

# **Molecular 2D Descriptors (Mold2) Generator Software, A step by step tutorial**

Version 2.0

Center for Bioinformatics  
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# Contact Information

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**Downloaded at:**

<http://www.fda.gov/ScienceResearch/BioinformaticsTools/Mold2/>

# Running Mold2, Initial View

Shown below is the initial view upon starting Mold2 (requires Java Runtime Environment JRE 1.6.0 or higher).

Windows:

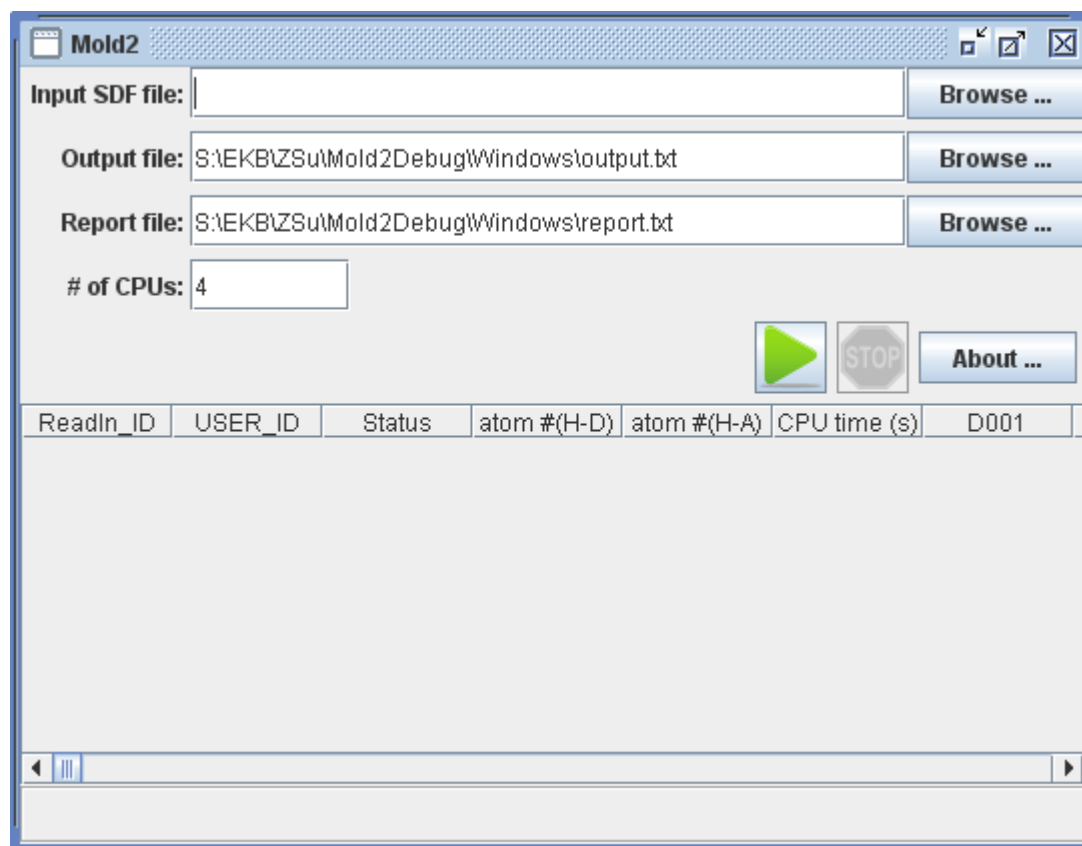
-double click

Mold2.bat

-Or run Mold2.bat in  
an Windows cmd  
line

Linux:

./Mold2.sh



# Running Mold2 by Java Web Start

Mold2 can be also launched by one click on any supported platforms.

<http://weblaunch.nctr.fda.gov/arraytracktesting/Mold2.html>

Mold2 Software Setup - Windows Internet Explorer

http://weblaunch.nctr.fda.gov/arraytracktesting/Mold2.html

## Welcome to Mold<sup>2</sup> Software Setup

[NCTR Toxicoinformatics Home](#) | [ArrayTrack Home](#) |

You'll be able to run Mold<sup>2</sup> on your local machine by following one or two simple steps, depending on whether Java is already installed on your machine.

**Step 1:** It appears that Java is already installed (good!), so you can go on to step 2.

*(In case of problems, you can [click here](#) to re-install the Java environment that is required by Mold<sup>2</sup>.)*

**Step 2:** **1** [Click here](#) to install and run Mold<sup>2</sup>.

You can also use this link in the future to run Mold<sup>2</sup>, or let Mold<sup>2</sup> place icons on your desktop and start menu when prompted.

Mold<sup>2</sup> is a product of [National Center for Toxicological Research](#)

**Warning - Security**

The application's digital signature cannot be verified.  
Do you want to run the application?

**Name:** Mold2 2.0.0  
**Publisher:** National Center for Toxicological Research  
**From:** http://weblaunch.nctr.fda.gov

Always trust content from this publisher.

