GriDock: An MPI-based software for virtual screening in drug discovery

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GriDock is a molecular modelling software developed to identify potentially bioactive compounds (*hit-compounds*) in order to speed-up the drug discovery process. It’s based on the *virtual-screening* approach in which the activity of a large set of molecules is predicted by multiple molecular docking calculations distributed on a Grid system. More in details, GriDock joints the VEGA flexibility and the AutoDock 4 power to take full advantage of the Grid technology.