data record containing blood pressure information might have a FAIR Profile where this facet is modelled using both the SNOMED vocabulary and the ICD10 vocabulary, since the data facet can be understood using either. We acknowledge that these meta-modelling concepts are not novel, and have been suggested by a variety of other projects such as DCAT and Dublin Core (the DC Application
Profile (Heery & Patel, 2000), and have been extensively described by the ISO 11179 standard for "metadata registries". It was then necessary to select a modelling framework for FAIR Profiles capable of representing arbitrary, and possibly redundant, semantic models.
Our investigation into relevant existing technologies and implementations revealed a relatively new, unofficial specification for a generic mapping language called "RDF Mapping Language" (RML (Dimou et al., 2014)). RML is an extension of R2RML (Das, Sundara & Cyganiak, 27 September, 2012), a W3C Recommendation for mapping relational databases to RDF, and is described as " <i>a uniform mapping formalization for data in different format, which [enables] reuse and exchange between tools and applied data</i> " (Dimou et al., 2014). An RML map describes the triple structure (subject, predicate, object, abbreviated as [S,P,O]), the semantic types of the subject and object, and their constituent URI structures, that would result from a transformation of non-RDF data (of any kind) into RDF data. RML

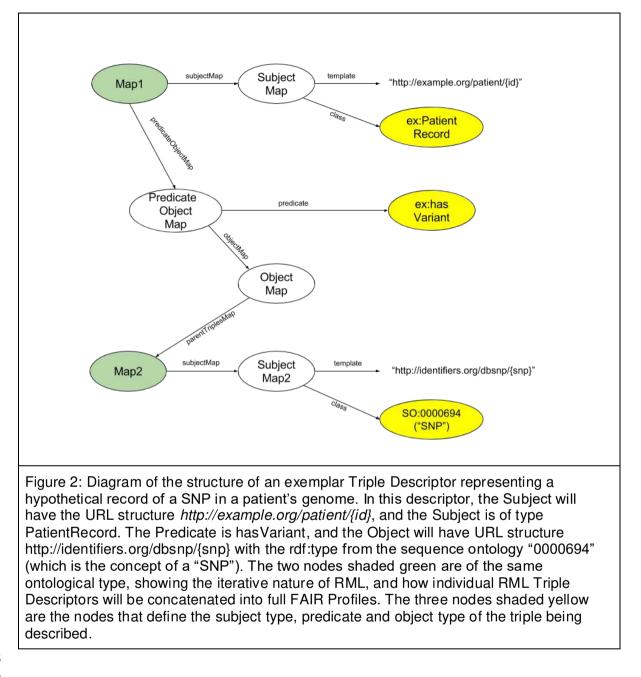
466 maps are modular documents where each component describes the schema for a single-467 resource-centric graph (i.e. a graph with all triples that share the same subject). The "object" 468 position in each of these map modules may be mapped to a literal, or may be mapped to 469 another RML module, thus allowing linkages between maps in much the same way that the 470 object of an RDF triple may become the subject of another triple. RML modules therefore 471 may then be assembled into a complete map representing both the structure and the 472 semantics of an RDF representation of a data source. RML maps themselves take the form 473 of RDF documents, and can be published on the Web, discovered, and reused, via standard 474 Web technologies and protocols. RML therefore fulfils each of the desiderata for FAIR 475 Profiles, and as such, we selected this technology as the candidate for their implementation. 476 Comparing with related technologies, this portion of our interoperability prototype serves a 477 similar purpose to the XML Schema (XSD: Fallside & Walmsley, 2004) definitions within the 478 output component of a Web Services Description Language (WSDL) document, but unlike 479 XSD, is capable of describing the structure and semantics of RDF graphs.

480

481 Of particular interest to us was the modularity of RML - its ability to model individual triples. 482 This speaks directly to our desiderata 4, where we do not wish to require (and should not 483 expect) a modeller to invest the time and effort required to fully model every facet of a 484 potentially very complex dataset. Far more often, individuals will have an interest in only one 485 or a few facets of a dataset. As such, we chose to utilize RML models at their highest level 486 of granularity - that is, we require a distinct RML model for each triple pattern (subject+type, 487 predicate, object+type) of interest. We call these small RML models "Triple Descriptors". 488 An exemplar Triple Descriptor is diagrammed in Figure 2. There may be many Triple 489 Descriptors associated with a single data resource. Moreover, multiple Triple Descriptors 490 may model the same facet within that data resource, using different URI structures, 491 subject/object semantic types, or predicates, thus acting as different "views" of that data 492 facet. Finally, then, the aggregation of all Triple Descriptors associated with a specific data 493 resource produces a FAIR Profile of that data. Note that FAIR Profiles are not necessarily comprehensive; however, by aggregating the efforts of all modellers, FAIR Profiles model 494 495 only the data facets that are most important to the community.

496

497 FAIR Profiles enable view harmonization over compatible but structurally non-integrable 498 data, possibly in distinct repositories. The Profiles of one data resource can be compared to 499 the Profiles of another data resource to identify commonalities between their Triple 500 Descriptors at the semantic level, even if the underlying data is semantically opaque and/or 501 structurally distinct - a key step toward Interoperability. FAIR Profiles, therefore, have utility, 502 independent of any actuated transformation of the underlying data, in that they facilitate 503 compatible data discovery. Moreover, with respect to desiderata 5, Triple Descriptors, and 504 sometimes entire FAIR Profiles, are RDF documents published on the Web, and therefore 505 may be reused to describe new data resources, anywhere on the Web, that contain similar 506 data elements, regardless of the native representation of that new resource, further 507 simplifying the goal of data harmonization.



508 509

510 Data Interoperability: Data transformation with FAIR Projectors and Triple

- 511 Pattern Fragments
- 512

513 The ability to identify *potentially* integrable data within opaque file formats is, itself, a notable

achievement compared to the *status quo*. Nevertheless, beyond just discovery of relevant

- 515 data, our interoperability layer aims to support and facilitate cross-resource data integration
- and query answering. This requires that the data is not only semantically described, but is
- also semantically and syntactically transformed into a common structure.
- 518

519 Having just presented a mechanism to describe the structure and semantics of data - Triple

520 Descriptors in RML - what remains lacking is a way to retrieve data consistent with those 521 Triple Descriptors. We require a means to expose transformed data without worsening the 522 existing critical barrier to interoperability - opaque, non-machine-readable interfaces and API 523 proliferation (Verborgh & Dumontier, 2016). What is required is a universally-applicable way 524 of retrieving data generated by a (user-defined) data extraction or transformation process, 525 that does not result in yet another API.

