

Please follow the instructions below to run Mold2 version 2.0:

A. Unzip the downloaded file Mold2.zip;

B. Run Mold2:

1. For Windows Operating System:
 - 1) Open the fold Mold2 in which you unzipped the downloaded file Mold2.zip;
 - 2) Open the sub-fold Windows;
 - 3) Rename file Mold2.doc to Mold2.exe;
 - 4) Rename file Mold2.txt to Mold2.bat;
 - 5) Double click Mold2.bat;
 - 6) Follow tutorial slides (file Mold2_Tutorial.sdf in the fold Mold2).
2. For Linux Operating system:
 - 1) Open the fold of Mold2 in which you unzipped the downloaded file Mold2.zip;
 - 2) Open the sub-fold Linux_x86-32 or Linux_x86-64;
 - 3) Change the permission of Mold2.sh to executable if necessary;
 - 4) Type “./Mold2.sh” to run Mold2 v2.0;
 - 5) Follow tutorial slides (file Mold2_Tutorial.sdf in the fold Mold2).

Mold2_Description.pdf has brief descriptions for the 777 descriptors. For details of the 777 description, please see the paper on Mold2 (Mold2paper.pdf).

A dataset of 232 compounds (TestCompounds.sdf) is provided for testing Mold2.

Please send your questions, comments, and suggestions to:

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