Breakmarking UniProt RDF: SPARQL that make your database cry....

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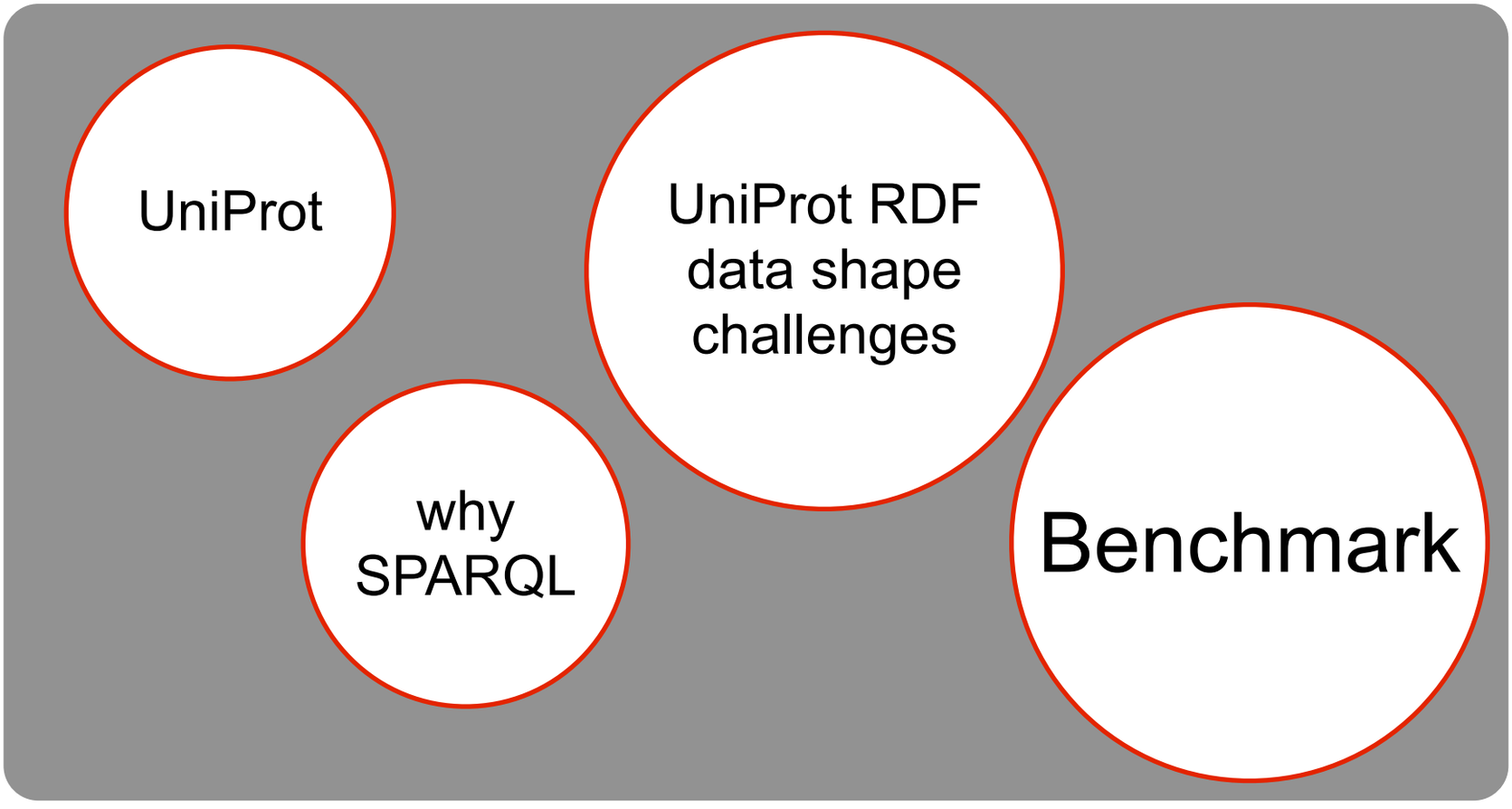
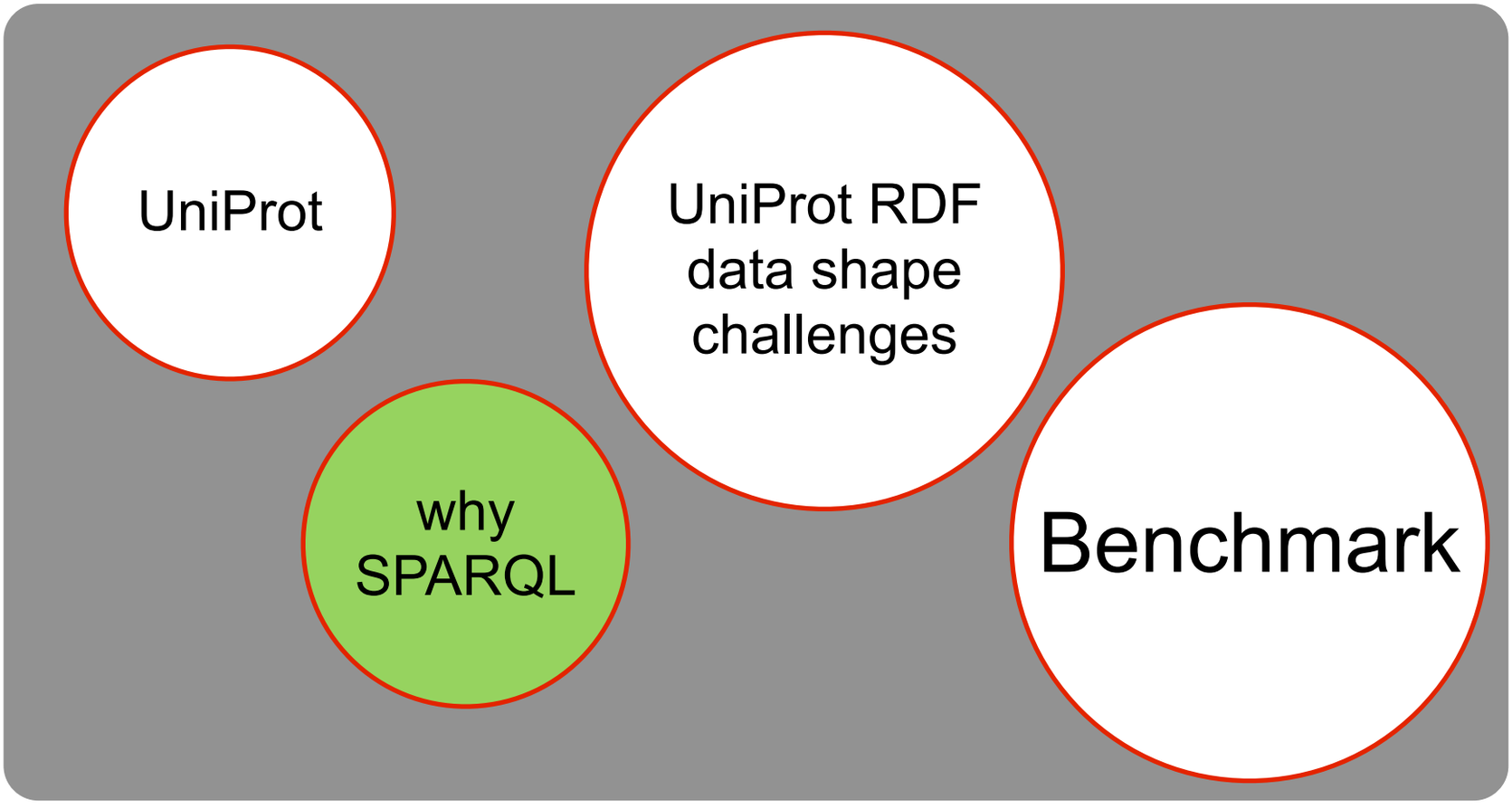
Swiss Institute of Bioinformatics

