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Poster presentation

XFb – a combined approach for 2D ring drawing

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The two-dimensional illustration of complex ring systems integrated in small molecules is an important feature for the visualization of results generated by computer-aided molecular design procedures. Important groups of drugs like the natural and semi-synthetical opioids contain bridged ring systems which can not be drawn by generic ring drawing methods. In this case, extensions like a ring template database (RDB) or force field (FF) based drawing methods are required [1]. We introduced an algorithm (XFb) that combines both methods – the RDB as well as the FF as extension for the structure diagram drawing tool 2D draw [2].

The order of methods in the computation of the ring system layout is chosen accordingly to the quality of the resulting coordinates. At first the RDB containing hand generated coordinates is scanned for a template of the given ring system. By using an unique linear representation of templates the time to check whether a set of coordinates exists or not can be significantly reduced in contrast to structural comparison. If in the following the generic algorithm fails to generate a set of coordinates which correspond to a collision free layout the FF method is called. As well as for the RDB method a time efficient implementation was one of the main goals during the development.

The method was integrated in the PoseView algorithm [3], which automatically generates two-dimensional layouts for protein-ligand complexes. A short overview concerning the resulting methods will be given on the poster. In the result part the advantages and limitations of the XFb approach will be discussed by means of several representative test cases.

References

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