

Backbones Generator (Bbgen2)

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Background

The software here presented (BB-Gen2) is dedicated to providing new answers to difficulties arising from protein structure prediction from an aminoacid sequence. As such, it takes off after BB-Gen1, an application that performs an aminoacid combination algorithm stemming from a simple model and an input angle set to generate probable residual chains. However, in this first version two problems arise: the size of the output and the time it takes to compute the algorithm (natural to combinatorial problems.)

Results

The new approach taken with BB-Gen2 addressed these issues in three key points. First, partial fragments are generated using a new algorithm. Then, a software tool designed for selection purposes compares the aminoacid input and chooses suitable representatives among them. To finish the cycle, these selected fragments return to the application for combination by the use of filters (steric clashes, end-to-end distance and volume) thus producing a final resulting chain.



This cycle can then be repeated as many times as deemed fit. Also, this tool can generate compressed output using pre-fragment indexes instead of extensive information about the chains.

Conclusion

This new tool is capable of solving, or at least considerably diminishing, the problems present in the first version of the tool. In combination with the selector, the potentially exponential size is reduced until a minimal amount of combinations is used. The new compressed format decreases even further any redundant data and accomplishes a critical downsizing of the generated output.

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