526

527 The Triple Pattern Fragments (TPF) specification (Verborgh et al., 2016) defines a REST 528 interface for publishing triples. The server receives HTTP GET calls on URLs that contain a 529 triple pattern [S,P,O], where any component of that pattern is either a constant or a variable. 530 In response, a TPF server returns pages with all triples from its data source that match the 531 incoming pattern. As such, any given triple pattern has a distinct URL.

532

533 We propose, therefore, to combine three elements - data transformed into RDF, which is 534 described by Triple Descriptors, and served via TPF-compliant URLs. We call this 535 combination of technologies a "FAIR Projector". A FAIR Projector, therefore, is a Web 536 resource (i.e., something identified by a URL) that is associated with both a particular data 537 source, and a particular Triple Descriptor. Calling HTTP GET on the URL of the FAIR 538 Projector produces RDF triples from the data source that match the format defined by that 539 Projector's Triple Descriptor. The originating data source behind a Projector may be a 540 database, a data transformation script, an analytical web service, another FAIR Projector, or 541 any other static or dynamic data-source. Note that we do not include a transformation 542 methodology in this proposal; however, we address this issue and provide suggestions in the 543 Discussion section. There may, of course, be multiple projectors associated with any given 544 data source, serving a variety of triples representing different facets of that data.

545

546 Linking the Components: FAIR Projectors and the FAIR Accessor

547

At this point, we have a means for requesting triples with a particular structure - TPF Servers - and we have a means of describing the structure and semantics of those triples - Triple Descriptors. Together with a source of RDF data, these define a FAIR Projector. However, we still lack a formal mechanism for linking TPF-compliant URLs with their associated Triple Descriptors, such that the discovery of a Triple Descriptor with the desired semantics for a particular data resource, also provides its associated Projector URL.

554

We propose that this association can be accomplished, without defining any novel API or 555 556 standard, if the output of a FAIR Projector is considered a DCAT Distribution of a particular 557 data source, and included within the MetaRecord of a FAIR Accessor. The URL of the 558 Projector, and its Triple Descriptor, become metadata facets of a new dcat:Distribution 559 element in the MetaRecord. This is diagrammed in Figure 3, where Distribution_3 and 560 Distribution 4 include Triple Pattern Fragment-formatted URLs representing the FAIR 561 Projector, and the Triple Descriptor RML model describing the structure and semantics of 562 the data returned by calling that Projector.

563

564 Thus, all components of this interoperability system - from the top level repository metadata,

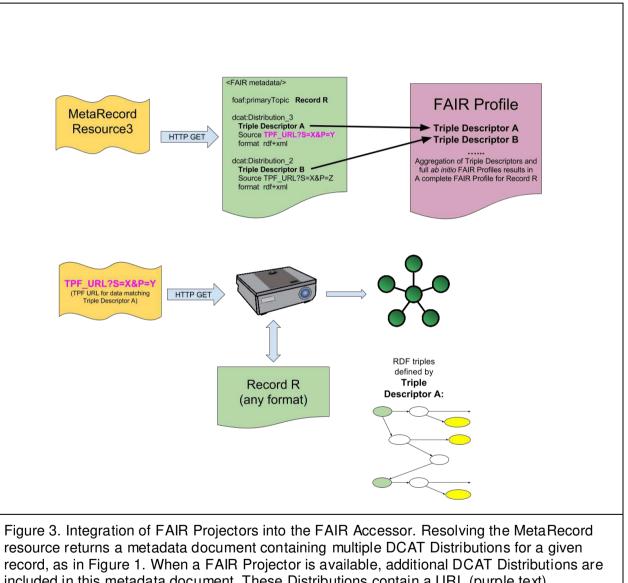
to the individual data cell - are now associated with one another in a manner that allows

mechanized data discovery, harmonization, and retrieval, including relevant citation

567 information. No novel technology or API was required, thus allowing this rich combination of

568 data and metadata to be explored using existing Web tools and crawlers.

569 570



record, as in Figure 1. When a FAIR Projector is available, additional DCAT Distributions are included in this metadata document. These Distributions contain a URL (purple text) representing a Projector, and a Triple Descriptor that describes, in RML, the structure and semantics of the Triple(s) that will be obtained from that Projector resource if it is resolved. These Triple Descriptors may be aggregated into FAIR Profiles, based on the Record that they are associated with (Record R, in the figure) to give a full mapping of all available representations of the data present in Record R.

572

573 Results

574

In the previous section, we provided the URL to a simple exemplar FAIR Accessor published 575 576 on Zenodo. To demonstrate the interoperability system in its entirety - including both the 577 Accessor and the Projector components - we will now proceed through a second exemplar 578 involving the special-purpose repository for protein sequence information, UniProt. In this 579 example, we examine a FAIR Accessor to a dataset, created through a database query, that consists of a specific "slice" of the Protein records within the UniProt database - that is, the 580 581 set of proteins in Aspergillus nidulans FGSC A4 (NCBI Taxonomy ID 227321) that are 582 annotated as being involved in mRNA Processing (Gene Ontology Accession GO:0006397). 583 We first demonstrate the functionality of the two layers of the FAIR Accessor in detail. We 584 then demonstrate a FAIR Projector, and show how its metadata integrates into the FAIR 585 Accessor. In this example, the Projector modifies the ontological framework of the UniProt 586 data such that the ontological terms used by UniProt are replaced by the terms specified in 587 EDAM - an ontology of bioinformatics operations, datatypes, and formats (lson et al., 2013). 588 We will demonstrate that this transformation is specified, in a machine-readable way, by the 589 FAIR Triple Descriptor that accompanies each Projector's metadata. 590

