

Google Wave robot for CDK functionality

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Cdk, Cheminf, Google, Wave

Abstract

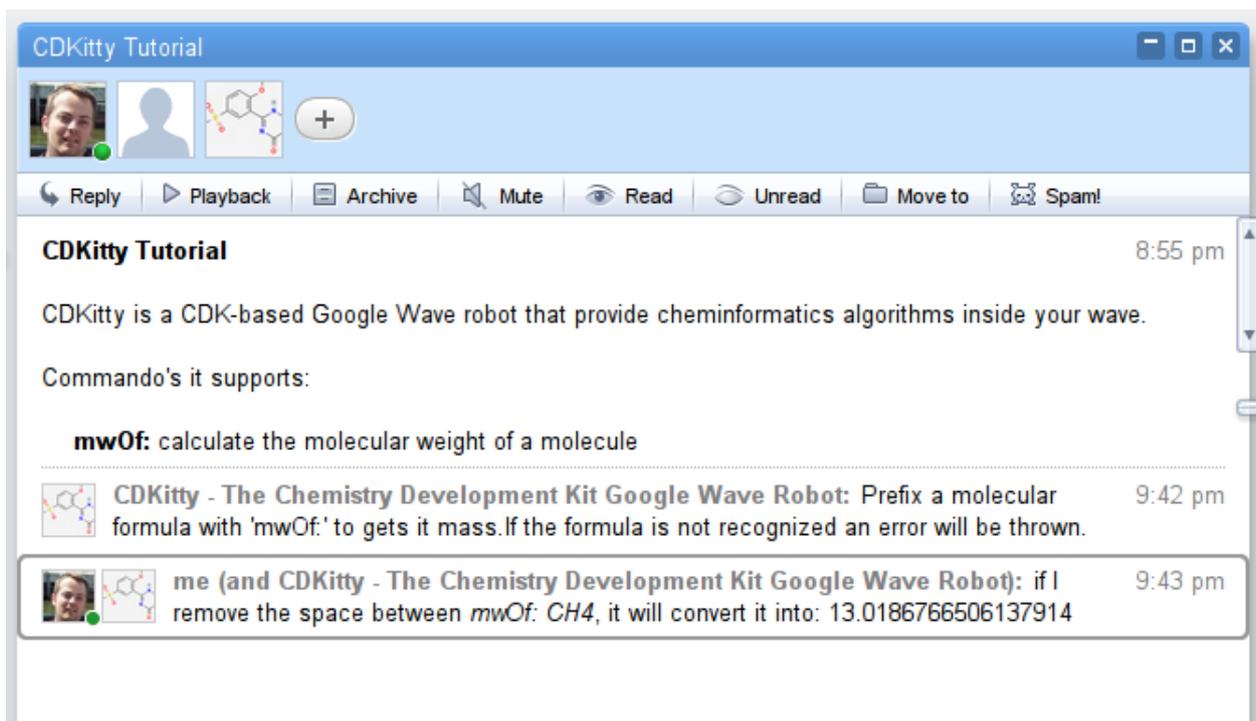
I was really happy to hear early last week that I was invited to take part in the Google Wave beta, and received my account details this Monday, while at attending (and speaking at) the GDCh Wissenschaftsforum Chemie 2009. Yesterday was a travel day, and while working on course material for the Pharmaceutical Bioinformatics course that uses Bioclipse, I set up an Eclipse environment for development of a wave robot.

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chem-bla-ics

I was really happy to hear early last week that I was invited to take part in the [Google Wave](#) beta, and received my account details this Monday, while at attending (and [speaking at](#)) the GDCh Wissenschaftsforum Chemie 2009. Yesterday was a travel day, and while working on course material for the [Pharmaceutical Bioinformatics](#) course that uses [Bioclipse](#), I set up an Eclipse environment for development of a wave robot. [Documentation](#) was very clear, and deployment on [Appspot](#) one click on the appropriate button. Great work from the people from Google! It was all so easy, I could not resist pushing things a bit further, and looked carefully at other robots, like [ChemSpidey](#) by [Cameron](#) and [Igor](#) by [Euan](#), to see how text replacement is done, and wrote my first functional robot, *CDKitty* (chemdevelkit@appspot.com):



It seems that it is a policy that wave robot names end with *-y*, so CDKitty sounded somewhat appropriate. Anyways, the robot is not overly functional yet, but it has a *profile* (which took some extra googling) and one function **mwOf**. Add the robot to your wave and prefix a molecular formula with **mwOf:**, and CDKitty will calculate the molecular formula on the fly. Clearly, this opens up a whole new application world for the [CDK](#), and you can leave feature requests at the [issue tracker](#) of the [project home at GitHub](#). Patches are most welcome too! :)

BTW, it seems I messed up the regular expression, which seems not to be including the last digit (filed as [issue 1](#)).

Almost forgot to add that: many thanx to [Cameron](#) for the insightful discussions we had over applecider, Weisse and German dinner on Monday evening!