UniProt.rdf



Talk two things
uniprot.rdf
SPARQL!

UniProt.rdf



Friday 4 April 14

Talk two things
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Quality!

UniProt

SIB Swiss Institute of Bioinformatics

Friday 4 April 14

SPARQL does not make a biologist happy
It makes you happier so you can make the biologist happy

SPARQL or CLAY

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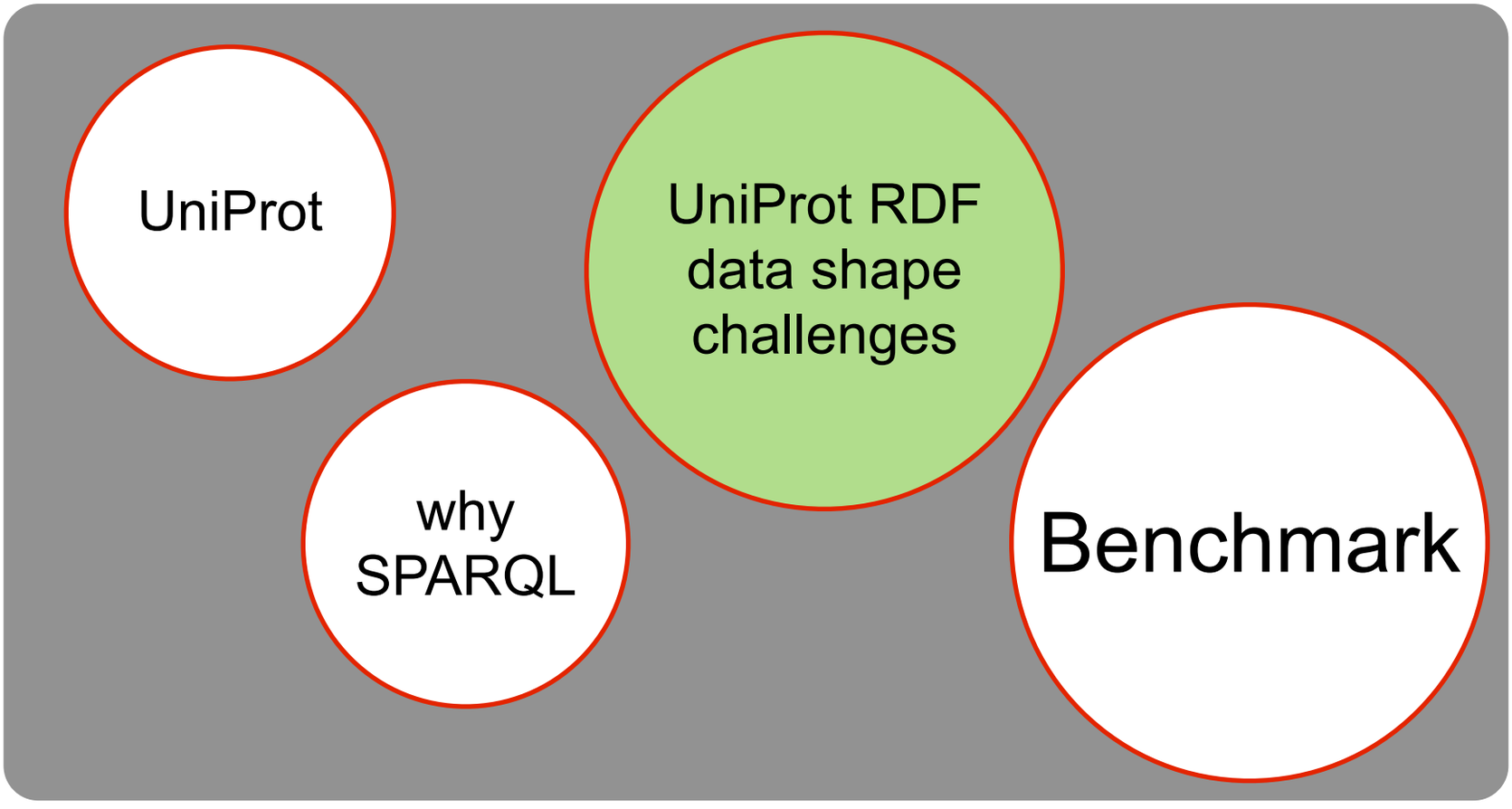
- Everything possible with SPARQL is possible with Clay tablets
- Information stays information
- Only difference is number of slaves, um I mean PhD students you need
- Clay is more expensive than FLASH ;)