- 591 The two-step FAIR Accessor
- 592

614

593 The example FAIR Accessor accesses a database of RDF hosted by UniProt, and issues 594 the following query over that database (expressed in the standard RDF query language 595 SPARQL):

```
596
597
             PREFIX up:<http://purl.uniprot.org/core/>
598
             PREFIX taxon:<http://purl.uniprot.org/taxonomy/>
599
             PREFIX rdf:<http://www.w3.org/1999/02/22-rdf-syntax-ns#>
600
             PREFIX GO:<http://purl.obolibrary.org/obo/GO >
601
             SELECT DISTINCT ?id
602
603
             WHERE
604
             {
605
                ?protein a up:Protein ;
606
                up:organism taxon:227321 ;
607
                up:classifiedWith/rdfs:subClassOf GO:0006397 .
608
                BIND(substr(str(?protein), 33) as ?id)
609
             }
610
611
      Accessor output is retrieved from the Container Resource URL:
612
613
             http://linkeddata.systems/Accessors/UniProtAccessor
```

- 615 The result of calling GET on the Container Resource URL is visualized in Figure 4, where
- 616 Tabulator (Tim Berners-lee et al., 2006) is used to render the output as HTML for human-
- 617 readability.
- 618
- 619

UniProt Slice FAIR Accessor	creator	wilkinsonlab.info/
- Aspergillus RNA	language	eng
Processing proteins	license	4.0/
	title	UniProt Slice FAIR Accessor - Aspergillus RNA Processing proteins
	authored By	0000 0002 9699 485X
	version	UniProt release 2016 09
	entities	82
	term has Principal	Dr. Mark Wilkinson
	Investigator	
	type	Dataset
		Basic Container
		Collection
	contact Point	Wilkinson.rdf
	description	Takes a SPARQL query of the UniProt database specific to proteins and their GO annotations related to RNA Procssing proteins in Aspergillus and makes it a FAIR Accessor source. The query being executed is:
		PREFIX up: <http: core="" purl.uniprot.org=""></http:>
		PREFIX taxon: <http: purl.uniprot.org="" taxonomy=""></http:>
		PREFIX rdf: <http: 02="" 1999="" 22-rdf-syntax-ns#="" www.w3.org=""></http:>
		PREFIX GO: <http: go_="" obo="" purl.obolibrary.org=""></http:>
		SELECT DISTINCT ?id
		WHERE
		{
		?protein a up:Protein ;
		up:organism taxon:227321 ;
		up:classifiedWith/rdfs:subClassOf GO:0006397 .
		BIND(substr(str(?protein), 33) as ?id)
		}
	identifier	Uni Prot Accessor
	keyword	Aspergillus nidulans
		Aspergillus
		Proteins
		RNA Processing
	landing Page	uniprot.org/
	language	en
	publisher	wilkinsonlab.info/
	theme	RNA Processing conceptscheme.rdf
	contains	C8V1L6
		C8V2B3
		C8V609
		C8V6T1
		C8V8F9
		C8V9C2
		C8V9G4
		C8VBS9
		C8VBV2
		COADAT

Figure 4. A representative portion of the output from resolving the Container Resource of the FAIR Accessor, rendered into HTML by the Tabulator Firefox plugin. The three columns show the label of the Subject node of all RDF Triples (left), the label of the URI in the predicate position of each Triple (middle), and the value of the Object position (right), where blue text indicates that the value is a Resource, and black text indicates that the value is a literal.

- 621
- 622 Of particular note are the following metadata elements:
- 623
- 624

http://purl.org/dc/elements/1.1/license	https://creativecommons.org/licenses/by-nd/4.0/
http://purl.org/pav/authoredBy	http://orcid.org/0000-0002-9699-485X
http://rdfs.org/ns/void#entities	82
a	http://purl.org/dc/dcmitype/Dataset
	http://www.w3.org/ns/ldp#BasicContainer
	http://www.w3.org/ns/prov#Collection
http://www.w3.org/ns/dcat#contactPoint	http://biordf.org/DataFairPort/MiscRDF/Wilkinson.rdf
http://www.w3.org/ns/dcat#keyword	"Aspergillus nidulans", "Aspergillus", "Proteins", "RNA Processing";
http://www.w3.org/ns/dcat#theme	http://linkeddata.systems/ConceptSchemes/RNA_Proces sing_conceptscheme.rdf
http://www.w3.org/ns/ldp#contains	http://linkeddata.systems/cgi-bin/Accessors/ UniProtAccessor/C8VIL6
	http://linkeddata.systems/cgi-bin/Accessors/ UniProtAccessor/C8V2B3

625 626

627

628

- License information is provided as an HTML + RDFa document, following one of the primary standard license forms published by Creative Commons. This allows the license to be unambiguously interpreted by both machines and people prior to accessing any data elements, an important feature that will be discussed later.
- Authorship is provided by name, using the Academic Research Project Funding
 Ontology (ARPFO), but is also unambiguously provided by a link to the author's
 ORCID, using the Provenance Authoring and Versioning (PAV; Ciccarese et al,
 2013) ontology.
- The repository descriptor is typed as being a Dublin Core Dataset, a Linked Data
 Platform container, and a Provenance Collection, allowing it to be interpreted by a
 variety of client agents, and conforming to several best-practices, such as the
 Healthcare and Life Science Dataset Description guidelines (Gray et al., 2015;
 Dumontier et al., 2016)
- 639 Contact information is provided in a machine-readable manner via the Friend of a
 640 Friend (FoaF) record of the author, and the DCAT ontology "contactPoint" property.
- Human readable keywords, using DCAT, are mirrored and/or enhanced by a
 machine-readable RDF document which is the value of the DCAT "theme" property.
 This RDF document follows the structure determined by the Simple Knowledge
 Organization System (SKOS) ontology, and lists the ontological terms that describe
 the repository for machine-processing.

- Finally, individual records within the dataset are represented as the value of the
 Linked Data Platform "contains" property, and provided as a possibly paginated list of
 URLs (a discussion of machine-actionable pagination will not be included here).
 These URLs are the MetaRecord Resource URLs shown in Figure 1.
- 650 651

Following the flow in Figure 1, the next step in the FAIR Accessor is to resolve a
MetaRecord Resource URL. For clarity, we will first show the metadata document that is
returned if there are no FAIR Projectors for that dataset. This will be similar to the document
returned by calling a FAIR MetaRecord URL in the Zenodo use case discussed in the earlier
Methods section.

