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AutoDockVinais an open source program for doing molecular docking. It was originally designed and implemented by Dr. Oleg Trott in the Molecular Graphics Lab now CCSB at The Scripps Research Institute. The latest version is available here

AutoDockVinais one of the docking engines of the AutoDock Suite. The image on the left illustrates the results of flexible docking green Download NOTE The latest stable version of AutoDockVinacan be downloaded from the GitHub repository. Older versions are available here

OS Files Installation instructions autodock_vina_1_1_2_linux_x86.tgz See instructions Linux AutoDockVinaManual Contents Features License Tutorial Frequently Asked Questions Platform Notes and Installation Windows Linux Mac Building from Source Other VinaVideo Tutorial This tutorial demonstrates molecular docking of imatinib usingVinawith AutoDock Tools and PyMOL

Note that the version ofVinaused in the tutorial is now old so some differences are unavoidable

Specifically the program option all is now called out and the predicted binding affinity is different in the current version of the software AutoDockVinais released under the permissive Apache license allowing flexible use for commercial or non commercial purposes Questions problems or suggestions? FAQ! If you have a question it may have already been answered

Please check the FAQ first. Otherwise use one of the following Email recommended Please subscribe to the AutoDock mailing list and send your messages there

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the output because of the subsequent refinement stage that could move different binding modes closer * Bug fix in some very unusual cases numerical rounding errors would accumulate leading internally to a distorted ligand structure About mgl admin This author has not yet filled in any details

So far mgl admin has created 0 blog entries for f in ligand_*.pdbqt do b=‘basename $f .pdbqt‘ echo Processing ligand $b j=${b}.job d=‘pwd‘ mkdir p $b echo ! bin bash > $j echo cd $d > $j echo vina AutoDockVinais an open source program for doing molecular docking

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