ETH zürich

Institute of Molecular Systems Biology

Where is the “*L*” in “ORD”?

Open Research Data – are we on track?
Hotel Kreuz, Zeughausgasse 41, Bern

Adriano Rutz, 2024-05-31

D BIOL

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Disclaimer

The “*L*” stands for *linked*,
as in “Linked Open (Research) Data”

What is Linked Open Data (LOD)?

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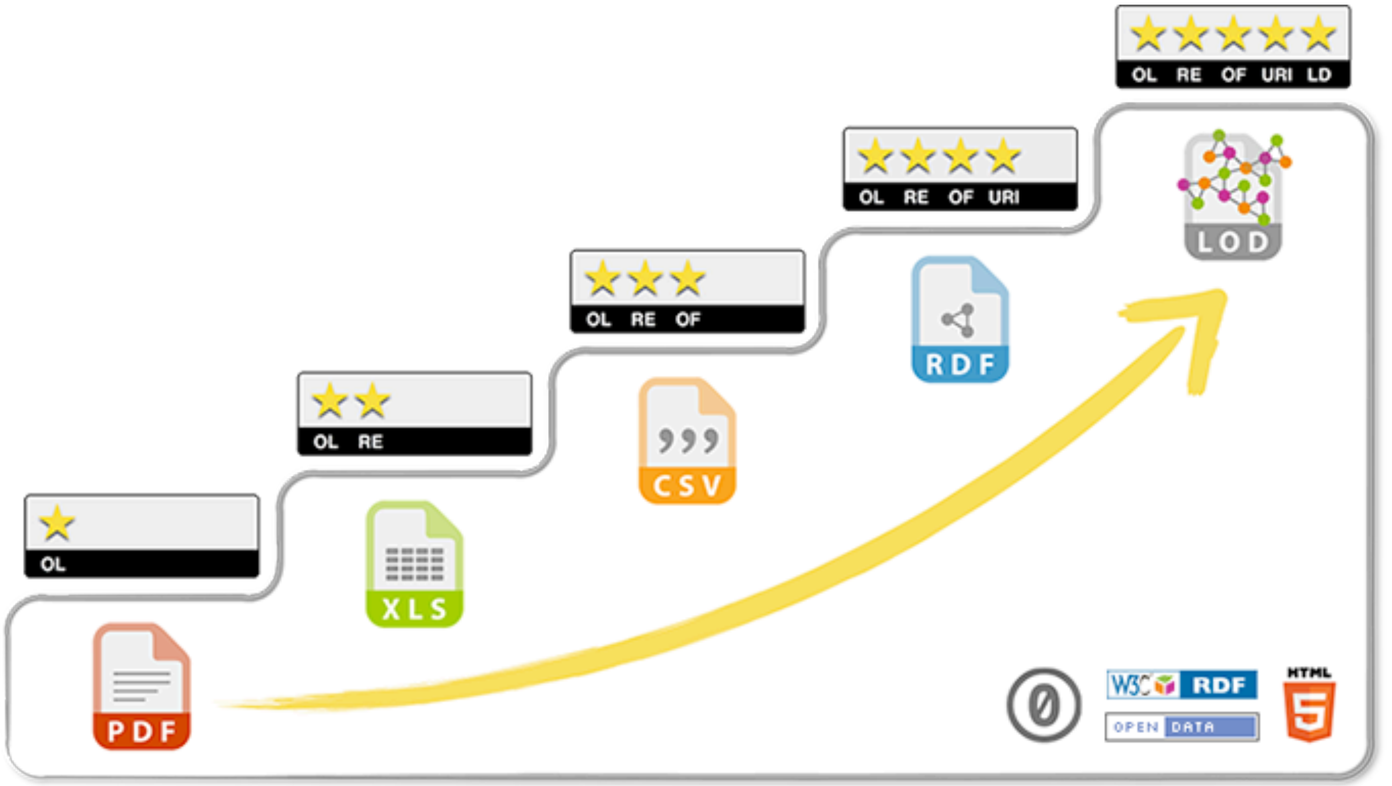

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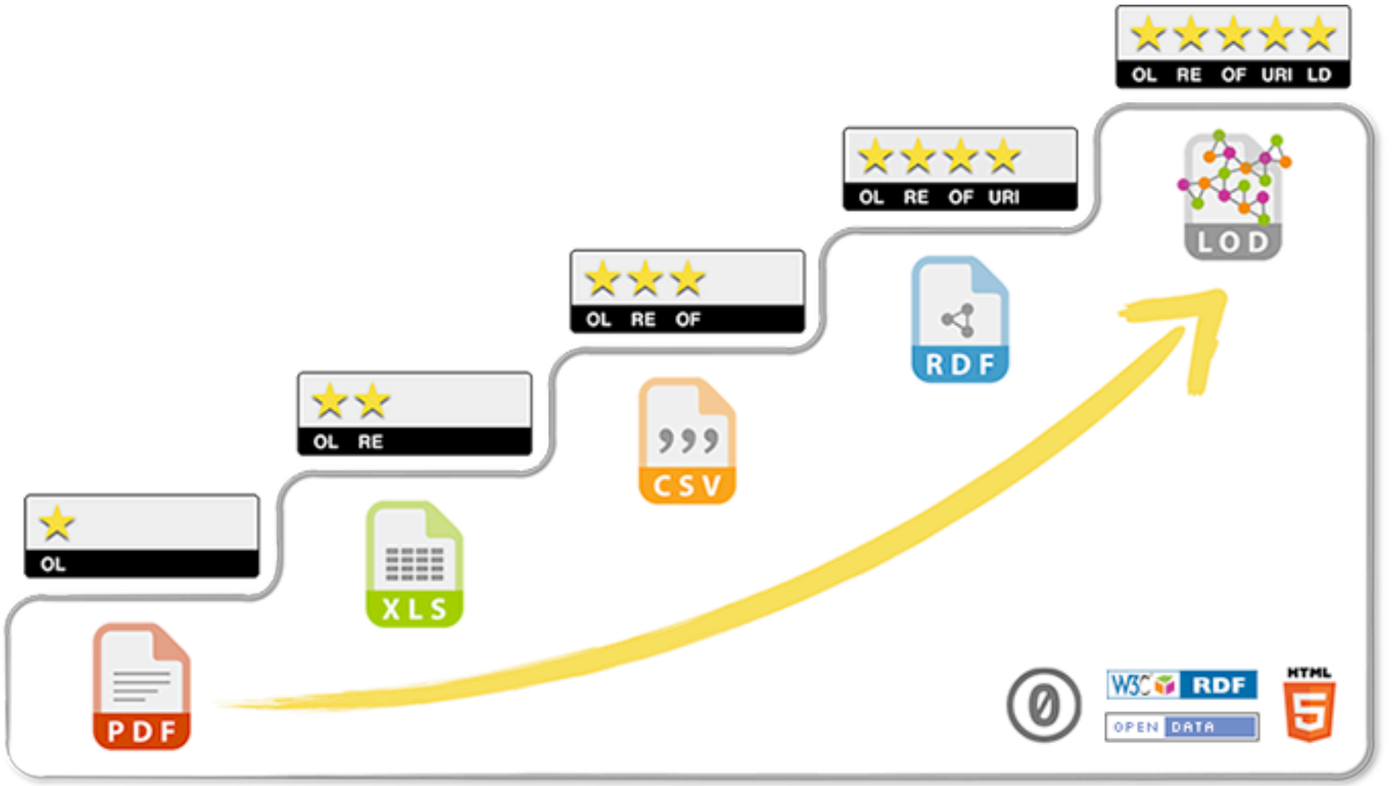
https://5stardata.info