657

658 Calling HTTP GET on a MetaRecord Resource URL returns a document that include

659 metadata elements and structure shown in Figure 5. Note that Figure 5 is not the complete

660 MetaRecord; rather it has been edited to include only those elements relevant to the aspects

of the interoperability infrastructure that have been discussed so far. More complete

662 examples of the MetaRecord RDF, including the elements describing a Projector, are

described in Figures 7, 8, and 9.

UniProt Protein C8V1L6	bibliographic Citation	The UniProt Consortium (2015). UniProt: a hub for protein information. Nucleic Acids Res. 43: D204-D212
	creator	UniProt Consortium
	language	eng
	license	3.0/
	title	UniProt Protein C8V1L6
	Version	UniProt release 2016 09
	in dataset	Uni Prot Accessor/
	contact point	contact
	description	Splicing factor u2af large subunit (AFU orthologue AFUA 7G05310)
	distribution	Distribution D7566F52 C143 11E6 897C 26245D07C3DD
		Distribution D75682F8 C143 11E6 897C 26245D07C3DD
	identifier	C8V1L6
	keyword	Annotation
	-	Aspergillus nidulans
		Aspergillus
		Functinal Annotation
		GO
		Gene Ontology
		Proteins
		RNA Processing
	landing page	uniprot.org
	language	en
	publisher	uniprot.org
	page	sparql
		uniprot.org/
	primary topic	C8V1L6
C8V1L6		
Distribution D7566F52 C143 11E6 897C	format	text/html
26245D07C3DD	type	Dataset
		Distribution
	download URL	C8V1L6.html
Distribution D75682F8 C143 11E6 897C	format	application/rdf+xml
26245D07C3DD	type	Dataset
	()pc	dataset
		Distribution
	download URL	C8V1L6.rdf
	dominoud one	eet mener

of the FAIR Accessor for record C8V1L6 (at *http://linkeddata.systems/Accessors/UniProtAccessor/C8V1L6*), rendered into HTML by the Tabulator Firefox plugin. The columns have the same meaning as in Figure 4.

666

667

668 Many properties in this metadata document are similar to those at the higher level of the 669 FAIR Accessor. Notably, however, the primary topic of this document is the UniProt record, 670 indicating a shift in the focus of the document from the provider of the Accessor to the provider of the originating Data. Therefore, the values of these facets now reflect the 671 672 authorship and contact information for that record. We do, recognize that MetaRecords are 673 themselves scholarly works and should be properly cited. The MetaRecord includes the "in 674 dataset" predicate, which refers back to the first level of the FAIR Accessor, thus this provides one avenue for capturing the provenance information for the MetaRecord. If 675 676 additional provenance detail is required, we propose (but no not describe further here) that 677 this information could be contained in a separate named graph, in a manner akin to that 678 used by NanoPublications (Kuhn et al., 2016). 679 680 The important distinctive property in this document is the "distribution" property, from the

681 DCAT ontology. For clarity, an abbreviated document in Turtle format is shown in Figure 6,

682 containing only the "distribution" elements and their values.

```
@prefix dc: <http://purl.org/dc/elements/1.1/>.
@prefix dcat: <http://www.w3.org/ns/dcat#>.
@prefix Uni: <http://linkeddata.systems/Accessors/UniProtAccessor/>.
Uni:C8V1L6
   dcat:distribution
       <#DistributionD7566F52-C143-11E6-897C-26245D07C3DD>,
       <#DistributionD75682F8-C143-11E6-897C-26245D07C3DD>;
<#DistributionD7566F52-C143-11E6-897C-26245D07C3DD>
   dc:format
      "text/html";
        dc:Dataset, dcat:Distribution;
   а
   dcat:downloadURL
      <http://www.uniprot.org/uniprot/C8V1L6.html>.
<#DistributionD75682F8-C143-11E6-897C-26245D07C3DD>
   dc:format
      "application/rdf+xml";
        dc:Dataset, void:Dataset, dcat:Distribution;
   а
   dcat:downloadURL
      <http://www.uniprot.org/uniprot/C8V1L6.rdf>.
```

Figure 6. Turtle representation of the subset of triples from the MetaRecord metadata pertaining to the two DCAT Distributions. Each distribution specifies an available representation (media type), and a URL from which that representation can be downloaded.

685 686

There are two DCAT Distributions in this document. The first is described as being in format 687 "application/rdf+xml", with its associated download URL. The second is described as being 688 689 in format "text/html", again with the correct URL for that representation. Both are typed as 690 Distributions from the DCAT ontology. These distributions are published by UniProt 691 themselves, and the UniProt URLs are used. Additional metadata in the FAIR Accessor (not 692 shown in Figure 6) describes the keywords that relate to that record in both machine and 693 human-readable formats, access policy, and license, allowing machines to more accurately 694 determine the utility of this record prior to retrieving it.

695

696 Several things are important to note before moving to a discussion of FAIR Projectors. First, 697 the two levels of the FAIR Accessor are not interdependent. The Container layer can 698 describe relevant information about the scope and nature of a repository, but might not 699 provide any further links to MetaRecords. Similarly, whether or not to provide a distribution 700 within a MetaRecord is entirely at the discretion of the data owner. For sensitive data, an 701 owner may chose to simply provide (even limited) metadata, but not provide any direct link to 702 the data itself, and this is perfectly conformant with the FAIR guidelines. Further, when 703 publishing a single data record, it is not obligatory to publish the Container level of the FAIR 704 Accessor; one could simply provide the MetaRecord document describing that data file, 705 together with an optional link to that file as a Distribution. Finally, it is also possible to publish 706 containers of containers, to any depth, if such is required to describe a multi-resource 707 scenario (e.g. an institution hosting multiple distinct databases).

708

709 The FAIR Projector

710

FAIR Projectors can be used for many purposes, including (but not limited to) publishing
transformed Linked Data from non-Linked Data; publishing transformed data from a Linked
Data source into a distinct structure or ontological framework; load-management/querymanagement; or as a means to explicitly describe the ontological structure of an underlying
data source in a searchable manner. In this demonstration, the FAIR Projector publishes
dynamically transformed data, where the transformation involves altering the semantics of
RDF provided by UniProt into a different ontological framework (EDAM).

