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Discovering Domain-Specific Public SPARQL Endpoints: A Life-Sciences Use-Case

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ABSTRACT
A significant portion of the LOD cloud consists of Life Sciences data sets. The LOD cloud contains billions of clinical facts linked together forming an interconnected “Web of Clinical Data”. However, tools for new publishers to find relevant datasets that could potentially be linked to are missing, particularly in specialist domain-specific settings. Based on a set of domain-specific keywords extracted from a local dataset, this paper proposes methods to automatically identify a list of public SPARQL endpoints whose content relates to the local dataset.

Keywords
Linked Open Data (LOD) Cloud, Web of Data, SPARQL, Healthcare and Life Sciences

1. INTRODUCTION

Over the past several years, a variety of publishers – coming from academia, governmental organisations, online communities and companies alike – have begun exposing their corpora on the Web as Linked Data. The Linking Open Data (LOD) Cloud\[^2\] provides an overview of 295 Linked Datasets, which, according to publisher statistics\[^2\], incorporate over 30 billion facts. Of these, 41 datasets relate to Life Sciences, incorporating 3 billion facts. With regards to accessing this content, aside from crawling the raw data, 68% of the LOD datasets offer a link to at least one SPARQL endpoint that can be used to directly query the dataset. The Datahub catalogue\[^3\] lists at least 427 such SPARQL endpoints available on the Web (though indeed some are offline or unreliable\[^1\]).

The LOD Cloud also comprises of 500 million links across datasets (191 million links specifically in the life-sciences domain\[^4\] following the fourth Linked Data principle: “link to related data”. From the perspective of a consumer, these links allow for recursively discovering and navigating detailed information about related entities elsewhere on the Web. From the perspective of a publisher, links encourage modularity, where high-quality links (once in place) can reduce the amount of content they need to host: for example, instead of each publisher redundantly providing a basic description of all the countries they mention in their data, each publisher can link to a detailed description for each country in a legacy dataset elsewhere (such as GeoNames or DBpedia). From the perspective of the Web, these links form the mesh upon which the Web of Data is based.

But creating links is a challenging task for publishers. Addressing this challenge, a number of linking frameworks, such as Silk\[^11\] and LIMES\[^6\], have been proposed to help publishers link their local datasets to a remote LOD dataset through a specified SPARQL endpoint. However, given that there are now hundreds of public SPARQL endpoints, a still-more fundamental question has not been tackled: how can publishers find SPARQL endpoints that are relevant targets for links in the first place? As we will see, answering this question is non-trivial, particularly for specialised domains.

Currently the selection of relevant endpoints relies on manual effort and requires experience and knowledge of available datasets and endpoints. One potential method is to manually inspect the list of datasets and endpoints listed on the DataHub catalogue, but only very high level dataset descriptions are available regarding the topic of the dataset and available access mechanisms. The content of SPARQL endpoints can be described using VoID\[^5\], SPARQL 1.1 Service Descriptions, and specialised vocabulary (or ontology)\[^2\], which may help, but these are not available for many endpoints\[^1,10\].

The most general option is to consider the SPARQL endpoints as black boxes whose content is opaque and directly query them to determine if they are relevant. In this paper, we explore this option. Based on a set of domain-specific keywords extracted from a dataset, we probe SPARQL endpoints with queries to determine their relevance. Initially, we identified three potential methods:

\[^{1}\]http://lod-cloud.net/\[^{1}a. 2014/04/07.\]
\[^{2}\]Statistics are quoted from http://lod-cloud.net/state/\[^{2}a. 2014/04/07.\]
\[^{3}\]http://datahub.io/group/lodcloud\[^{3}a. 2014/04/07.\]

\[^{5}\]http://www.w3.org/TR/void/\[^{5}a. 2014/04/07.\]
Full-text Search: SPARQL does not provide any standard full-text search functionality. Although some SPARQL vendors offer custom full-text search features implemented by efficient inverted indexes (e.g., Virtuoso provides a `bif:contains` keyword), not all SPARQL endpoints will support such features.

REGEF Filters: SPARQL allows for matching literals with `REGEF` filter expressions. However, filter expressions are applied as a post-processing step: using `REGEF` for full-text search would involve scanning all object literals in the dataset, rendering this method inefficient and impractical.

