

JChemPaint-Primary being picked up...

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Jchempaint

Abstract

Backporting the JChemPaint-Primary patch for master to the cdk-1.2.x branch turned out to be fairly easy, but is a major step forward as we now have a patch to extend CDK 1.2.x with rendering support again, a major thing we lost when going from the CDK 1.0 to the 1.2 series.

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chem-bla-ics

Backporting the [JChemPaint-Primary patch for master](#) to the cdk-1.2.x branch turned out to be fairly easy, but is a major step forward as we now have a patch to extend CDK 1.2.x with rendering support again, a major thing we lost when going from the CDK 1.0 to the 1.2 series.

For example, [KNIME](#) delayed moving to CDK 1.2 because of the lack of the renderer. Another project that really wanted to have the renderer was Ruby CDK ([rcdk-ng](#), but not the same as the [R rcdk package](#) :), originally [started by Rich](#), now maintained by Sebastian Klemm at the [Institute for Pharmatechnology of the University of Applied Science](#), Switzerland.

Ruby CDK is a web environment for molecular structures, and based on the new rendering code, it looks like (copyright by Sebastian):

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Compound: Aspirin
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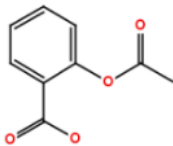
Name
Aspirin

Comment
The prototypical analgesic used in the treatment of mild to moderate pain. It has anti-inflammatory and antipyretic properties and acts as an inhibitor of cyclooxygenase which results in the inhibition of the biosynthesis of prostaglandins. Aspirin also inhibits platelet aggregation and is used in the prevention of arterial and venous thrombosis. (From Martindale, The Extra Pharmacopoeia, 30th ed, p5)

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