

AutoDock-GPU 1.5.3

Webpage

<https://autodock.scripps.edu/>
<https://github.com/ccsb-scripps/AutoDock-GPU>

Version

v1.5.3

Build Environment

- GCC 8.5.0
- CUDA Toolkit 12.0
-

Files Required

(will be downloaded in the following procedure)

Build Procedure

```
#!/bin/sh

VERSION=1.5.3
INSTALL_DIR=/apl/autodock-gpu/${VERSION}

module -s purge
module -s load cuda/12.0

export GPU_INCLUDE_PATH=/apl/cuda/12.0/include
export GPU_LIBRARY_PATH=/apl/cuda/12.0/lib64

# -----

cd ${INSTALL_DIR}

git clone https://github.com/ccsb-scripps/AutoDock-GPU.git
mv AutoDock-GPU/{*,.git*} .
rmdir AutoDock-GPU
git checkout refs/tags/v${VERSION}
# build for A30, A100 (compute capability)
sed -i -e "s/52 60 61 70/80/" Makefile.Cuda
make DEVICE=CUDA NUMWI=128
```

Notes

- Built for NVIDIA A100 and A30.
- Input data should be prepared with MGLTools (<https://ccsb.scripps.edu/mgltools/>).
 - autogrid command is not included in MGLTools (Linux version)? You may need to use autogrid in AutoDock 4.2.6 package.
 - Python scripts in AutoDock Vina (under example directory) might be used for building input data.