Exact Literal Matching: A final option is to create exact literals from the domain keywords that can be looked up directly. However, this method requires an exact literal to be matched, meaning an exact case-sensitive phrase match with the correct language tag.

Herein we focus on the third option given that it will work for any SPARQL endpoint and will involve efficient lookups (as opposed to inefficient post-filtering). In previous work, we proposed an algorithm (called QTERMEX) for combining raw clinical terms into literals [5]. The QTERMEX algorithm takes as input a terminology, in this case a set of Clinical Terms (`CTerms`), and generates a set of Query Terms (`QTerms`). The QTERMEX algorithm incorporates stop-word removal, word permutations, and resolving unique tokens from `CTerms` represented as sentences (e.g., “Migraine cumulative (with aura)”) or URIs (e.g., `http://www.chuv.ch/variables/schizophrenia/code:SZAPU2`). In the former case, for example, the `QTerms` extracted would be “Migraine”, “cumulative”, and “Migraine cumulative” after the punctuation and stop-words “aura” and “with” are removed. To keep the output succinct, the order of words is preserved in the QTERMEX algorithm (i.e., it would not produce “cumulative Migraine”). We then query endpoints for the `QTerm` literals created from the terminology in this fashion.

We take the output from the QTERMEX algorithm and expand it by creating multiple case and language-tag variants for each `QTerm` so as to generate more hits. We also present comparative evaluation of our methods for a real-world use-case involving three clinical partners who wish to publish Linked Data and need to find existing relevant datasets that can be linked to.

The rest of the paper is as follows: Section 2 presents the methodology towards term extraction and a multi-matching algorithm that creates literal variants for each `QTerm` so as to generate more hits. We also present comparative evaluation of our methods for a real-world use-case involving three clinical partners who wish to publish Linked Data and need to find existing relevant datasets that can be linked to.

The first algorithm, `Query Term Extractor` (QTERMEX, Algorithm 1), takes as input a terminology, in this case a set of Clinical Terms (`CTerms`), and generates a set of Query Terms (`QTerms`). Each `QTerm` ε `QTerms` will subsequently be used to generate an RDF literal that can be queried against the SPARQL endpoints of various LOD datasets.

### 2. TERM EXTRACTION AND MULTI MATCHING

As discussed earlier, we use our previously proposed algorithm (QTERMEX) [5] for extraction of literals from `CTerms` (as exemplified in Table 1). These literals are then searched against public endpoints. We propose an algorithm in this paper that queries for case and language-tag variants for extracted literals.

#### 2.1 QTermEx Algorithm

The first algorithm, `Query Term Extractor` (QTERMEX, Algorithm 1), takes as input a terminology, in this case a set of Clinical Terms (`CTerms`), and generates a set of Query Terms (`QTerms`). Each `QTerm` ∈ `QTerms` will subsequently be used to generate an RDF literal that can be queried against the SPARQL endpoints of various LOD datasets.

All `QTerms` in the terminology are iterated over. The input `QTerm` is first pre-processed by replacing junk characters with spaces (JunkCharSet; e.g., punctuation, par-
entheses, symbols, etc.), by removing stop words (SWSet, e.g., “the”, “and”, etc.) and by removing general terms (GTSet; e.g., “duration”, “rate”, “family”, etc.). Junk characters are pre-defined. Stop words are collected from the terminology using the Ranks.nl text-analysis tool. General terms are specific to a given terminology and are defined by domain experts; these general terms are used to reduce the number of queries SPARQL endpoints for multiple case variants of each QTerm and for literals with language tags.

We call this a Direct Matching (DM) approach, where each QTerm is used to generate a single query literal. Each literal is then used to generate a simple SPARQL query as “SELECT ?s ?p WHERE {?s ?p “Term”}”. This can be used to probe for relevant endpoints.

However, querying for exact literals is case sensitive and many literals in LOD datasets contain language tags. Our second algorithm, Multi Matching (μMatch; Algorithm 2), queries SPARQL endpoints for multiple case variants of each QTerm and for literals with language tags.

