CDK Bug Squash Party - Day 2

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Abstract

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.

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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 commited 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.