- Excellent retention times :D

SPARQL against

- RDBMS
  - R2RML -> D2RQ, Ultrawrap, XSPARQL...
- Programs
  - SADI...
- Triplestore
  - Mark logic, Jena, Virtuoso, OWLIM, uRiKA, Oracle spatial, Oracle NoSQL, IBM DB2, etc...
- Biological flat file formats
  - sparql-bed
- CSV/TSV/Spreadsheats
  - Tarql, Sparqlify

No matter what query language you currently use:
Translating from SPARQL is possible
Data storage is decoupled from querying
Only speed for some query types is affected

UniProt.rdf



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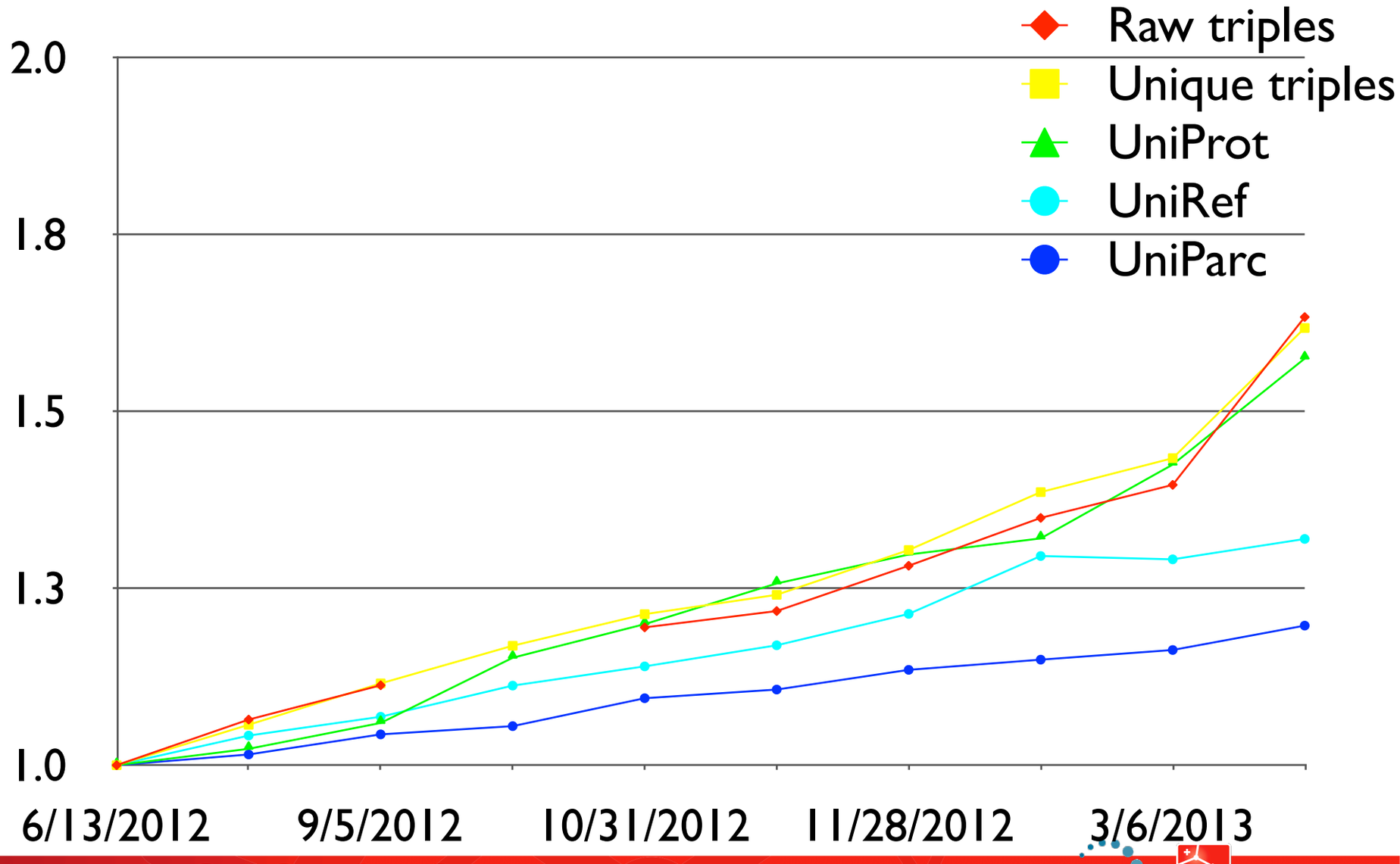
Growing & Living knowledgebase