719 This FAIR Projector's TPF interface is available at:

721 http://linkeddata.systems:3001/fragments

722

723 Data exposed as a TPF-compliant Resource require a subject and/or predicate and/or object

value to be specified in the URL; a request for the all-variable pattern (blank, as above) will return nothing. How can a software agent know what URLs are valid, and what will be

726 returned from such a request?

727

In this interoperability infrastructure, we propose that Projectors should be considered as

729 DCAT Distributions, and thus TPF URLs, with appropriate parameters bound, are included in

the distribution section of the MetaRecord metadata. An example is shown in Figure 7, againrendered using Tabulator.

732

-	0	\mathbf{a}
1	·	· 🖌 👘
1	J	J

UniProt Protein C8V1L6	bibliographic Citation	The UniProt Consortium (2015). UniProt: a hub for protein information. Nucleic Acids Res. 43: D204-D212
	creator	UniProt Consortium
	language	eng
	license	3.0/
	title	UniProt Protein C8V1L6
	Version	UniProt release 2016 09
	in dataset	Uni Prot Accessor/
	contact point	contact
	description	Splicing factor u2af large subunit (AFU orthologue AFUA 7G05310)
	distribution	Distribution9E275EC2 C1F6 11E6 8812 3E445D07C3DD
		Distribution9E2771E6 C1F6 11E6 8812 3E445D07C3DD
		Distribution9EFD1238 C1F6 11E6 8812 3E445D07C3DD
		Distribution9EFD2458 C1F6 11E6 8812 3E445D07C3DD
	identifier	C8V1L6
	keyword	Annotation
		Aspergillus nidulans
		Aspergillus
		Functinal Annotation
		GO
		Gene Ontology
		Proteins
		RNA Processing
	landing page	uniprot.org
	language	en
	publisher	uniprot.org
	page	sparql
		uniprot.org/
	primary topic	C8V1L6

Figure 7. A portion of the output from resolving the MetaRecord Resource of the FAIR Accessor for record C8UZX9, rendered into HTML by the Tabulator Firefox plugin. The columns have the same meaning as in Figure 4. Comparing the structure of this document to that in Figure 5 shows that there are now four values for the "distribution" predicate. An RDF and HTML representation, as in Figure 5, and two additional distributions with URLs conforming to the TPF design pattern (highlighted).

734

735

- Note that there are now four distributions two of them are the html and rdf distributions
 discussed above (Figure 5). The two new distributions are those provided by a FAIR
 Projector. Again, looking at an abbreviated and simplified Turtle document for clarity (Figure
 8) we can see the metadata structure of one of these two new distributions.
- 740

@prefix dc: <http://purl.org/dc/elements/1.1/>.
@prefix dcat: <http://www.w3.org/ns/dcat#>.

```
@prefix rr: <http://www.w3.org/ns/r2rml#>.
@prefix gl: <http://semweb.mmlab.be/ns/gl#>.
@prefix rml: <http://semweb.mmlab.be/ns/rml#>.
@prefix Uni: <http://linkeddata.systems/Accessors/UniProtAccessor//>.
@prefix void: <http://rdfs.org/ns/void#>.
@prefix Uni: </cgi-bin/Accessors/UniProtAccessor/>.
@prefix FAI: <http://datafairport.org/ontology/FAIR-schema.owl#>.
@prefix core: <http://purl.uniprot.org/core/>.
@prefix edam: <http://edamontology.org/>.
Uni:C8V1L6
   dcat:distribution
       <#Distribution9EFD1238-C1F6-11E6-8812-3E445D07C3DD>,
<#Distribution9EFD1238-C1F6-11E6-8812-3E445D07C3DD>
  dc:format
      "application/rdf+xml", "application/x-turtle", "text/html";
  rml:hasMapping
      <#Mappings9EFD1238-C1F6-11E6-8812-3E445D07C3DD>;
        FAI: Projector, dc:Dataset, void:Dataset, dcat:Distribution;
   а
   dcat:downloadURL
   <http://linkeddata.systems:3001/fragments?subject=http%3A%2F%2Fidentifiers%2Eorg
%2Funiprot%2FC8V1L6&predicate=http%3A%2F%2Fpur1%2Euniprot%2Eorg%2Fcore%2Fclassified
With>.
<#Mappings9EFD1238-C1F6-11E6-8812-3E445D07C3DD>
  rr:subjectMap
      <#SubjectMap9EFD1238-C1F6-11E6-8812-3E445D07C3DD>.
  rr:predicateObjectMap
      <#POMap9EFD1238-C1F6-11E6-8812-3E445D07C3DD>;
<#SubjectMap9EFD1238-C1F6-11E6-8812-3E445D07C3DD>
  rr:class edam:data 0896; rr:template "http://identifiers.org/uniprot/{ID}".
<#POMap9EFD1238-C1F6-11E6-8812-3E445D07C3DD>
   rr:objectMap
      <#ObjectMap9EFD1238-C1F6-11E6-8812-3E445D07C3DD>;
  rr:predicate
      core:classifiedWith.
<#ObjectMap9EFD1238-C1F6-11E6-8812-3E445D07C3DD>
  rr:parentTriplesMap <#SubjectMap29EFD1238-C1F6-11E6-8812-3E445D07C3DD>.
<#SubjectMap29EFD1238-C1F6-11E6-8812-3E445D07C3DD>
```

rr:class ed:data 1176; rr:template "http://identifiers.org/taxon/{TAX}".

Figure 8. Turtle representation of the subset of triples from the MetaRecord metadata pertaining to one of the FAIR Projector DCAT Distributions of the MetaRecord shown in Figure 7. The text is colour-coded to assist in visual exploration of the RDF. The DCAT Distribution blocks of the two Projector distributions (black bold) have multiple media-type representations (red), and are connected to an RML Map (Dark blue) by the hasMapping predicate, which is a block of RML that semantically describes the subject, predicate, and object (green, orange, and purple respectively) of the Triple Descriptor for that Projector. This block of RML is schematically diagrammed in Figure 2. The three media-types (red) indicate that the URL will respond to HTTP Content Negotiation, and may return any of those three formats.