Algorithm 2: μMatch: Multi Matching Algorithm

Input: A Term (C Term or Q Term), A language tag (lang-tag)
Output: A finite set of dataset endpoints (EPSet)
SEndpoints := set of catalogued Dataset Endpoints;
for EP in SEndpoints do
    add := QueryAndLog(Term, lang-tag, EP);
    PCase := Proper Case Term;
    add := add ∨ QueryAndLog(PCase, lang-tag, EP);
    LCase := lower case Term;
    add := add ∨ QueryAndLog(LCase, lang-tag, EP);
    UCase := UPPER CASE Term;
    add := add ∨ QueryAndLog(UCase, lang-tag, EP);
    if add = true then
        EPSet := EPSet ∪ {EP};
return EPSet;

QueryAndLog(Term, lang-tag, EP)
match := false;
Query := create SPARQL query for Term;
Result := supply Query to EP and retrieve results;
if Result not empty then
    match := true;
    log Result;
    LanguageQuery := add lang-tag to supplied Term
    and create query;
    Result := supply LangCaseQuery to EP and retrieve results;
if Result not empty then
    match := true;
    log Result;
return match;

μMatch (Algorithm 2) takes as input the set of QTerms generated by QTERMEX and a list of URLs for different SPARQL endpoints (SEndpoints). We generate SEndpoints by logging URLs of all candidate SPARQL endpoints in a particular domain. For our use-case, we created a list of SEndpoints specifically for the life-sciences domain. We considered SPARQL endpoints made publicly available by Bio2RDF[11] or that are tagged in the Datahub[12] repository with “life sciences” or “healthcare”.

In the μMatch algorithm, for each Term, we queried SEndpoints by executing the SPARQL query presented before. Since SPARQL is case-sensitive – for example, a literal value “cancer” is not same as “Cancer” or “CANCER” – the algorithm is refined to check for proper case, upper case and lower case literals. Furthermore, language tags are of-

2.2 Multi-Matching: μMatch Algorithm

The QTerms generated from our algorithm QTERMEX can be used to query the SPARQL endpoints of LOD datasets.

Table 2: Distribution of KwList cardinalities

<table>
<thead>
<tr>
<th>KwList</th>
<th>1</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>CHUV</td>
<td>140</td>
<td>70</td>
<td>5</td>
</tr>
<tr>
<td>CING</td>
<td>92</td>
<td>58</td>
<td>24</td>
</tr>
<tr>
<td>ZEINCR</td>
<td>138</td>
<td>7</td>
<td>5</td>
</tr>
</tbody>
</table>

http://www.ranks.nl/

http://download.bio2rdf.org/release/2/release.html
http://datahub.io/
ten used with literal values, for example, in some cases the literal value “cancer” is defined as “cancer”\@en. Our algorithm is thus refined to check for literals with language tags. We use the \@en language tag since the clinical terminologies contained in the datasets from our scenario are primarily in English. However, the proposed algorithm can easily accommodate other regional settings (for example: \@de, \@en-us, \@en-uk, etc.), with the caveat that four additional queries will be required for each additional language tag.

For each Term supplied to the algorithm, we run \muMatch with a set of 8 queries: \{ original-case, proper-case, lowercase, uppercase \} \times \{ no-lang-tag, \@en-tag \}. All non-empty results are logged along with the URLs and names of the respective SPARQL endpoints in \EPSet. In addition, the bindings returned for the ?s (subject) and ?p (predicate) query variables are also recorded and logged when a Term match is found on some particular SPARQL endpoint. The subjects bindings are useful to count the number of unique entities in the remote dataset that are matched by some literal term. The predicates bindings are returned are potentially useful for linking frameworks, like LIMES [6] or SILK [7], that are dependent on mapping information for generating links, such as which predicates to use. For example, the predicates found when searching for “cancer” on different SPARQL endpoints (given in Listing [1]) could provide an entry point for linking based on string-similarity functions.

Listing 1: Set of predicates for “Cancer”

3. EVALUATION

We carried out a series of experiments to compare our proposed algorithms using the three datasets provided by the three clinical partners mentioned in Table [1].