- Dataset grew from
  - 80 million in 2006
  - 12 billion 2014
  - more every **4 weeks** regular release

- Data model changes over time
  - owl:sameAs -> skos:exactMatch
  - FALDO for positions
  - more structure
  - sha checksums
  - uniparc (drop reification 2014_05)

63% more triples in a year



In 364 days! Doubling time 15 months instead of 18 months!
Information growth is faster than entry growth!
250% in 18 months instead of 200%

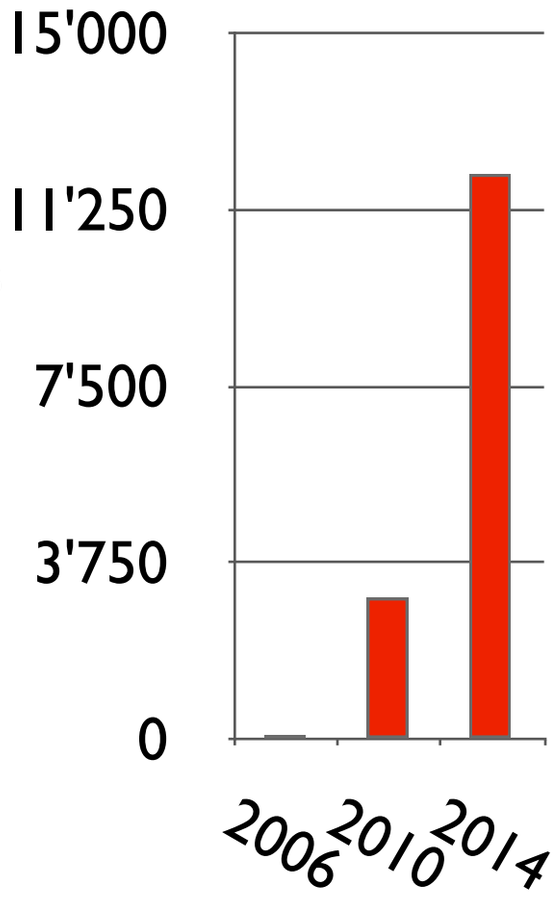
RDF normalization

- Entry based view is 40% repetitive data
  - 1 annotation in 12 entries (average)
  - high throughput papers
  - species names etc...

- Significantly changes number of triples

UniProt.rdf: An **improving** experience

- 2006 powerful server of the day
  - 80 **million** triples take a week to load in a triple store
  - **SERQL** queries **may** return results
- 2014 powerful server of the day
  - 12 **billion** triples take a week to load in a triple store (32 hours for key-value store)
  - **SPARQL** queries **do** return results