741

742 Following the Triple Pattern Fragments behaviour, requesting the downloadURL with HTTP 743 GET will trigger the Projector to restrict its output to only those data from UniProt where the 744 subject is UniProt record C8V1L6, and the property of interest is "classifiedWith" from the 745 UniProt Core ontology. The triples returned in response to this call, however, will not match 746 the native semantics of UniProt, but rather will match the semantics and structure defined in 747 the RML Mappings block. The schematic structure of this Mapping RML is diagrammed in 748 Figure 2. The Mappings describes a Triple where the subject will be of type 749 edam: data 0896 ("Protein record"), the predicate will be "classifiedWith" from the UniProt Core ontology, and the object will be of type edam: data 1176 ("GO Concept ID"). 750 751

753 Specifically, the triples returned are:

755 @prefix uni: <http://identifiers.org/uniprot/>.
756 @prefix obo: <http://purl.obolibrary.org/obo/>.
757 uni:C8V1L6 core:classifiedWith obo:G0_0000245, obo:G0_0045292 .

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This is accompanied by a block of hypermedia controls (not shown) using the Hydra
vocabulary (Lanthaler & Gütl; Das, Sundara & Cyganiak, 27 September, 2012) that provide
machine-readable instructions for how to navigate the remainder of that dataset - for
example, how to get the entire row, or the entire column for the current data-point.

Though the subject and object are not explicitly typed in the output from this call to the Projector, further exploration of the Projector's output, via those TPF's hypermedia controls, would reveal that the Subject and Object are in fact typed according to the EDAM ontology, as declared in the RML Mapping. Thus, this FAIR Projector served data transformed from UniProt Core semantic types, to the equivalent data represented within the EDAM semantic framework, as shown in Figure 9. Also note that the URI structure for the UniProt entity has been changed from the UniProt URI scheme to a URI following the Identifiers.org scheme.

The FAIR Projector, in this case, is a script that dynamically transforms data from a query of
UniProt into the appropriately formatted triples; however, this is opaque to the client. The
Projector's TPF interface, from the perspective of the client, would be identical if the
Projector was serving pre-transformed data from a static document, or even generating

novel data from an analytical service. Thus, FAIR Projectors harmonize the interface to
retrieving RDF data in a desired semantic/structure, regardless of the underlying mechanism
for generating that data.

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780 This example was chosen for a number of reasons. First, to contrast with the static Zenodo 781 example provided earlier, where this Accessor/Projector combination are querying the 782 UniProt database dynamically. In addition, because we wished to demonstrate the utility of 783 the Projector's ability to transform the semantic framework of existing FAIR data in a 784 discoverable way. For example, in UniProt, Gene Ontology terms do not have a richer 785 semantic classification than "owl: Class". With respect to interoperability, this is problematic, 786 as the lack of rich semantic typing prevents them from being used for automated discovery 787 of resources that could potentially consume them, or use them for integrative, cross-domain 788 queries. This FAIR Accessor/Projector advertises that it is possible to obtain EDAM-789 classified data, from UniProt, simply by resolving the Projector URL.

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In UniProt	http://purl.uniprot.org/uniprot/C8UZX9		
	a		
	<pre>http://purl.uniprot.org/core/Protein ;</pre>		
	<pre>http://purl.uniprot.org/core/classifiedWith http://purl.obolibrary.org/obo/G0_0000462 .</pre>		
	http://purl.obolibrary.org/obo/GO_0000462		
	a http://www.w3.org/2002/07/owl#Class		
After Projection	http://identifiers.org/uniprot/C8UZX9		
	http://edamontology.org/data_0896 ;		
	<pre>http://purl.uniprot.org/core/classifiedWith http://purl.obolibrary.org/obo/G0_0000462 .</pre>		
	http://purl.obolibrary.org/obo/GO_0000462		
	a http://edamontology.org/data_1176		

Figure 9: Data before and after FAIR Projection. Bolded segments show how the URI structure and the semantics of the data were modified, according to the mapping defined in the Triple Descriptor (data_0896 = "Protein report" and data_1176 = "GO Concept ID"). URI structure transformations may be useful for integrative queries against datasets that utilize the Identifiers.org URI scheme such as OpenLifeData (González et al., 2014). Semantic transformations allow integrative queries across datasets that utilize diverse and redundant ontologies for describing their data, and in this example, may also be used to add semantics where there were none before.

793 Discussion

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795 Interoperability is hard. It was immediately evident that, of the four FAIR principles, 796 Interoperability was going to be the most challenging. Here we have designed a novel 797 infrastructure with the primary objective of interoperability for both metadata and data, but 798 with an eye to all four of the FAIR Principles. We wished to provide discoverable and 799 interoperable access to a wide range of underlying data sources - even those in 800 computationally opaque formats - as well as supporting a wide array of both academic and 801 commercial end-user applications above these data sources. In addition, we imposed 802 constraints on our selection of technologies; in particular, that the implementation should re-803 use existing technologies as much as possible, and should support multiple and 804 unpredictable end-uses. Moreover, it was accepted from the outset that the trade-off 805 between simplicity and power was one that could not be avoided, since a key objective was 806 to maximize uptake over the broadest range of data repositories, spanning all domains - this 807 would be nearly impossible to achieve through, for example, attempting to impose a 808 'universal' API or novel query language. Thus, with the goal of maximizing global uptake and 809 adoption of this interoperability infrastructure, and democratizing the cost of implementation 810 over the entire stakeholder community - both users and providers - we opted for lightweight, 811 weakly integrative, REST solutions, that nevertheless lend themselves to significant degrees 812 of mechanization in both discovery and integration. 813

- We now look more closely at how this interoperability infrastructure meets the expectationswithin the FAIR Principles.
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- FAIR facet(s) addressed by the Container Resource:
- **Findable** The container has a distinct globally unique and resolvable identifier, allowing it to be discovered and explicitly, unambiguously cited. This is important because, in many cases, the dataset being described does not natively possess an identifier, as in our example above where the dataset represented the results of a query. In addition, the container's metadata describes the research object, allowing humans and machines to evaluate the potential utility of that object for their task.
- Accessible the Container URL resolves to a metadata record using standard HTTP GET. In addition to describing the nature of the research object, the metadata record should include information regarding licensing, access restrictions, and/or the access protocol for the research object.
 Importantly, the container metadata exists independently of the research object it describes, where FAIR Accessibility requires metadata to be persistently available even if the data itself is not.
- Interoperable The metadata is provided in RDF a globally-applicable
 syntax for data and knowledge sharing. In addition, the metadata uses
 shared, widely-adopted public ontologies and vocabularies to facilitate
 interoperability at the metadata level.