3.1 Experimental Setup

All experiments were conducted on a computer running 64-bit Windows 7 OS, with 4GB RAM and an Intel Core i5 (2.53 GHz) CPU. We use a MySQL RDBMS to store experimental data, including the endpoints to search and the results of successful queries. As previously discussed, we consider a total of 44 public endpoints from the Bio2RDF project and from the Datahub catalogue with “LIFESCIENCES” or “HEALTHCARE” tags. Queries are sent to the public endpoints over HTTP using the standard SPARQL protocol.

Given three sets of raw clinical terms (CTerms) as input, we generate three sets of query terms (QTerms) by applying the QTermEx algorithm [3]. Based on these sets of terms, we then perform the following four experiments:

- **CTerms–DM**: We query endpoints using the raw clinical terms with the Direct Matching (DM) approach: each CTerm creates a single literal and a single query.
- **CTerms–\muM**: We query endpoints using the raw clinical terms with the Multi Matching (\muM) approach: each CTerm creates eight literals with combinations of case and language tags, resulting in eight queries per term.
- **QTerms–DM**: We query endpoints using the extended query terms with the Direct Matching (DM) approach: each QTerm creates a single literal and a single query.
- **QTerms–\muM**: We query endpoints using the extended query terms with the Multi Matching (\muM) approach: each QTerm creates eight literals and eight queries.

The total number of queries generated for each of the three datasets and each of the four experiments is shown in Table [3]. We can see that the query load of Multi Matching approach is fixed at 8× that of the Direct Matching approach. We see that when using the expanded set of query terms, the query load increases by 1.3–2.5× versus the raw clinical terms. Furthermore, we see that our approach generates a non-trivial load of thousands of queries per dataset. However, the queries we issue are single-pattern atomic lookups, which should be efficient for the endpoint to execute.

Figure [1] shows the query generation time (in milliseconds) categorized along two dimensions (1) \muMatch using CTerms; and (2) \muMatch using QTerms. Three different runtime cases (Best, Average, and Worst cases) have been used to provide further insight into the execution time for generating queries for each dataset. We observe that execution time for CTerms Vs. QTerms on all three cases does not deviate significantly. Therefore an increase in query load is trivial in terms of query generation.

![Figure 1: Query Generation Time](image-url)

Table 3: Number of Queries generated per dataset per experiment

<table>
<thead>
<tr>
<th>Dataset</th>
<th>CTerms</th>
<th>QTerms</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>\muM</td>
<td>\muM</td>
</tr>
<tr>
<td>CHUV</td>
<td>173</td>
<td>174</td>
</tr>
<tr>
<td>CING</td>
<td>1444.2</td>
<td>1432</td>
</tr>
<tr>
<td>ZEINCRO</td>
<td>1528</td>
<td>1444.2</td>
</tr>
</tbody>
</table>

Table 3: Number of Queries generated per dataset per experiment.
3.2 Results

We compare the results of our four experiments based on three metrics:

**Matched Results (MR)**: represents the total number of query results obtained for all terms against all SPARQL endpoints.

**Matched Terms (MT)**: represents the number of distinct terms for which non-empty results were found for at least one SPARQL endpoint.

**Matched Endpoints (ME)**: represents the number of distinct endpoints for which some term generated a non-empty result.

To illustrate these metrics, consider an example where a set of two Terms = {“lung”, “cancer”} is searched (using DM or µM) on SEndpoints = {“GeneBank”, “DrugBank”, “PubMed”}, where the results contained 5 matches of “lung” in “GeneBank”, 0 matches in “DrugBank” and 2 matches in “PubMed”. Similarly, the returned results for “cancer” had 0 matches in “GeneBank”, “DrugBank” and “PubMed”. In this example, MR = 7, MT = 1 and ME = 2.

A detailed comparison of MR, MT and ME for all datasets and experiments is presented in Figures 2–4 respectively. In general, we see a small increase in the number of matches when considering DM versus µM; whether or not the 8× query-load of µM is cost effective depends on the scenario, where the trade-off is the completeness of results versus the efficiency of the discovery process. Conversely, we see a more significant increase for QTerm versus CTerm, which is associated with an increased query load of 1.3–2.5×: the process of removing junk characters, stop words and general terms, and generating a variety of n-grams, leads to a significant increase in matches, particularly for the dataset provided by the second clinical partner (i.e., CING).