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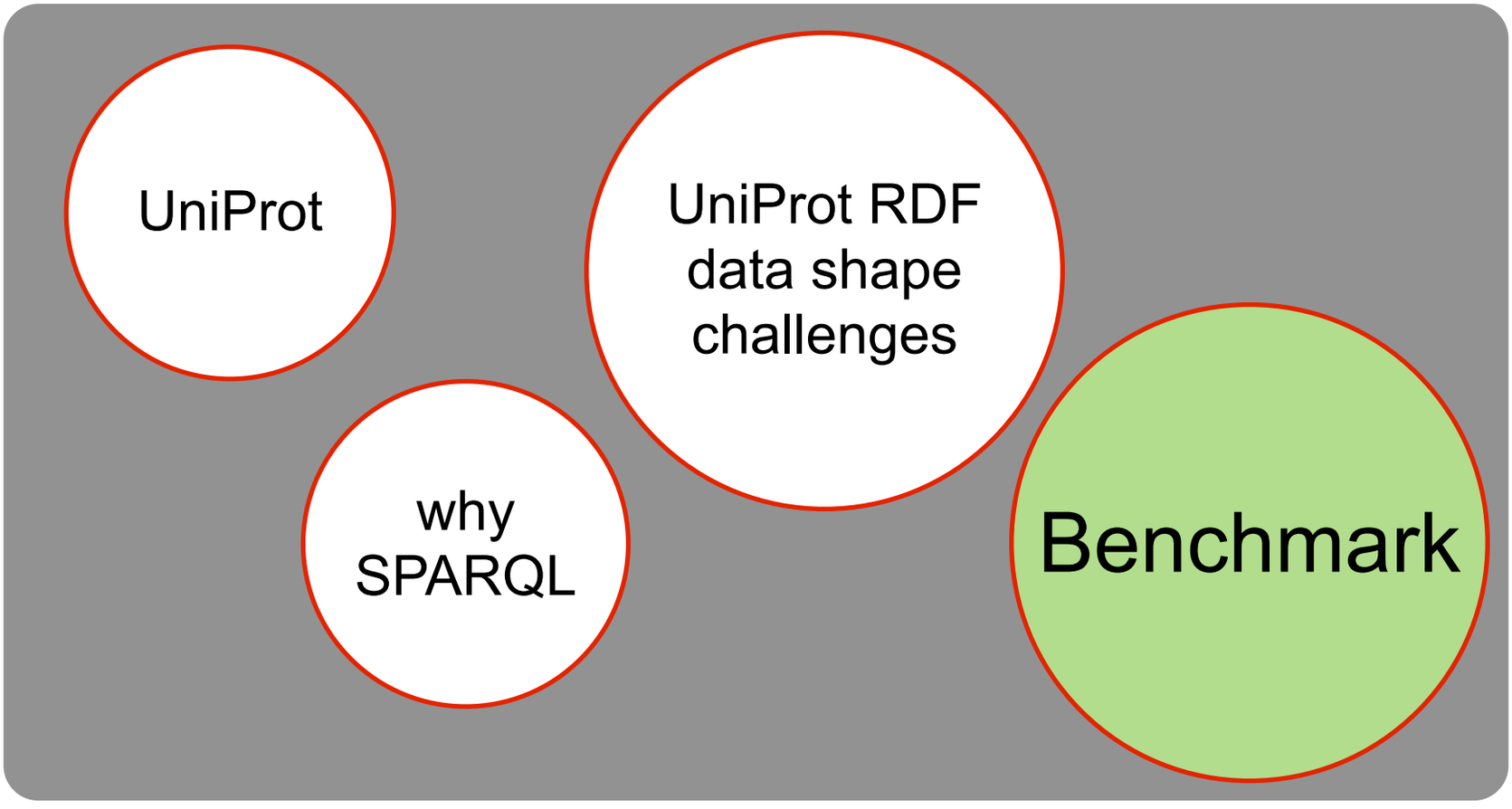

