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Potential for ligand generation using *de novo* structure construction method LEGEND

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LEGEND is an efficient tool for *de novo* ligand design. It automatically generates ligand candidate structures based on 3D structures of target macromolecules. It is the main advantage that a wide variety of structures which fit well to the target cavity can be constructed, by adding atoms one by one using force field and random numbers. For dealing with the problems of how the designed structures can be obtained for assay, our database search system, EUREKA, is a promising method, because it can find analogous structures that might also bind stably to the target cavity, from the databases of available compounds or literature information. We have greatly improved both LEGEND and EUREKA, and show the practical and effective strategy for *de novo* design of novel ligand structures, using our methods. Also, we will show the validation of our strategy, using two protein systems.