

Editorial

by Egon Willighagen

Welcome to the third and last issue of 2006, the eight issue overall, or 1000th in binary. With twenty pages in this issue, the total number of pages this year sums up to 58, which is ten pages less than the second volume. Indeed, the last two issues lacked articles from the FAQ and Literature series. A CDK ChangeLog has not been published either, which together, explains the drop in number of pages. Additionally, the number of tutorials since the start has steadily been dropping to nothing at this moment, while publishing tutorials was one of the goals of CDK News.

Looking on the bright side, the adoption of the Open Journal Systems (OJS) went more than smoothly. The editorial board is, therefore, happy to announce a new website: <http://www.cdknews.org/>. This new website in the CDK family uses the OJS, and includes a as-soon-as-publishable (ASAP) section and has a corresponding RSS feed! This is quite a step forward, because now contributions are put online as soon as they come out of the process of reviewing, copy-editing and laying out.

This issue contains four articles, among which one about the new functionality in the CDK to calculate Gasteiger-Marsili charges. While these charges are much less accurate than quantum chemistry derived charges, calculation of them also requires fewer computational resources, and, therefore, still often used in chemoinformatics. Rojas Chertó describes in his article the details of his CDK implementation.

Steinbeck gives an overview on the state of CDK's structure diagram generation implementation, and Guha gives an update on the interface between CDK and the statistical software R in one article, and describes the new CDK implementation of the Kier-Hall descriptors.

New editors needed

The editorial board thanks Noel O'Boyle for his work as reviewer for CDK News, and would like to take this as an opportunity to advertise the open positions we have in the editorial board. We seek two or three new reviewers who would like to review one or two articles per issue, two copy-editors with good English skills, and two persons who are interesting in continuing the Frequently Asked Questions, and Literature series. Please send me email if you are interested in helping publish CDK News.

The next issue is scheduled for March 2007, with a formal deadline at 16 February. Submissions after this date may be published in the next issue, but going-to-print is not delayed for these submissions. As always, submissions may include comments on current code, discuss certain algorithms in general, or just describe any work related to the CDK library.

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Front Page Rojas Chertó has implemented Garsteiger-Marsili charges for the CDK (sigma charges in top plot, full partial charges in bottom plot). While the algorithm is not published in detail, the correlation with the commercial Petra package is quite satisfactory.