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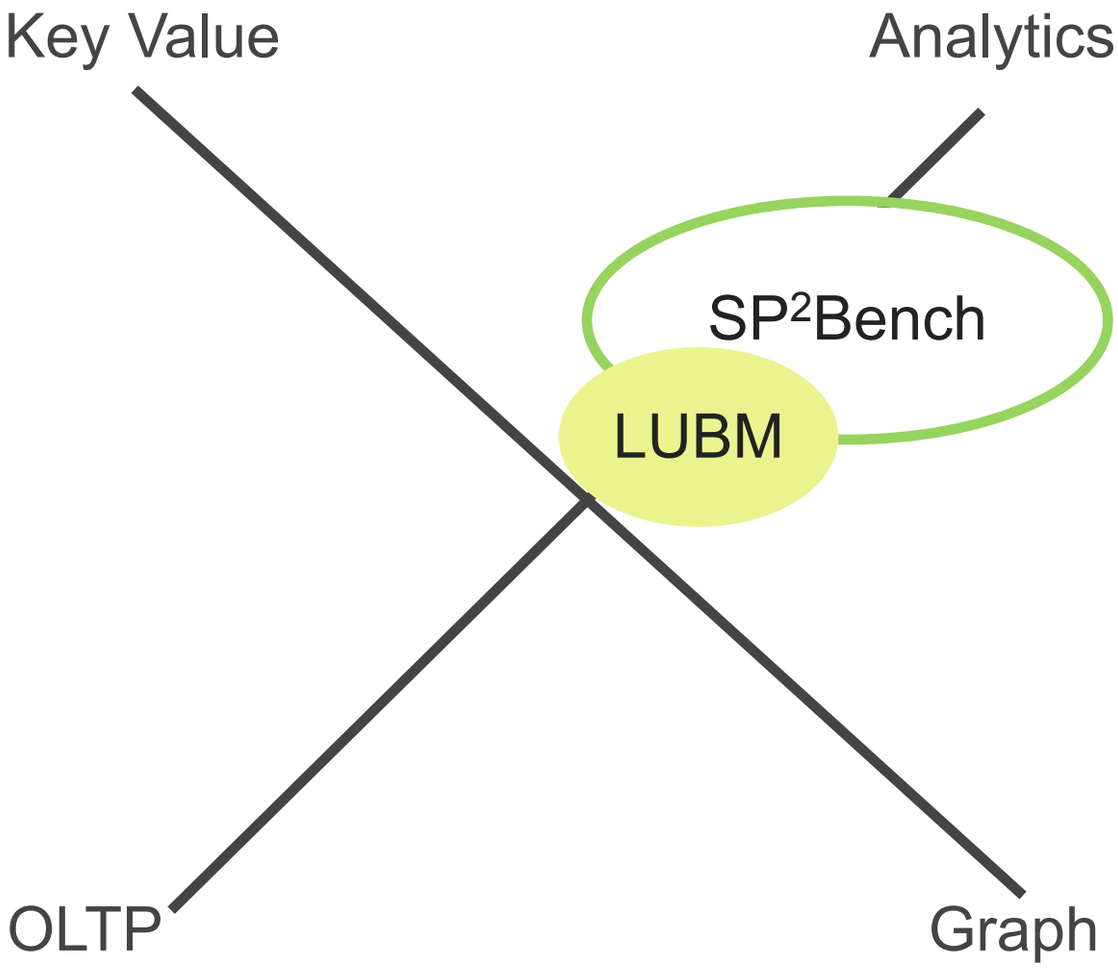
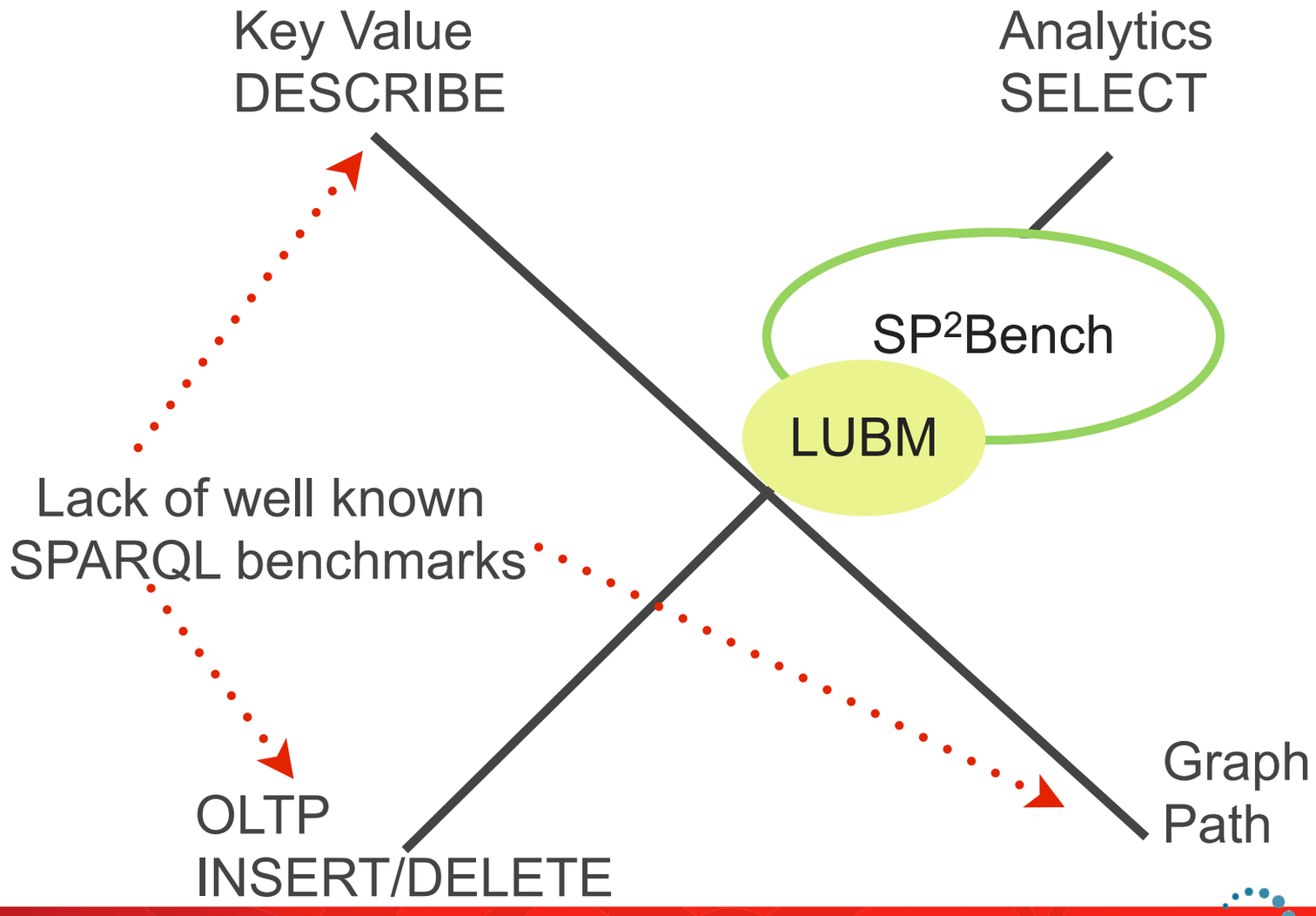
Stats

