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The 3D structures of small molecules were retrieved from the PubChem compound database and the ZINC Database. In order to be suitable for a molecular docking calculation, both chemical structures must be stored in a file as 3D (3-dimensional) objects. The 3D files were also converted to 2D files (2-dimensional) that can be directly read and written by the Gold program. The 2D files generated by the program are readable by other programs, such as ChemDraw. Moreover, the above list contains the ligands that Gold has already placed in the protein structure or an active site, provided that the protein cavity is wide enough to receive these molecules. Other ligands are placed by the docking program according to their GOLD score. This is a 1 billion ligand database containing crystal structures, with druglike and biologically active fragments being on average longer. The database does not include molecules with water molecules, which can be removed. The database can be downloaded in a single file and no intermediate files are required. The resulting database is named CCDC_DB. The database contains a total of 3.2 million unique molecules and has been split into 6 M files, in which molecules are stored on average at different distances from one another. The sizes of the files, depending on distance, range from 14 to 1,000,000,000. The names of the files are formed from the numerical file IDs and a suffix indicating the distance from one another. A file name is formed by adding an integer ID to the file number, and to the maximum distance between molecules. For example, File 3.2.14.2.250.000 has files 3.2.14, 3.2.14.1, 3.2.14.2, 3.2.14.2.250, etc. 5ec8ef588b

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