What is Linked Open Data (LOD)?

make your *content* available on the Web (whatever format) under an open license



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What is Linked Open Data (LOD)?

make it available as structured data (e.g., Excel instead of image scan of a table)

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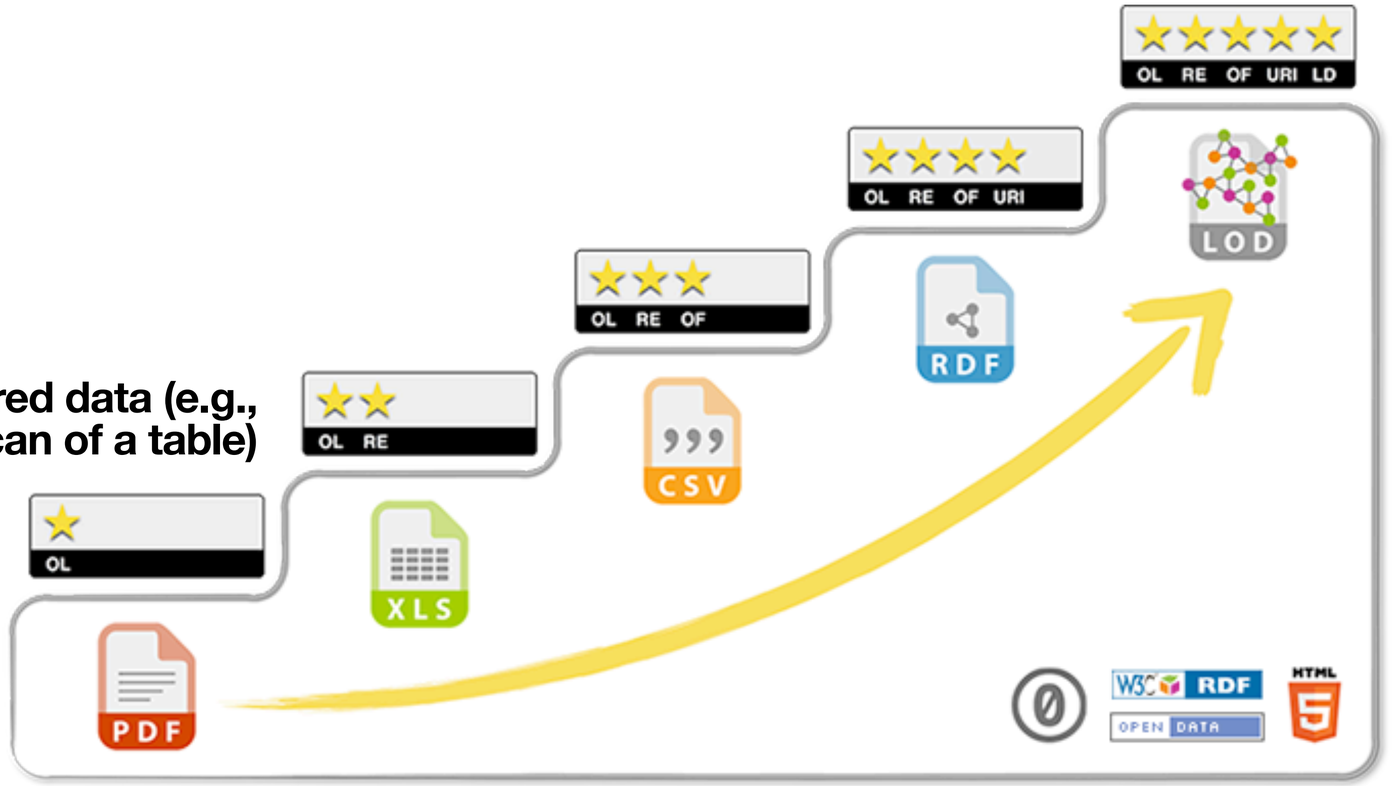

