

cdk2024 #3: an unexpected downstream project



Published June 16, 2024

Citation

Willighagen, E. (2024, June 16). cdk2024 #3: an unexpected downstream project. *Chem-bla-ics*. <https://doi.org/10.59350/dtfq8-5x011>

Keywords

Cdk, Grant, Cdk2024

Abstract

In the CDK2024 grant we wrote about updating various software projects using the Chemistry Development Kit. We even wrote that “[r]equired API changes will be publicly shared and disseminated with the Groovy Cheminformatics with the Chemistry Development Kit book (egonw.github.io/cdkbook/)”. The Groovy Cheminformatics with the Chemistry Development Kit book is a project that has run since 2009.

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In [the CDK2024 grant](#) we wrote about updating various software projects using the [Chemistry Development Kit](#). We even wrote that “[r]equired API changes will be publicly shared and disseminated with the Groovy Cheminformatics with the Chemistry Development Kit book (egonw.github.io/cdkbook/)”. The *Groovy Cheminformatics with the Chemistry Development Kit* book is a project that has run since 2009.

```
commit c5cbf9b5dd49baf582afc595c9cbafc714c5199f
Author: Egon Willighagen <egon.willighagen@gmail.com>
Date:   Fri Apr 10 12:34:42 2009 +0200
```

```
Initial copy of the current draft; converted into separate project for
easier branching
for tunes of the book for workshops and sorts
```

The original version was in LaTeX and [sold online via Lulu.com](#). Because all code examples were run (the first public edition had 72 pages with 75 code examples), like RMarkdown of Jupyter Notebooks by design, I was able to make [many releases](#). The big advantage of this was that when [API](#) changes happened, this would be visible by code not compiling or by output changing.

At some point I open sourced the book ([doi:10.6084/M9.FIGSHARE.2057790.V1](https://doi.org/10.6084/M9.FIGSHARE.2057790.V1)) and then realized that I can [convert the book to Markdown](#):

```
commit 2630699aa280200188f2ae9ef3f0698964926752
Author: Egon Willighagen <egon.willighagen@gmail.com>
Date:   Mon Dec 24 16:59:14 2018 +0100
```

```
Create chapter3.md
```

This is the version available at egonw.github.io/cdkbook/ for some time now. So, now that for SMARTCyp I need to update the visualization, I went back to my book of code examples (I have a collection of more than 200 examples), but then found that the chapter on [Depiction](#) was missing. I was not looking forward to this, because I know that the code examples predate a massive improvement by [John Mayfield](#) of the rendering stack and I never got around to see if the examples from the book work well enough with that new API (one is actually updated).

That is when I realized that the *Groovy Cheminformatics* book actually also is a downstream project that needs updating. I have been doing this already and it's fairly smooth so that I did not think of including it in the grant, other than updating the [Migration](#) chapter. I now had enough time to dive into [this project](#). I need that, because the goal of the project is also to learn about all the meta science aspects of project maintenance, roles, communication, etc. Therefore also this blog post: we need a track record, to collect data.

Anyway, porting [the first script](#) went fairly easy, but I am now running into a stacktrace:

chem-bla-ics

```
Processing RenderSelection.groovyin
doing RenderSelection.out ...
org.codehaus.groovy.control.MultipleCompilationErrorsException: startup
failed:
/home/egonw/var/Projects/hub/cdkbook-source/code/RenderSelection.groovy: 39:
unable to resolve class ExternalHighlightGenerator
@ line 39, column 16.
    generators.add(new ExternalHighlightGenerator());
                      ^
org.codehaus.groovy.syntax.SyntaxException: unable to resolve class
ExternalHighlightGenerator
@ line 39, column 16.
```

That brings us to the task of how to find where that class is coming from, which happens to be something I already [had to write up](#) for up for `RingSearch`. Dependency galore.