836	Reusable - the metadata includes citation information related to the
837	authorship of the container and/or its contents, and license information related
838	to the reuse of the data, by whom, and for what purpose.
839	to the reduce of the data, by whom, and for what purpose.
840	Other features of the Container Resource
841	Privacy protection - The container metadata provides access to a rich
842	description of the content of a resource, without exposing any data within that
843	resource. While a provider may choose to include MetaRecord URLs within
844	this container, they are not required to do so if, for example, the data is highly
845	sensitive, or no longer easily accessible; however, the contact information
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847	provided within the container allows potential users of that data to inquire as
	to the possibility of gaining access in some other way. As such, this container
848	facilitates a high degree of FAIRness, while still providing a high degree of
849 850	privacy protection.
851	FAIR Facet(s) Addressed by the MetaRecord:
852	• Findable - The MetaRecord URL is a globally-unique and resolvable identifier
853	for a data entity, regardless of whether or not it natively possesses an
854	identifier. The metadata it resolves to allows both humans and machines to
855	interrogate the nature of a data element before deciding to access it.
856	Accessible - the metadata provided by accessing the MetaRecord URL
857	describes the accessibility protocol and license information for that record,
858	and describes all available formats.
859	 Interoperable - as with the Container metadata, the use of shared ontologies
860	and RDF ensures that the metadata is interoperable.
861	Reusable - the MetaRecord metadata should carry record-level citation
862	information to ensure proper attribution if the data is used. We further
863	propose, but do not demonstrate, that authorship of the MetaRecord itself
864	could be carried in a second named-graph, in a manner similar to that
865	proposed by the NanoPublication specification.
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867	Other features of the MetaRecord
868	• Privacy protection - the MetaRecord provides for rich descriptive information
869	about a specific member of a collection, where the granularity of that
870	description is entirely under the control of the data owner. As such, the
871	MetaRecord can provide a high degree of FAIRness at the level of an
872	individual record, without necessarily exposing any identifiable information. In
873	addition, the provider may choose to stop at this level of FAIRness, and not
874	include further URLs giving access to the data itself.
875	• Symmetry of traversal - Since we predict that clients will, in the future, query
876	over indexes of FAIR metadata searching for dataset or records of interest, it
877	is not possible to predict the position at which a client or their agent will enter
878	your FAIR Accessor. While the container metadata provides links to individual
879	MetaRecords, the MetaRecord similarly provides a reference back "upwards"
013	metal cecords, the metal cecord similarly provides a reference back upwards

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to its container. Thus a client can access repository-level metadata (e.g. curation policy, ownership, linking policy) for any given data element it discovers. This became particularly relevant as a result of the European Court of Justice decision (Court of Justice, 2016) that puts the burden of proof on those who create hyperlinks to ensure the document they link to is not, itself, in violation of copyright.

 High granularity of access control - individual elements of a collection may have distinct access constraints or licenses. For example, individual patients within a study may have provided different consent. MetaRecords allow each element within a collection to possess, and publish, its own access policy, access protocol, license, and/or usage-constraints, thus providing finegrained control of the access/use of individual elements within a repository.

FAIR Facet(s) Addressed by the Triple Descriptors and FAIR Projectors:

- **Findable** Triple Descriptors, in isolation or when aggregated into FAIR Profiles, provide one or more semantic interpretations of data elements. By indexing these descriptors, it would become possible to search over datasets for those that contain data-types of interest. Moreover, FAIR Projectors, as a result of the TPF URI structure, create a unique URL for every data-point within a record. This has striking consequences with respect to scholarly communication. For example, it becomes possible to unambiguously refer-to, and therefore "discuss" and/or annotate, individual spreadsheet cells from any data repository.
- 904 Accessible - Using the TPF design patterns, all data retrieval is • 905 accomplished in exactly the same way - via HTTP GET. The response 906 includes machine-readable instructions that guide further exploration of the 907 data without the need to define an API. FAIR Projectors also give the data 908 owner high granularity access control; rather than publishing their entire 909 dataset, they can select to publish only certain components of that dataset, 910 and/or can put different access controls on different data elements, for 911 example, down to the level of an individual spreadsheet cell.
 - Interoperable FAIR Projectors provide a standardized way to export any type of underlying data in a machine-readable structure, using widely used, public shared vocabularies. Data linkages that were initially implicit in the datastore, identifiers for example, become explicit when converted into URIs, resulting in qualified linkages between formerly opaque data deposits. Similarly, data that resides within computationally opaque structures or formats can also be exposed, and published in a FAIR manner if there is an algorithm capable of extracting it and exposing it via the TPF interface.
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Other features of FAIR Projection

- Native formats are preserved - As in many research domains, bioinformatics has created a large number of data/file formats. Many of these, especially those that hold "big data", are specially formatted flat-files that focus on size-efficient representation of data, at the expense of general machine-accessibility. The analytical tooling that exists in this domain is capable of consuming these various formats. While the FAIR Data 932 community has never advocated for wholesale Interoperable representations 933 of these kinds of data - which would be inefficient, wasteful, and lacking in 934 utility - the FAIR Projector provides a middle-ground. Projection allows 935 software to query the core content of a file in a repository prior to downloading 936 it; for example, to determine if it contains data about an entity or identifier of 937 interest. FAIR Projectors, therefore, enable efficient discovery of data of-938 interest, without requiring wasteful transformation of all data content into a 939 FAIR format.
- 940 Semantic conversion of existing Triplestores - It is customary to re-cast 941 the semantic types of entities within triplestores using customized SPARQL 942 BIND or CONSTRUCT clauses. FAIR Projectors provide a standardized, 943 SPARQL-free, and discoverable way to accomplish the same task. This 944 further harmonizes data, and simplifies interoperability.
- 945 Standardized interface to (some) Web APIs - Many Web APIs in the 946 biomedical domain have a single input parameter, generally representing an 947 identifier for some biochemical entity. FAIR Projectors can easily replace 948 these myriad Web APIs with a common TPF interface, thus dramatically 949 enhancing discoverability, machine-readability, and interoperability between 950 these currently widely disparate services.
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952 Incentives and Barriers to Implementation