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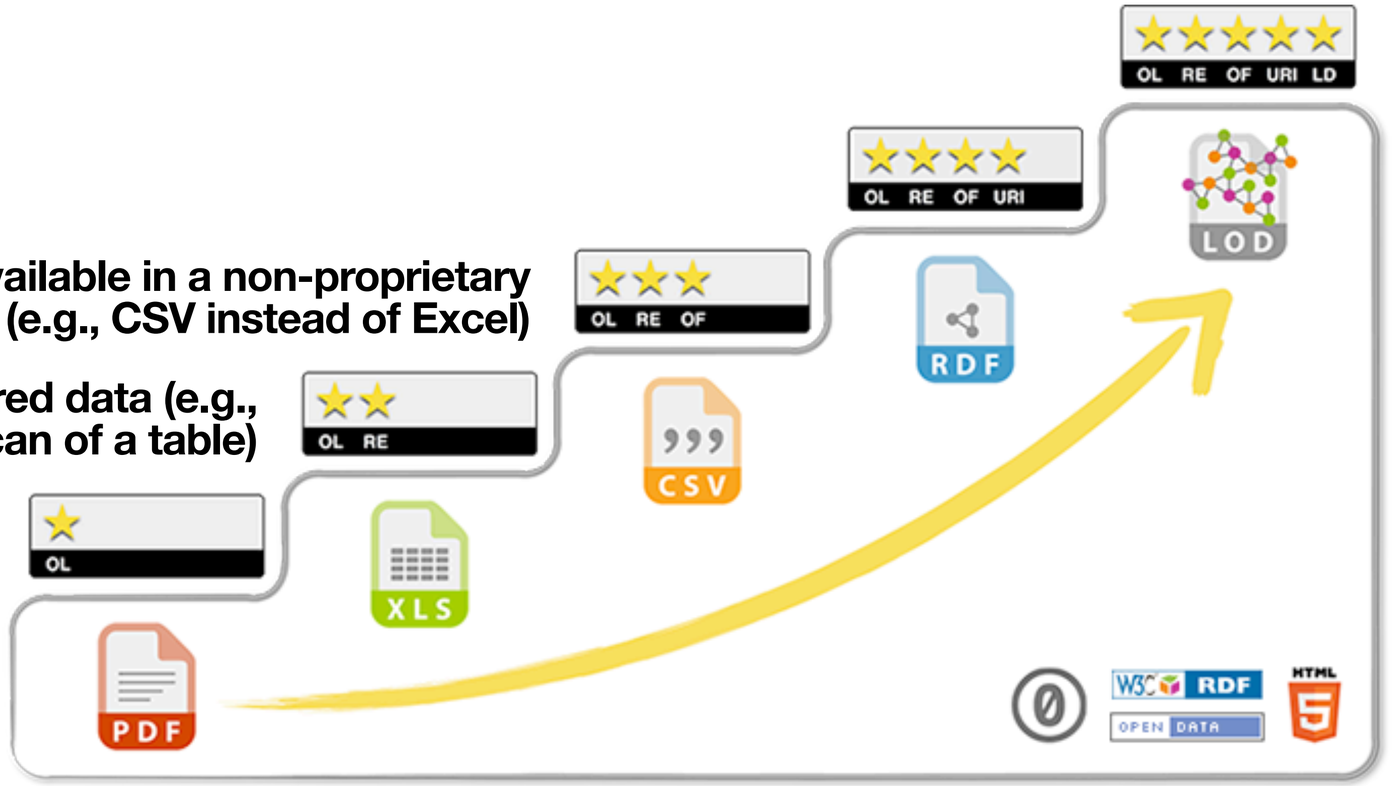
What is Linked Open Data (LOD)?

make it available in a non-proprietary open format (e.g., CSV instead of Excel)

make it available as structured data (e.g., Excel instead of image scan of a table)

make your *content* available on the Web (whatever format) under an open license



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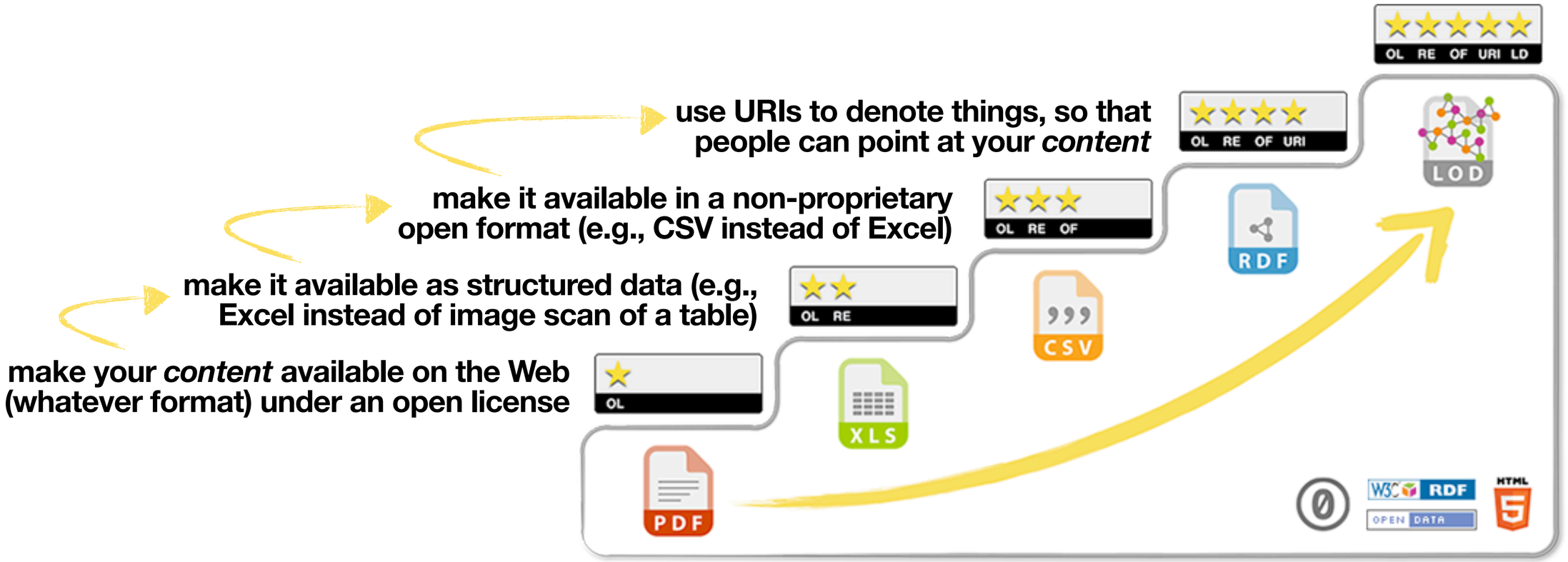

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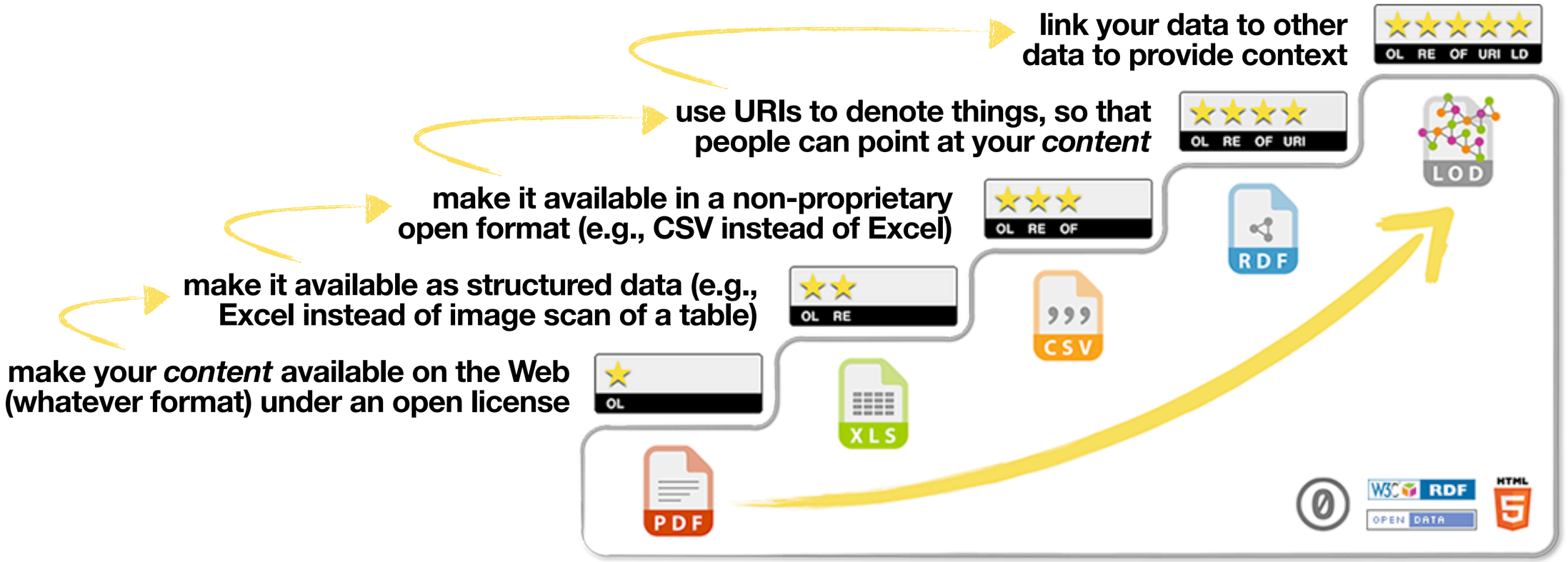

