

chem-bla-ics

Creating nanopublications with Groovy

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Yesterday, I struggled some with creating [nanopublications](#) with [Groovy](#). My first attempt was an utter failure, but then I discovered [Thomas Kuhn's NanopubCreator](#) and it was downhill from there.

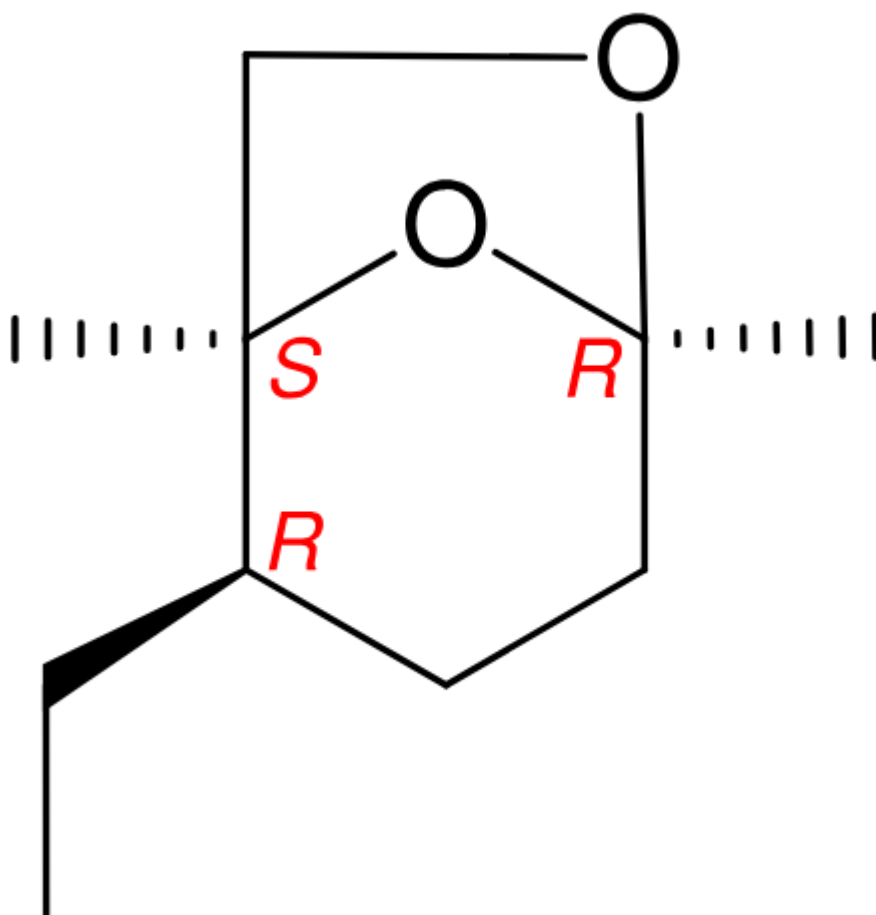
On the right, a depiction is given of a compound found in *Taphrorychus bicolor* (doi:[10.1002/JLAC.199619961005](https://doi.org/10.1002/JLAC.199619961005)). Published in *Liebigs Annalen*, see [this post](#) about the history of that journal.

There are two good things about this. First, I now have a [code base](#) that I can easily repurpose to make *trusty nanopublications* (doi:[10.1007/978-3-319-07443-6_27](https://doi.org/10.1007/978-3-319-07443-6_27)) about anything structured as a table (so can you).

Second, I now about almost 1200 CCZero nanopublications that tell you in which species a certain metabolite has been found. Sourced from [Wikidata](#), using [their SPARQL end point](#). This collection is a bit boring that this moment, and most of them are human metabolites, where the source is either [Recon 2.2](#) or [WikiPathways](#). But I expect (hope) to see more DOIs to show up. Think [We challenge you to reuse Additional Files](#).

Finally, you are probably interested in learning what one of the created nanopublications looks like, so I put [a Gist online](#):

```
@prefix this: <http://www.bigcat.unimaas.nl/nanopubs/wikidata/tmp/np742.RAwXcetTykN6UPVzB> .
@prefix sub: <http://www.bigcat.unimaas.nl/nanopubs/wikidata/tmp/np742.RAwXcetTykN6UPVzB> .
@prefix wd: <http://www.wikidata.org/entity/> .
@prefix np: <http://www.nanopub.org/nschema#> .
@prefix has-source: <http://semanticscience.org/resource/SIO_000253> .
@prefix has-inchikey: <http://semanticscience.org/resource/CHEMINF_000399> .
@prefix orcid: <http://orcid.org/> .
@prefix wdt: <http://www.wikidata.org/prop/direct/> .
@prefix owl: <http://www.w3.org/2002/07/owl#> .
@prefix pav: <http://purl.org/pav/> .
```



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@prefix rdfs: <http://www.w3.org/2000/01/rdf-schema#> .

@prefix skos: <http://www.w3.org/2004/02/skos/core#> .

sub:Head {

 this: np:hasAssertion sub:assertion ;
 np:hasProvenance sub:provenance ;
 np:hasPublicationInfo sub:pubinfo ;
 a np:Nanopublication .

}

sub:assertion {

 wd:Q15978631 rdfs:label "Homo sapiens"@en ;
 skos:exactMatch <http://purl.obolibrary.org/obo/NCBITaxon_9606> .

 wd:Q27125029 has-inchikey: "APJYDQYYACXCRM-UHFFFA0YSA-0" ;
 rdfs:label "tryptaminium"@en ;
 wdt:P703 wd:Q15978631 .

}

sub:provenance {

 sub:assertion has-source: wd:Q2013 , wd:Q28601559 .

 wd:Q28601559 rdfs:label "Recon 2.2: from reconstruction to model of human metabolism"
 owl:sameAs <https://doi.org/10.1007/S11306-016-1051-4> .

}

sub:pubinfo {

 this: pav:createdBy orcid:0000-0001-7542-0286 .

}