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BEmuse: a tool for drug design on the Grid

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BEmuse (Bias-Exchange Metadynamics Submission Environment) is a Grid-enabled tool developed within EU-IndiaGrid project. It is capable of folding a 36-residue protein in less than a year of single CPU time, significantly reducing the high number of CPU years needed with other techniques. BEmuse has been successfully tested on the EU-IndiaGrid infrastructure and was developed with interoperability among different computational platforms in mind. At the moment it could easily run on different computational grids with minimum effort. BEmuse is now ready to tackle key challenges in drug design, which requires the atomistic simulation of biological systems. This brief presentation highlights the benefits delivered by this innovative tool for companies involved in computational biology.

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