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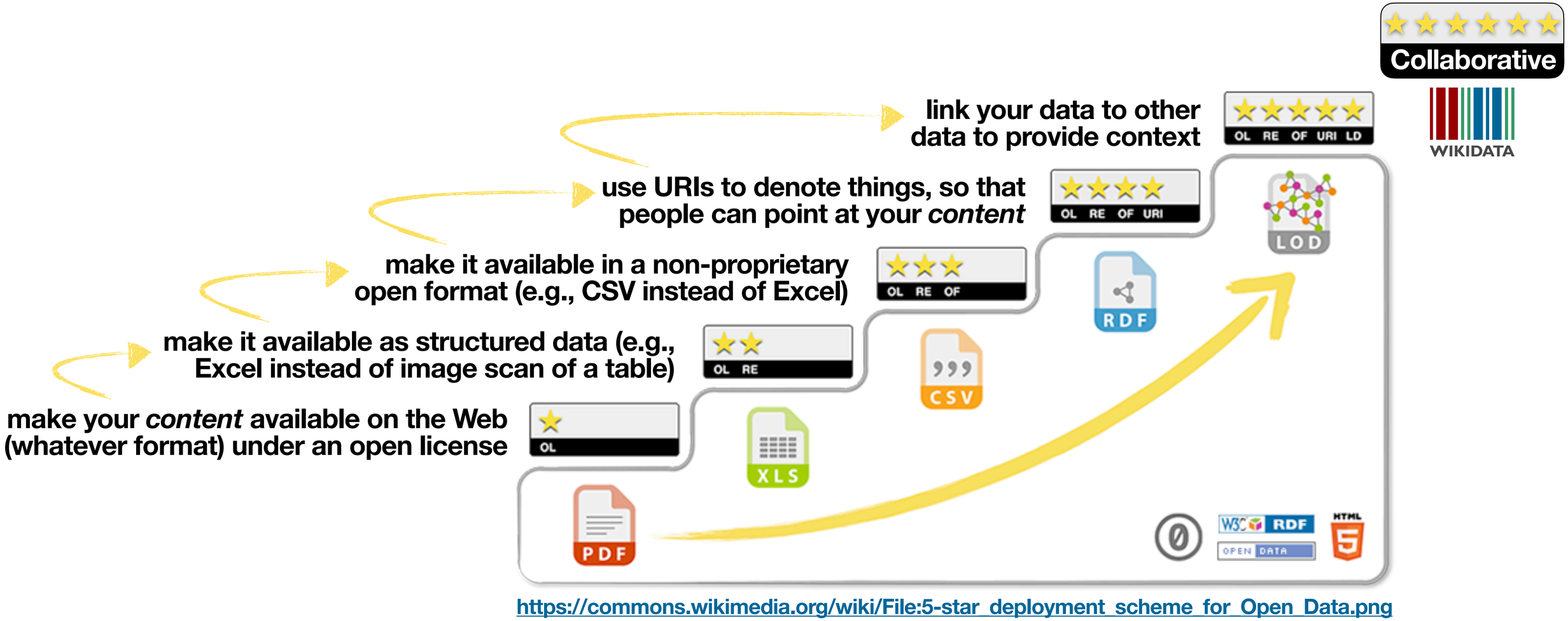

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The “L”OTUS initiative

Available Natural Product Data

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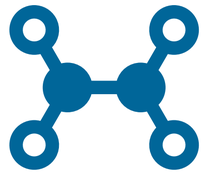
Available Natural Product Data