Looking forward, there is every indication that FAIRness will soon be a requirement of 953 954 funding agencies and/or journals. As such, infrastructures such as the one described in this 955 exemplar will almost certainly become a natural part of scholarly data publishing in the 956 future. Though the FAIR infrastructure proposed here may appear difficult to achieve, we 957 argue that a large portion of these behaviours - for example, the first two layers of the 958 Accessor - can be accomplished using simple fill-in-the-blank templates. Such templating 959 tools are, in fact, already being created by several of the co-authors, and will be tested on 960 the biomedical data publishing community in the near future to ensure they are clear and 961 usable by this key target-audience.

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963 Projection, however, is clearly a complex undertaking, and one that is unlikely to be accomplished by non-informaticians on their own. Transformation from unstructured or 964 965 semi-structured formats into interoperable formats cannot be fully automated, and we do not 966 claim to have fully solved the interoperability bottleneck. We do, however, claim to have 967 created an infrastructure that improves on the status quo in two ways: First, we propose to

968 replace the wasteful, one-off, "reuseless" data transformation activities currently undertaken 969 on a daily basis throughout the biomedical community (and beyond), with a common, 970 reusable, and machine-readable approach, by suggesting that all data transformations 971 should be described in RML and transformed data exposed using TPF. Second, the solution 972 we propose may, in many cases, partially automate the data transformation process itself. 973 RML can be used, in combination with generic software such as RML Processor 974 (http://github.com/RMLio) to actuate a data transformation over many common file formats 975 such as CSV or XML. As such, by focusing on building RML models, in lieu of reuseless 976 data transformation scripts, data publishers achieve both the desired data transformation, as 977 well as a machine-readable interface that provides that transformed data to all other users. 978 This may be incentivized even more by creating repositories of RML models that can be reused by those needing to do data transformations. Though the infrastructure for capturing 979 980 these user-driven transformation events and formalizing them into FAIR Projectors does not 981 yet exist, it does not appear on its surface to be a complex problem. Thus, we expect that 982 such infrastructure should appear soon after FAIRness becomes a scholarly publishing 983 requirement, and early prototypes of these infrastructures are being built by our co-authors. 984

985 Several communities of data providers are already planning to use this, or related FAIR 986 implementations, to assist their communities to find, access, and reuse their valuable data 987 holdings. For example, the Biobanking and Rare disease communities will be given end-988 user tools that utilize/generate such FAIR infrastructures to: guide discovery by researchers; 989 help both biobankers and researchers to re-code their data to standard ontologies building 990 on the SORTA system (Pang et al., 2015); assist to extend the MOLGENIS/BiobankConnect 991 system (Pang et al., 2016); add FAIR interfaces to the BBMRI (Biobanking and BioMolecular 992 resources Research Infrastructure) and RD-connect national and European biobank data 993 and sample catalogues. There are also a core group of FAIR infrastructure authors who are 994 creating large-scale indexing and discovery systems that will facilitate the automated identification and retrieval of relevant information, from any repository, in response to end-995 996 user queries, portending a day when currently unused - "lost" - data deposits once again 997 provide return-on-investment through their discovery and reuse. 998

999 Conclusions

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1001 There is a growing movement of governing bodies and funding organizations towards a 1002 requirement for open data publishing, following the FAIR Principles. It is, therefore, useful to 1003 have an exemplar "reference implementation" that demonstrates the kinds of behaviours that 1004 are expected from FAIR resources.

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1006 Of the four FAIR Principles, Interoperability is arguably the most difficult FAIR facet to 1007 achieve, and has been the topic of decades of informatics research. Several new standards 1008 and frameworks have appeared in recent months that addressed various aspects of the 1009 Interoperability problem. Here, we apply these in a novel combination, and show that the

1010 result is capable of providing interoperability between formerly incompatible data formats

- 1011 published anywhere on the Web. In addition, we note that the other three aspects of FAIR -1012 Findability, Accessibility, and Reusability - are easily addressed by the resulting 1013 infrastructure. The outcome, therefore, provides machine-discoverable access to richly 1014 described data resources in any format, in any repository, with the possibility of 1015 interoperability of the contained data down to the level of an individual "cell". No new 1016 standards or APIs were required; rather, we rely on REST behaviour, with all entities being 1017 resources with a resolvable identifier that allow hypermedia-driven "drill-down" from the level 1018 of a repository descriptor, all the way to an individual data point in the record. 1019 1020 Such an interoperability layer may be created and published by anyone, for any data source, 1021 without necessitating an interaction with the data owner. Moreover, the majority of the 1022 interoperability layer we describe may be achieved through dynamically generated files from 1023 software, or even (for the Accessor portion) through static, manually-edited files deposited in 1024 any public repository. As such, knowledge of how to build or deploy Web infrastructure is not 1025 required to achieve a large portion of these FAIR behaviours. 1026 1027 The trade-off between power and simplicity was considered acceptable, as a means to 1028 hopefully encourage wide adoption. The modularity of the solution was also important 1029 because, in a manner akin to crowdsourcing, we anticipate that the implementation will 1030 spread through the community on a needs-driven basis, with the most critical resource
- 1031 components being targeted early the result of individual researchers requiring interoperable
- access to datasets/subsets of interest to them. The interoperability design patterns
 presented here provide a structured way for these individuals to contribute and share their
- 1034 individual effort effort they would have invested anyway in a collaborative manner, piece-
- 1035 by-piece building a much larger interoperable and FAIR data infrastructure to benefit the 1036 global community.

1037

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1039

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