Of the 44 endpoints we consider, the querying process generates positive hits for 9–33 endpoints. With a high ratio of potentially relevant endpoints being found, we thus deem it important to rank the relevance of these endpoints, allowing domain experts to consider more highly ranked endpoints as better candidates for the linking process. Thus, in addition to comparing MR, MT and ME, we also investigated two intuitive ranking schemes for endpoint-relevance with respect to each of the three local datasets, as follows. Both ranking schemes are illustrated using the results collected from QTerms–µM experiment.

**In the first step**: we computed a ranking based on the number of distinct terms found per SPARQL endpoint, which we call the “EndPoint Ranking (EPR)”. This metric is a per-endpoint version of MT that indicates how broad the coverage of domain terms is for each endpoint. The top-10 most relevant endpoints according to this metric for each of the three datasets is shown in Figures 5–7 respectively, where the x-axis represents the names of the SPARQL endpoints and the y-axis represents the number of distinct terms with non-empty results. From these figures, it can be seen that the DBpedia endpoint had the broadest coverage of terms. We considered DBpedia for our experiments due to its cross-domain characteristics.

**In the second step**: we computed a ranking based on the number of results found per SPARQL endpoint across all terms, which we call the “Frequency of results per EndPoint Ranking (Fre-EPR)”. This metric is a per-endpoint version of MR that indicates how deep the coverage of specific domain terms is for each endpoint. A top-5 ranked comparison of the total number of matches found in different SPARQL endpoints for each dataset is provided by Table 4. As opposed to the EPR metric, which focuses on how broad the coverage of domain-specific terms, Fre-EPR captures the depth of matches. Whereas DBpedia was most highly ranked for EPR, we find that more specialised endpints are ranked more highly for Fre-EPR: the highest-ranked SPARQL endpoint for both CHUV and CING is “PubMed” and for ZEINCRO is “BIO2RDF Atlas”. More specialised datasets offer more hits for specific terms, suggesting that there are many potential entities that could be

<table>
<thead>
<tr>
<th>Dataset</th>
<th># Terminology Name</th>
<th>Results</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bio2RDF Atlas</td>
<td>12672</td>
<td></td>
</tr>
<tr>
<td>Pubmed</td>
<td>2671</td>
<td></td>
</tr>
<tr>
<td>SGD</td>
<td>11112</td>
<td></td>
</tr>
<tr>
<td>KEGG Pathway</td>
<td>17241</td>
<td></td>
</tr>
<tr>
<td>NCBI-Gene</td>
<td>432</td>
<td></td>
</tr>
<tr>
<td>Toxkb</td>
<td>345</td>
<td></td>
</tr>
</tbody>
</table>

### Table 4: Fre-EPR for all datasets

- **CHUV**
  - 1 Pubmed: 190651
  - 2 UniProt UniRef: 51460
  - 3 Toxkb: 5518
  - 4 CKAN: 5044
  - 5 DBpedia: 885

- **CING**
  - 1 Pubmed: 187153
  - 2 UniProt UniRef: 31938
  - 3 Toxkb: 25614
  - 4 KEGG Pathway: 17241
  - 5 SGD: 11112

- **ZEINCRO**
  - 3 GOA: 736
  - 4 NCBI-Gene: 432
  - 5 Toxkb: 345
In the third step: we additionally look at the ratio of terms for which some results were returned, which we refer to (loosely) as “recall”. Based on a subset of already identified CTerms and/or QTerms on endpoints, we executed our experiments and computed recall using the $\mu$MATCH algorithm.

Table 5 presents the recall results for $\mu$MATCH algorithm. The QTerms recall results for CHUV and CING improved significantly over the CTerms recall results. Furthermore, we also notice a significant recall improvement after adding a language tag in queries. The language tag is applied in two settings: 1) applying a language tag to a complete term and not for individual case variants; and 2) applying a language tag to each individual case variant. Figure 8 highlights the impact of applying a language tag. The results for CHUV and CING in the second scenario are again significantly improved. The terminologies provided by CHUV and CING are self-descriptive whereas the one provided by ZEINCRO is a coded terminology: hence the improved results for CHUV and CING.

### 4. RELATED WORK

With respect to finding relevant datasets on the Web, a variety of keyword-based search engines have been proposed in the literature, including, for example, Sindice [9]. However, such search engines return entities as results and do not directly allow for finding relevant SPARQL endpoints.