	UniProt	LUBM	SP2Bench
Graphs	16	1	1
types	164	19	13
object properties	58	25	20...
datatype properties	81	7	

Benchmarks should help us make choices



Benchmarks should help us make choices




```
CONSTRUCT
{    ?subject ?predicate ?object .}
WHERE {
        GRAPH<http://purl.uniprot.org/uniprot/P05067>{
                ?subject ?predicate ?object .
        }
}
```

Our benchmark

- Rule base classification turned into SPARQL
  - 1250 queries (now 1600)
  - 54 BGP avg per query (construct)
    - 175 max
    - 20 min
  - 50% have negation

- Run on10 billion + triples

Halve that for select.

Equivalent variants of queries

- MINUS or NOT EXISTS
  - May be different semantics, made sure queries match
- UNION or VALUES

- Different engines have different optimizations
  - Try to find the form they have optimized

Example

```
SELECT (COUNT(DISTINCT ?this) AS ?countTotal)
WHERE {
      ?this a up:Protein .
      ?this up:reviewed false .
      ?this rdfs:seeAlso panther:PTHR11361 .
            {?this rdfs:seeAlso smart:SM00533> .}
      UNION {?this rdfs:seeAlso pfam:PF05192> .}
      FILTER (
            NOT EXISTS
                  {       {?this rdfs:seeAlso interpro:IPR006153 .}
                  UNION {?this rdfs:seeAlso interpro:IPR000626 .}
                  UNION {?this rdfs:seeAlso interpro:IPR005061 .}
                  UNION {?this rdfs:seeAlso interpro:IPR007720 .}
                  UNION {?this rdfs:seeAlso interpro:IPR003583 .}
                  UNION {?this rdfs:seeAlso interpro:IPR004771 .}
                  UNION {?this rdfs:seeAlso interpro:IPR016040 .}
                  UNION {?this rdfs:seeAlso interpro:IPR003148 .}
                  UNION {?this rdfs:seeAlso interpro:IPR006055 .}
                  UNION {?this rdfs:seeAlso interpro:IPR000727 .}
                  UNION {?this rdfs:seeAlso interpro:IPR013520 .}
                  UNION {?this rdfs:seeAlso interpro:IPR000160 .}
                  UNION {?this rdfs:seeAlso interpro:IPR000873 .}}
      )
      ?this up:organism ?taxon .
            {?taxon rdfs:subClassOf* taxonomy:2157. }
      UNION {?taxon rdfs:subClassOf* taxonomy:2759. }
      UNION {?taxon rdfs:subClassOf* taxonomy:2 . }}
```


Example

```
SELECT (COUNT(DISTINCT ?this) AS ?countTotal)
WHERE {
      ?this a up:Protein .
      ?this up:reviewed false .
      ?this rdfs:seeAlso panther:PTHR11361 .
      VALUES (?theseLinks) {(smart:SM00533) (pfam:PF05192) }
      ?this rdfs:seeAlso ?theseLinks .
      VALUES (?notTheseLinks) { (interpro:IPR006153)
                                (interpro:IPR000626)
                                (interpro:IPR005061)
                                (interpro:IPR007720)
                                (interpro:IPR003583)
                                (interpro:IPR004771)
                                (interpro:IPR016040)
                                (interpro:IPR003148)
                                (interpro:IPR006055)
                                (interpro:IPR000727)
                                (interpro:IPR013520)
                                (interpro:IPR000160)
                                (interpro:IPR000873)}
      MINUS { ?this rdfs:seeAlso ?notTheseLinks . }
      VALUES (?supertaxon) {(taxonomy:2157)
                            (taxonomy:2759)
                            (taxonomy:2) }
      ?this up:organism/rdfs:subClassOf* ?supertaxon .  }
```

Example

```
SELECT (COUNT(DISTINCT ?this) AS ?countTotal)
WHERE {
      ?this a up:Protein .
      ?this up:reviewed false .
      ?this rdfs:seeAlso panther:PTHR11361 .
      VALUES (?theseLinks) {(smart:SM00533) (pfam:PF05192) }
      ?this rdfs:seeAlso ?theseLinks .
      VALUES (?notTheseLinks) { (interpro:IPR006153)
                                (interpro:IPR000626)
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                                (interpro:IPR000160)
                                (interpro:IPR000873)}
      MINUS { ?this rdfs:seeAlso ?notTheseLinks . }
      VALUES (?supertaxon) {(taxonomy:2157)
                            (taxonomy:2759)
                            (taxonomy:2) }
      ?this up:organism/rdfs:subClassOf* ?supertaxon .  }
```

