chem-bla-ics

Creating nanopublications with Groovy

Egon Willighagen

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Abstract
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.

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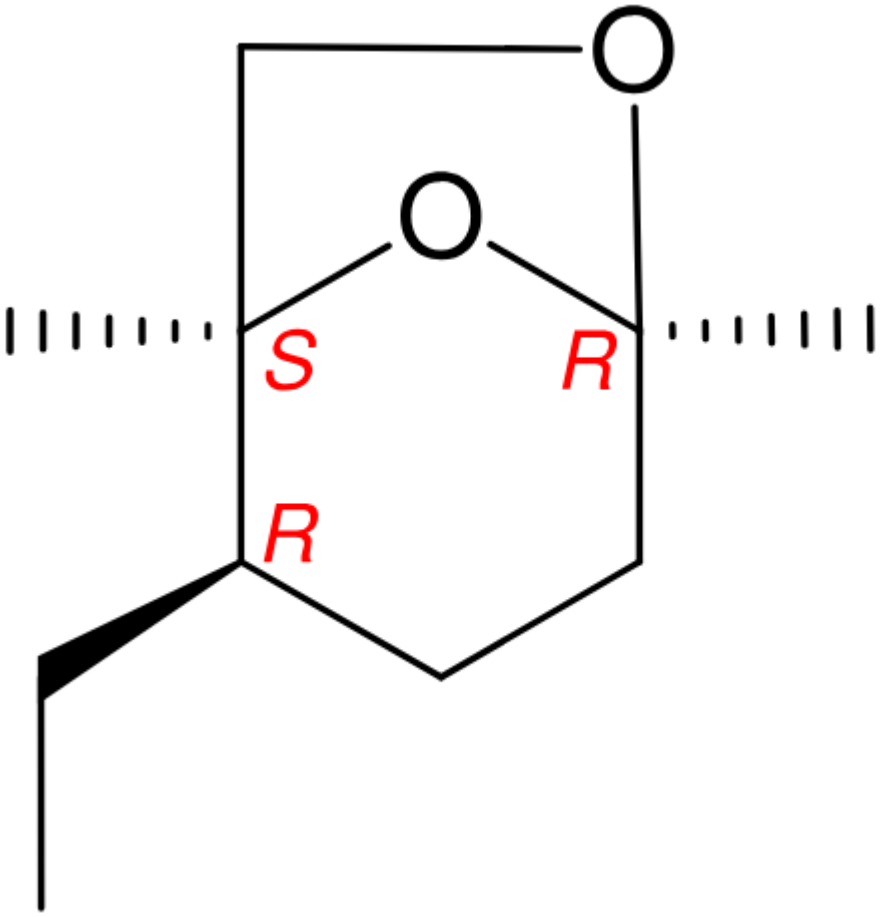

Yesterday, I struggled some with creating nanopublications with Groovy. My first attempt was an utter failure, but then I discovered Thomas Kuhn's NanopubCreator and it was downhill from there.

On the right, a depiction is given of a compound found in Taphrorychus bicolor (doi:10.1002/JLAC.199619961005). 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) 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, to I put a Gist online:

```
@prefix this: <http://www.bigcat.unimaas.nl/nanopubs/wikidata/tmp/np742.RAwXcetTykN6UPVzE
@prefix sub: <http://www.bigcat.unimaas.nl/nanopubs/wikidata/tmp/np742.RAwXcetTykN6UPVzBC
@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-UHFFFAOYSA-O" ;
                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 metabol
                owl:sameAs <https://doi.org/10.1007/S11306-016-1051-4> .
}

sub:pubinfo {
        this: pav:createdBy orcid:0000-0001-7542-0286 .
}
```