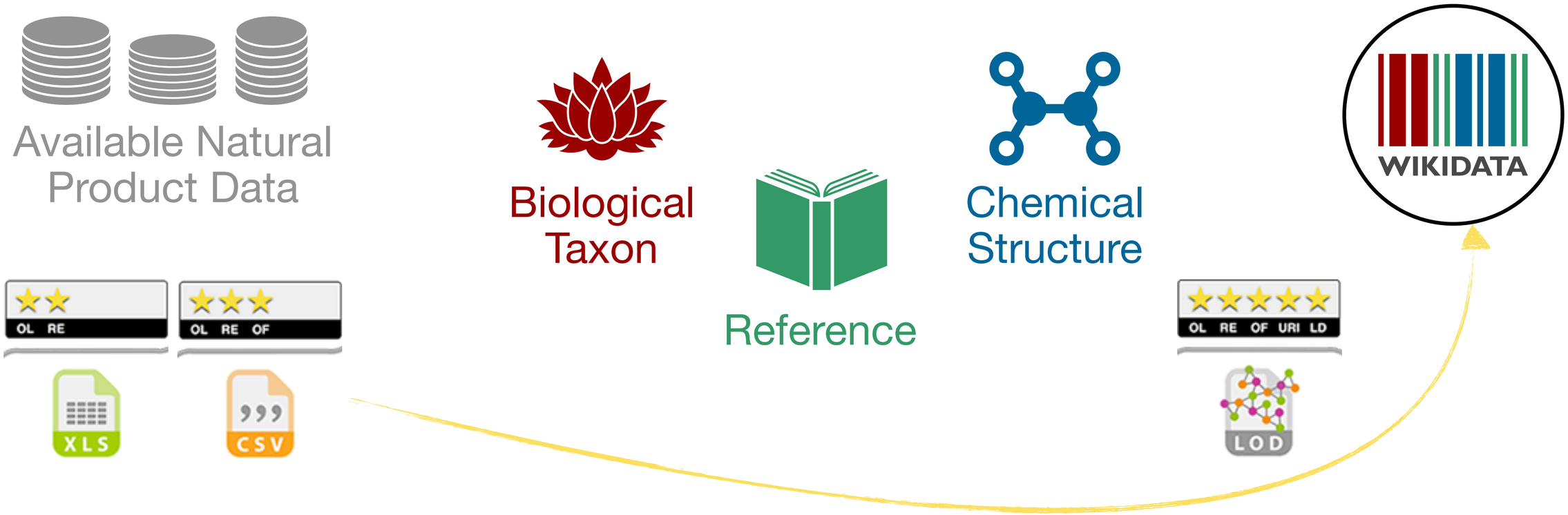
Biological Taxon

Reference



Chemical Structure

The “L”OTUS initiative



The “L”OTUS initiative - Wikidata

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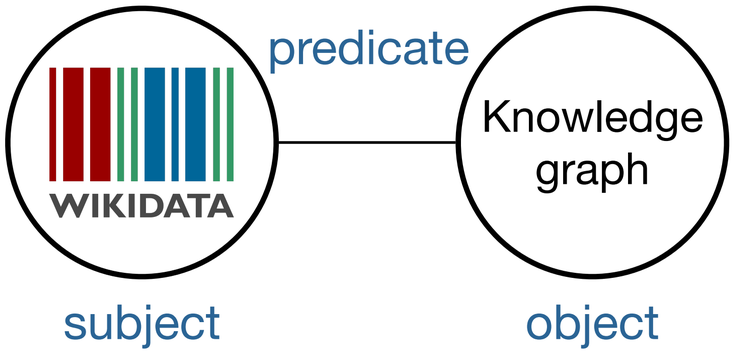
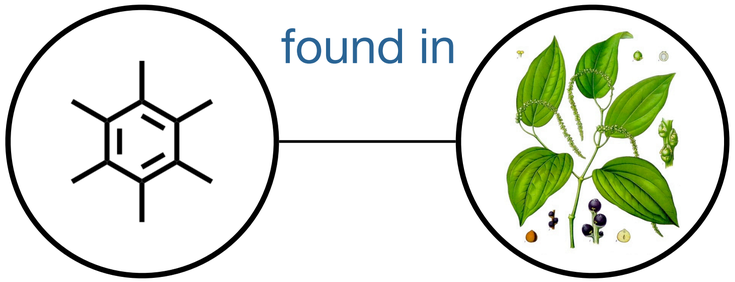


The “L”OTUS initiative - Wikidata

The initiative - SPARQ“L”

« Hey Wiki, what are the compounds found in Piper nigrum L.*? »*



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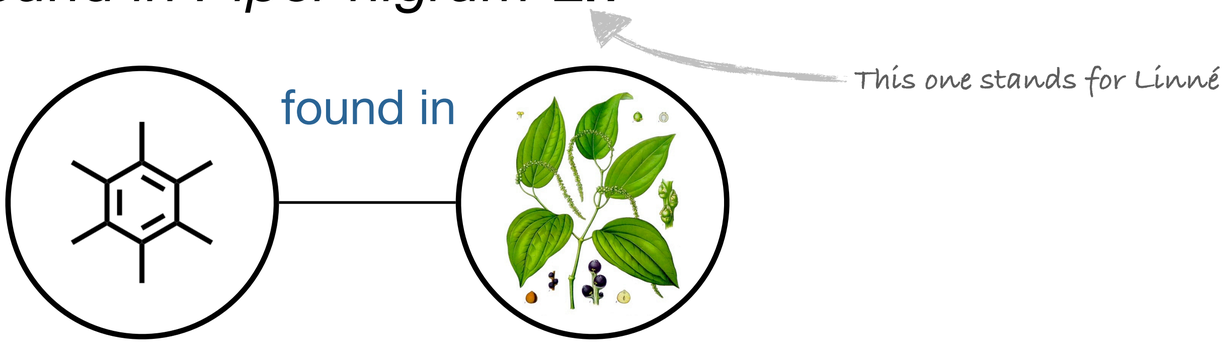

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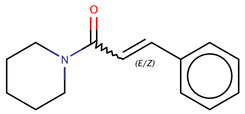
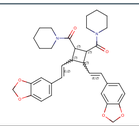
« Hey Wiki, what are the compounds found in Piper nigrum L.*? »*

```
SELECT DISTINCT
?structure ?structure_smiles ?structure_inchikey
WHERE {
    VALUES ?organism {
        wd:Q43084 # Piper nigrum
        }
        ?organism_child (wdt:P171*) ?organism.
        ?structure wdt:P233 ?structure_smiles;
            wdt:P235 ?structure_inchikey;
            (p:P703/ps:P703) ?organism_child.
}
```

row	structure	structure_smiles	structure_inchikey
1	wd:Q105143500		KNOXUMZPTHELAO-UHFFFAOYSA-N
…	…	…	…
419	wd:Q105224845		QOESZPJYTVEXNN-UHFFFAOYSA-N

419 results in 0.5 second

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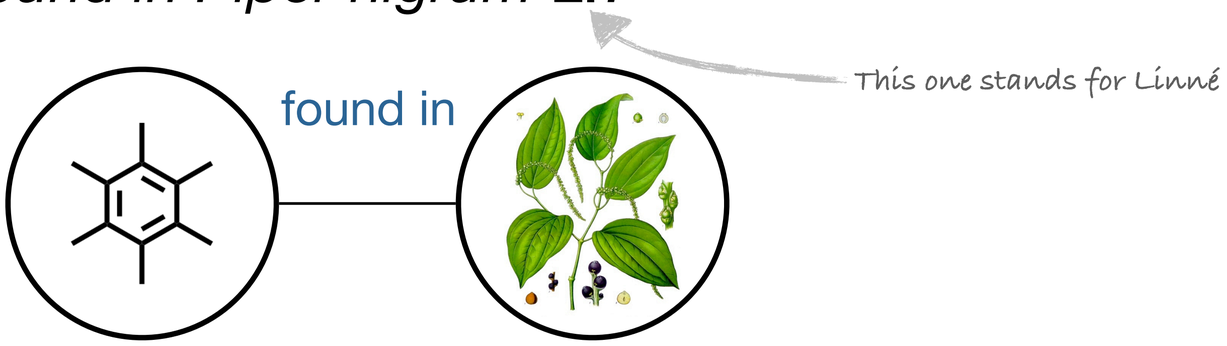