2 billion

56 million

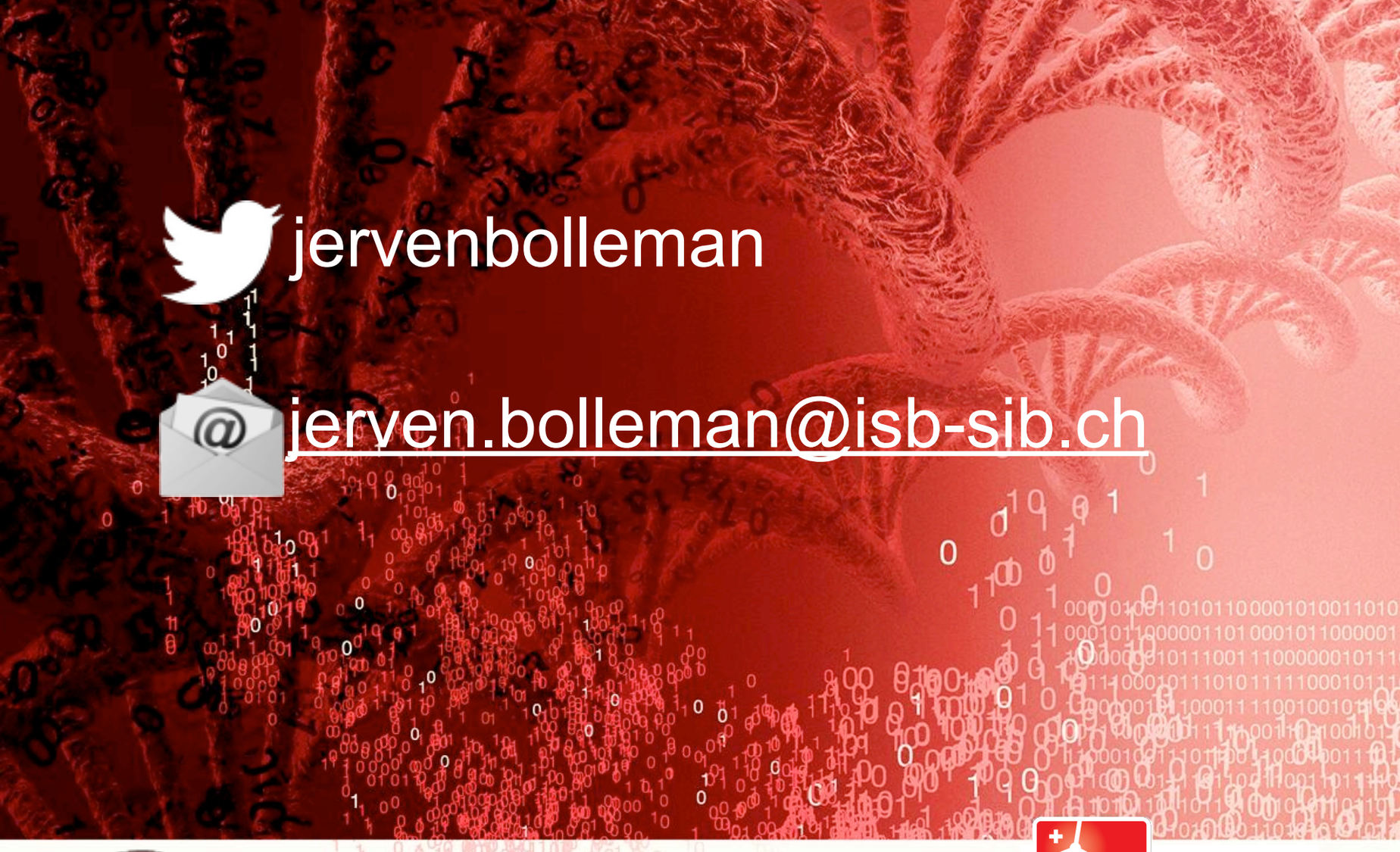
1 million taxnodes

Hardware/Software qualitative

- Owlim 5.2 (5.4 is faster)
  - Completes the test
  - 256GB ram/200GB java heap
  - 2 slow disks (5.4 gets SSDs)
  - 64 core AMD
- uRiKa
  - Matthorn at CSCS 2TB Ram
- Oracle almost 12c
  - 1/4 exadata

Future systems to test

- Virtuoso 7.1
  - Promising candidate
  - Not reviewed yet
- BigData
  - 1.0 never finished loading
  - Retest after 2 years
    - Looking into the cluster



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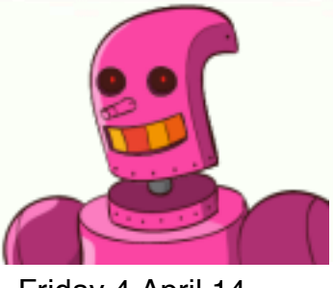

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answers semanticweb.com

```
PREFIX rdfs:<http://www.w3.org/2000/01/rdf-schema#>
PREFIX up:<http://purl.uniprot.org/core/>
PREFIX ko:<http://purl.uniprot.org/ko/>
SELECT ?protein ?taxon ?cluster ?pathway
WHERE
{
?protein up:organism ?taxon ;
         rdfs:seeAlso ko:K00399 ;
         up:annotation ?annotation ;
         ^(up:member/up:sequenceFor) ?cluster .
?annotation a up:Pathway_Annotation ;
  rdfs:seeAlso  ?pathway .
}
```