chem-bla-ics

CDK Bug Squash Party - Day 2



Published September 20, 2006

Citation

Willighagen, E. (2006, September 20). CDK Bug Squash Party - Day 2. *Chem-bla-ics*. https://doi.org/10.59350/wzs4m-9ky43

Keywords

Cdk, Bsp, Conference

Copyright

Copyright © None 2006. Distributed under the terms of the Creative Commons Attribution 4.0 International License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original author and source are credited.

chem-bla-ics

Like yesterday I will give short overview of things done at the Chemistry Development Kit Bug Squash Party (BSP). I think Stefan was the only to fix and close a bug report yesterday. Rajarshi added the MDE descriptor (yes, during a BSP new code might be committed too;)

More interestingly, discussion on the developers mailing list on the patch by Todd Martin of the EPA to address deducing bond orders in SMILES parsing (the major source of current open bugs!). A problem seems to be when his tool should be called in the SmilesParser class.

More details on the proceedings can be found on the BSP wiki page.