To the best of our knowledge, few works have looked at identifying candidate datasets for interlinking. One such example is the work of Leme at al. [3], which identifies datasets for interlinking and ranks them using probability measures based on a set of analysed features. The proposed approach suggests links amongst different data sources using high level information, while schema- or instance-level information is not taken into account.

Nikolov et al. [7, 8] propose an approach to identify relevant datasets for interlinking consisting of two steps: (1) searching relevant entities in other datasets using keywords; and (2) filtering irrelevant datasets based on semantic concept similarities using ontology matching techniques.

We previously mentioned that there are a number of linking frameworks available for Linked Data, including Silk [11] and LIMES [6]. Both of these works provide a declarative language for guiding the creation of links between datasets based on predicates. However, both of these tools presume that a SPARQL endpoint for the target dataset is specified in the input. Our work addresses the prior step of identifying public endpoints of LOD datasets that are interesting to link to.

Maali et al. [4] propose an extension of the Google Refine tool to curate and RDFise local datasets. The extension can help find legacy URIs for entities from target endpoints specified by the user. The authors propose using custom full-text search over SPARQL endpoints to find relevant URIs for keyword terms in the local dataset; e.g., using bif:contains over Virtuoso endpoints. However, they presume that the endpoints of interest are manually specified by the user. As previously argued, we do not rely on the vendor-specific

<table>
<thead>
<tr>
<th>Dataset</th>
<th>CTerms DM</th>
<th>CTerms $\mu$M</th>
<th>QTerms DM</th>
<th>QTerms $\mu$M</th>
</tr>
</thead>
<tbody>
<tr>
<td>CHUV</td>
<td>0.17</td>
<td>0.23</td>
<td>0.64</td>
<td>0.88</td>
</tr>
<tr>
<td>CING</td>
<td>0.04</td>
<td>0.06</td>
<td>0.67</td>
<td>0.90</td>
</tr>
<tr>
<td>ZEINCRO</td>
<td>0.09</td>
<td>0.19</td>
<td>0.35</td>
<td>0.62</td>
</tr>
</tbody>
</table>
full-text search features that are supported only by some SPARQL endpoints.

Other works have discussed the difficulties of discovering relevant SPARQL endpoints on the Web. For example, Buil Aranda et al. note that few structured descriptions are available for endpoints. Paulheim and Hertling also note that the discovery of endpoints is a difficult problem and propose methods to find endpoints given a URI of interest.

To the best of our knowledge, no work has presented methods to discover public SPARQL endpoints that are most relevant to a list of domain-specific keywords (as needed by our three clinical partners).

5. CONCLUSION

In this paper, we propose methods for automatically discovering public SPARQL endpoints that are candidates for linking with a local domain-specific dataset. We are inspired by the needs of three clinical organisations that wish to generate Linked Data but are unsure which datasets are most relevant to link to.

Given a set of domain-specific keywords, we discussed three possible methods by which the relevance of SPARQL endpoints could be determined: we choose to investigate algorithms that seek exact literal matches since the generated queries (1) would involve standard SPARQL features supported by all endpoints, unlike vendor-specific full-text search primitives and (2) would involve efficient lookups, unlike REGEX filters that would need to scan all indexed data.

However, exact literal matches require precise phrase matching and are sensitive to case and the presence/omission of language tags. We thus presented two algorithms to generate a variety of phrases from input keywords and to query for variations of case and language-tag. In experimental results for three real-world clinical terminologies, we showed that these algorithms increase the number of hits generated versus the raw keywords. We also discussed some preliminary ranking methods for the relevance of individual endpoints.

In an extended work, we would like to investigate using the full-text search API of a Linked Data warehouse, such as Sindice, to generate a list of relevant entity URIs, querying the endpoint for the presence of these entities rather than for exact literal matches. We would also like to investigate the effectiveness of our methods for other domains. Finally, we would like to investigate ranking metrics for the relevance of endpoints in more depth, in particular how well they indicate the potential for generating high-quality links.

(Note to reviewer: we plan to submit a demo/poster to ‘Call For Posters’ session of IDEAS’14, therefore, the datasets, the tool and a demo website will be made publicly available.)

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6. REFERENCES