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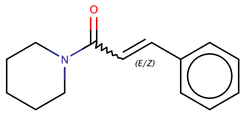
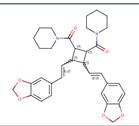
SELECT DISTINCT
?structure ?structure_smiles ?structure_inchikey
WHERE {
    VALUES ?organism {
        wd:Q43084 # Piper nigrum
        }
        ?organism_child (wdt:P171*) ?organism.
        ?structure wdt:P233 ?structure_smiles;
            wdt:P235 ?structure_inchikey;
            (p:P703/ps:P703) ?organism_child.
}
```

row	structure	structure_smiles	structure_inchikey
1	wd:Q105143500		KNOXUMZPTHELAO-UHFFFAOYSA-N
…	…	…	…
419	wd:Q105224845		QOESZPJYTVEXNN-UHFFFAOYSA-N

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« Hey Wiki, what are the compounds found in Gentianaceae? »

984 results in 0.9 second

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« Hey Wiki, how many articles does that correspond to? »

396 results in 0.6 second

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« And how many of them are open access? »

67 results in 0.6 second

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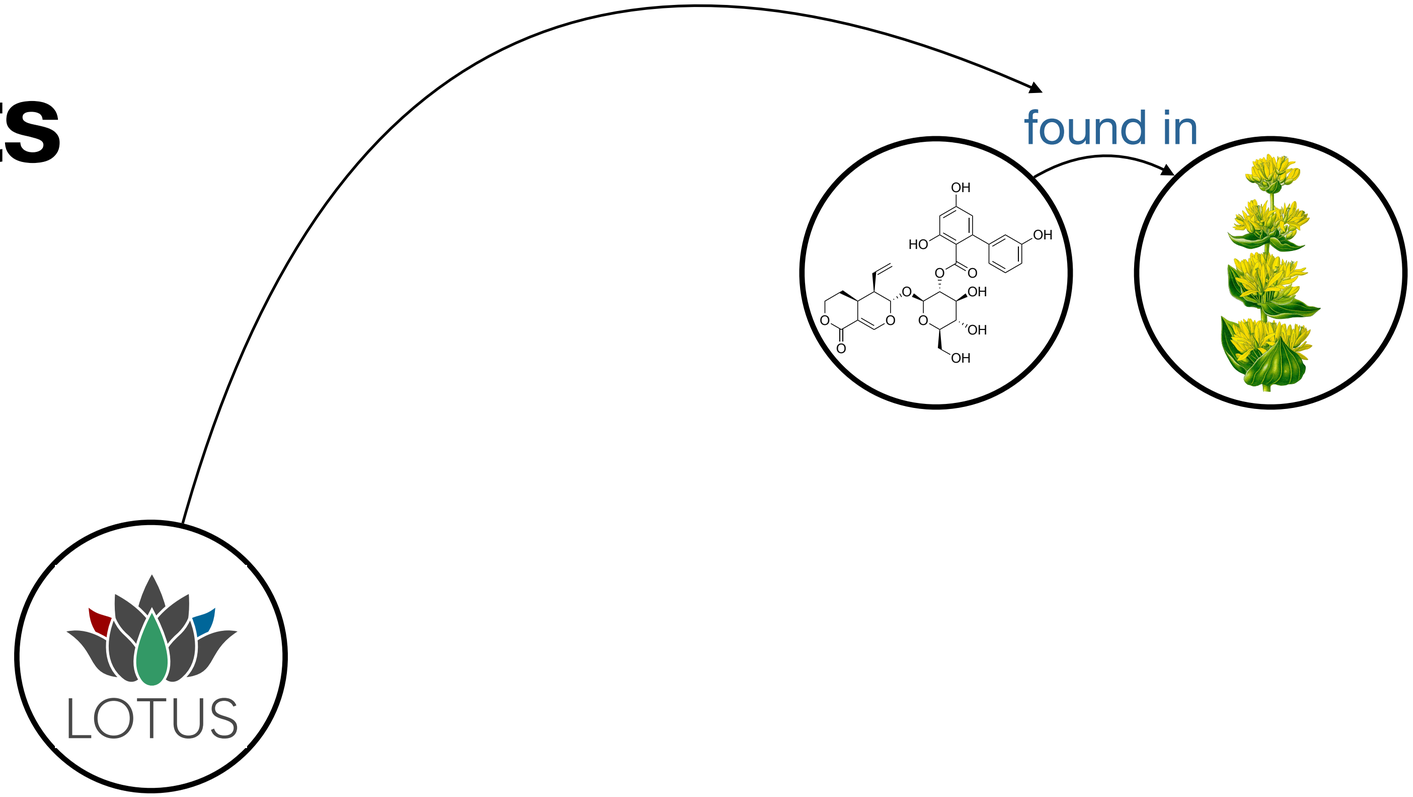
LO(R)D has no limits



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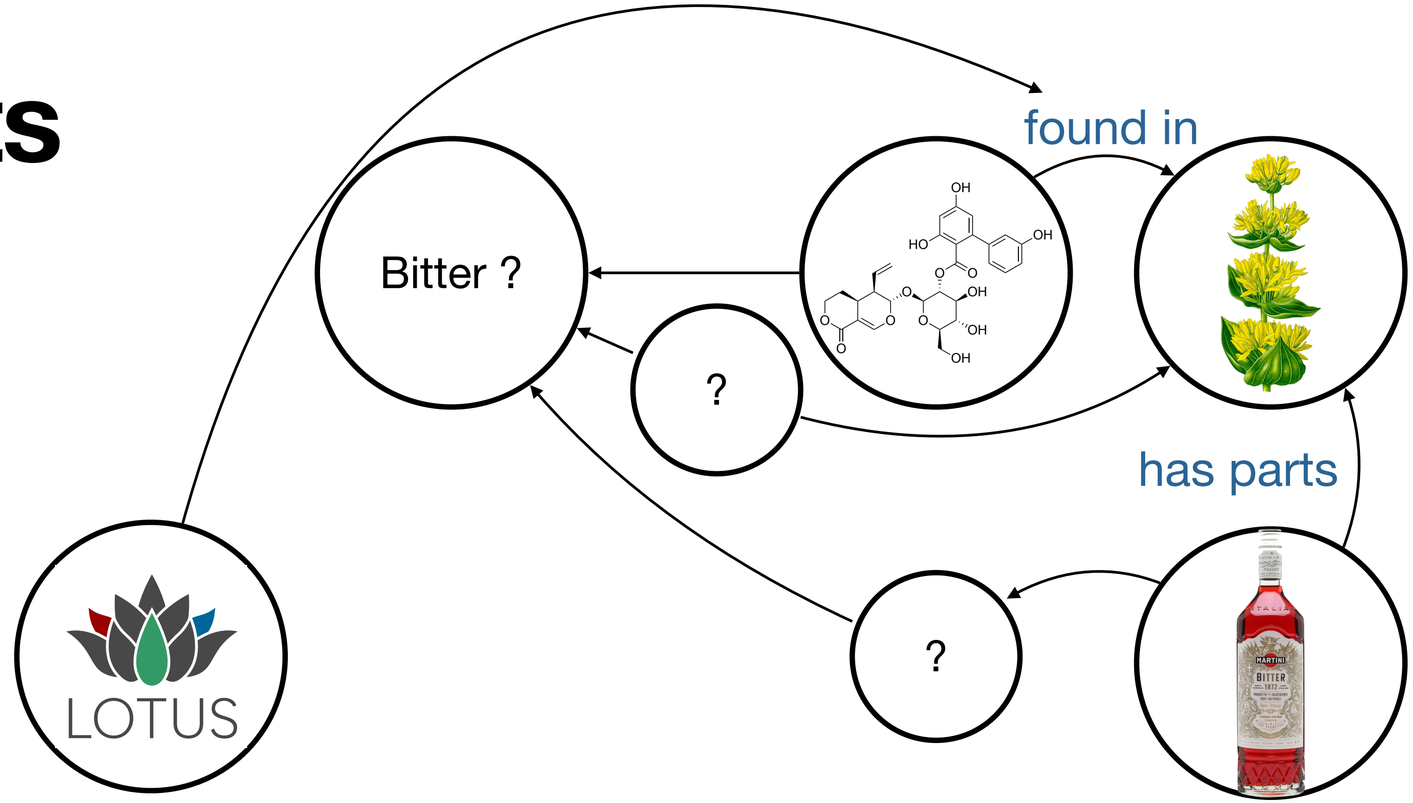

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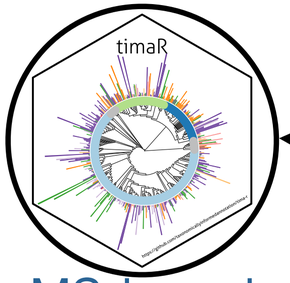
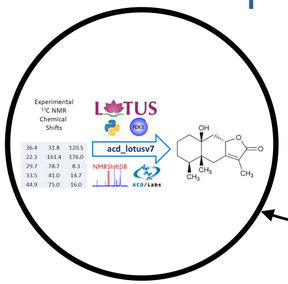


MS-based dereplication



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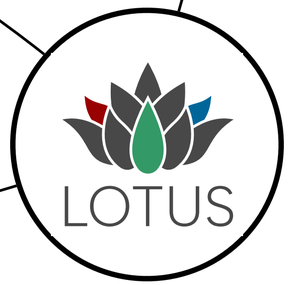

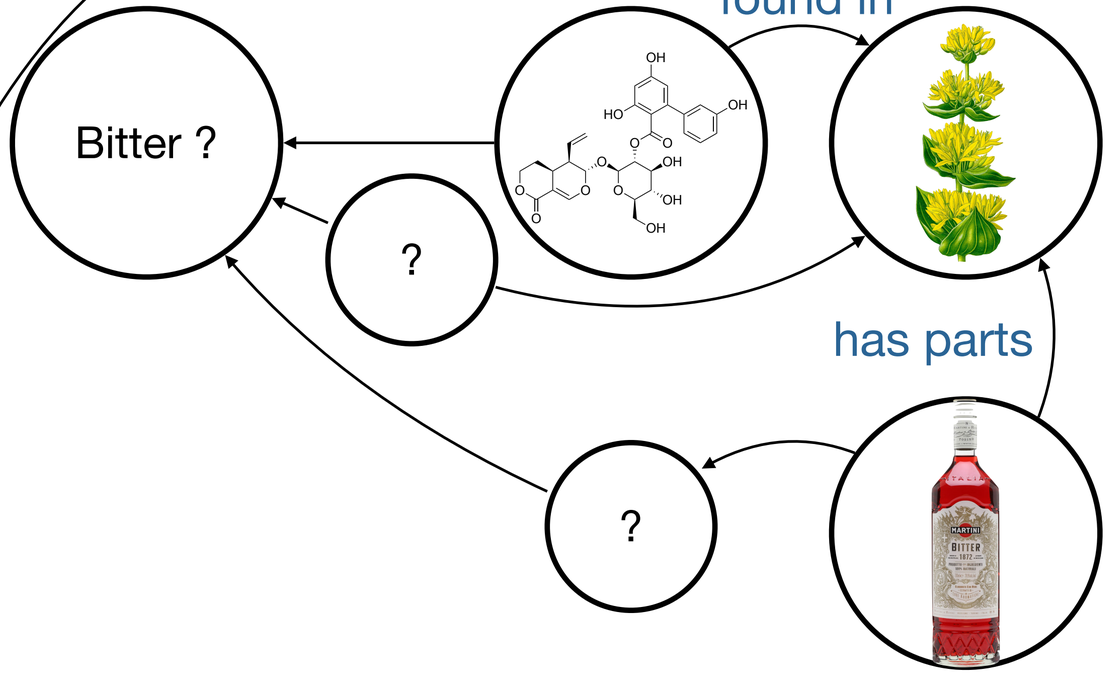

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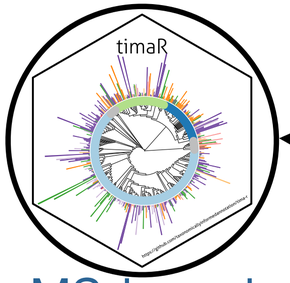

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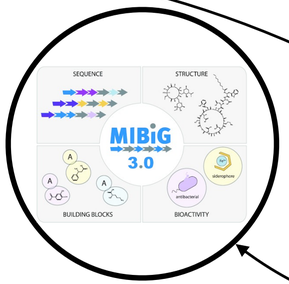
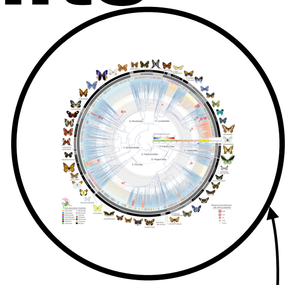
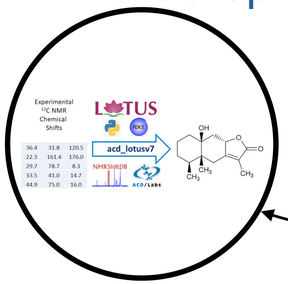


Biosynthetic Gene Clusters



Butterflies



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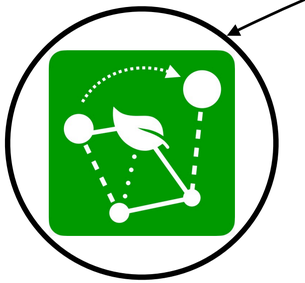

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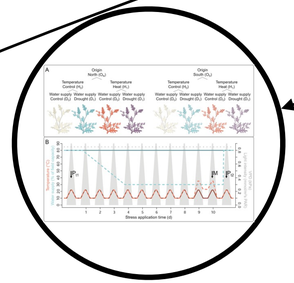

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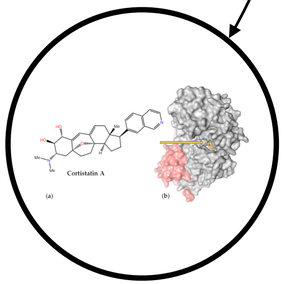
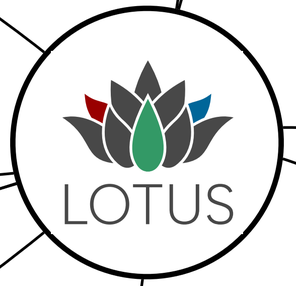
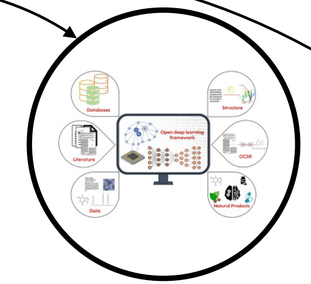
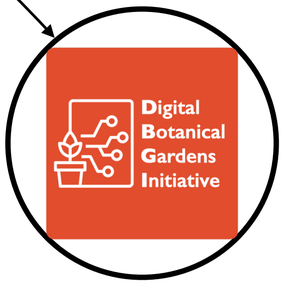


Enzyme inhibition with marine NPs





Natural Products & Machine Learning



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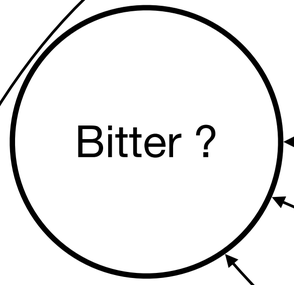

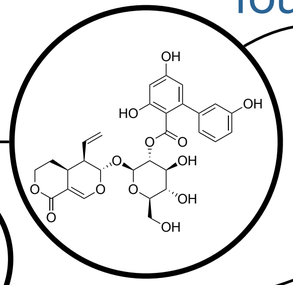

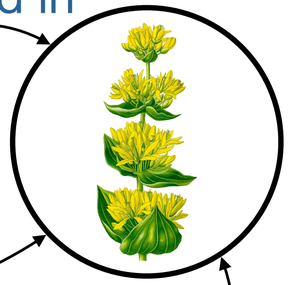

has parts

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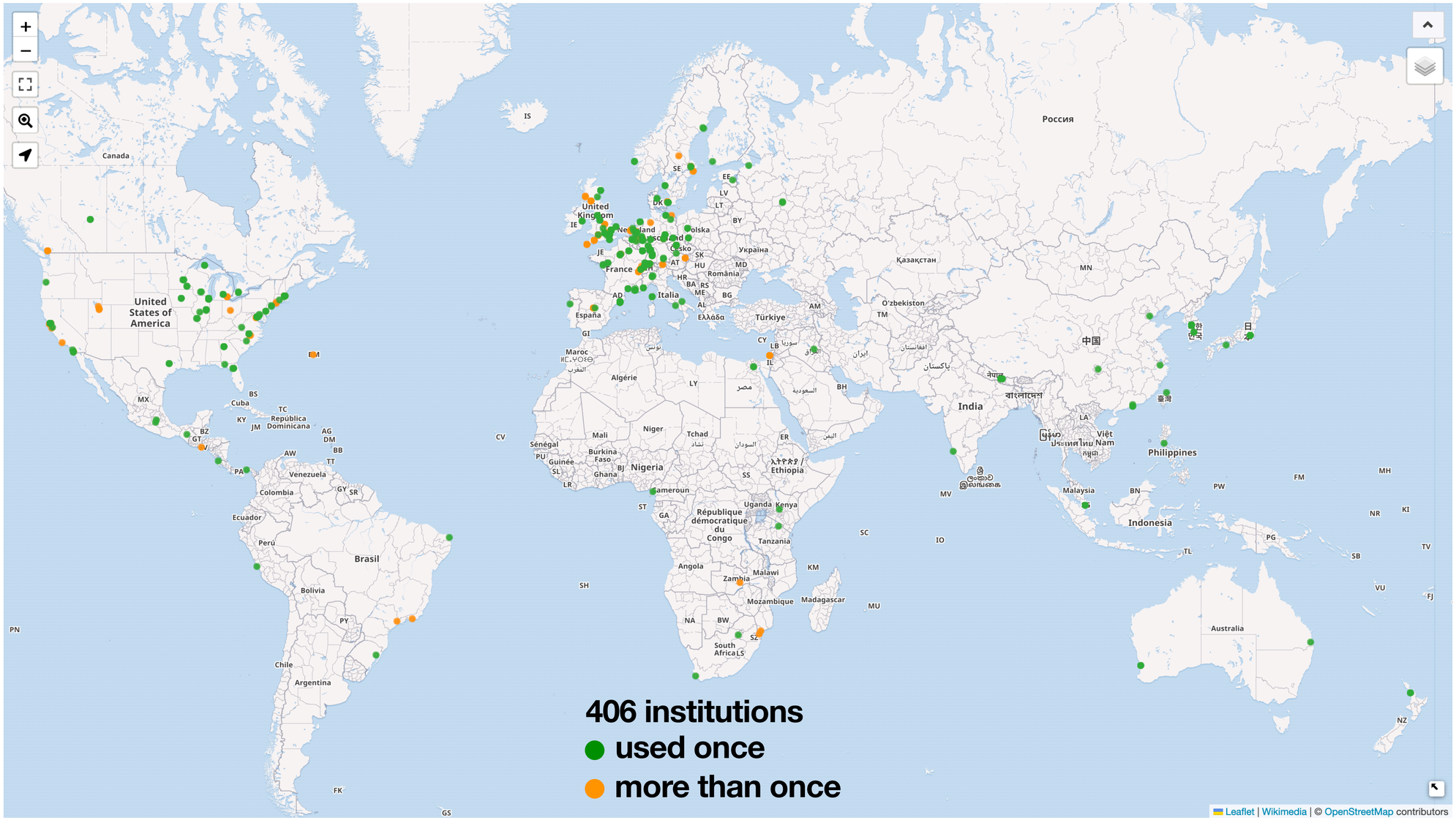

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Institute of Molecular Systems Biology

Prof. Nicola Zamboni

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rutz@imsb.biol.ethz.ch