**2** Run Cancel

The digital signature cannot be verified by a trusted source. Only run if you trust the origin of the application. [More Information...](#)

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**Mold2**

Input SDF file:  **Browse ...**

Output file: C:\Documents and Settings\zsu.FDA\output.txt **Browse ...**

Report file: C:\Documents and Settings\zsu.FDA\report.txt **Browse ...**

# of CPUs:

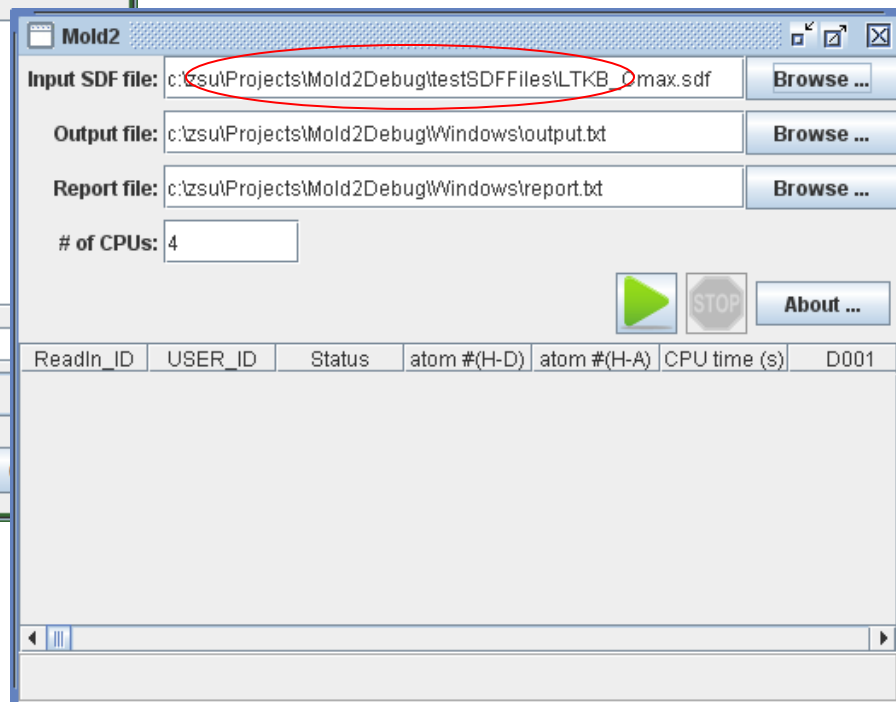
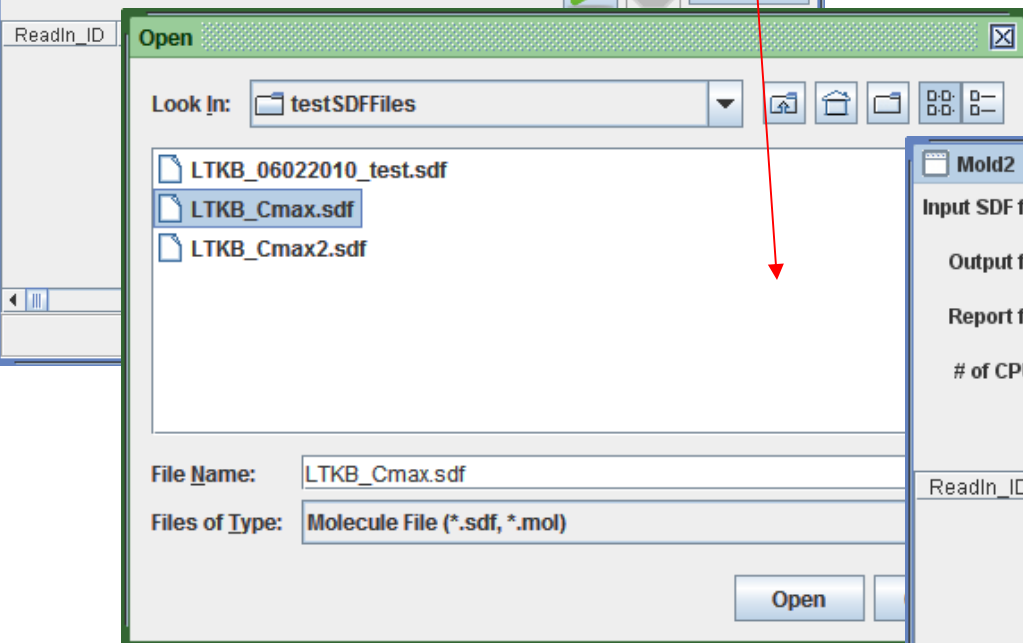
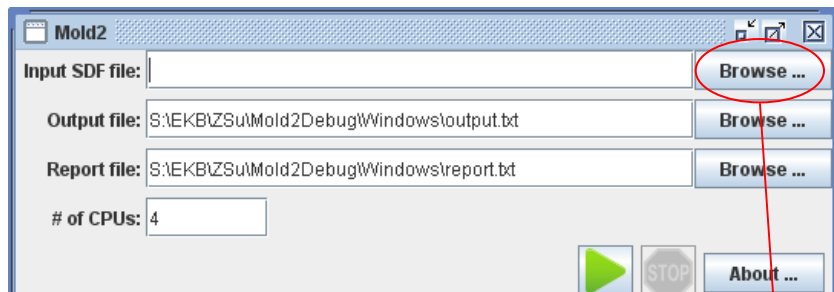
**Run** **STOP** **About ...**

ReadIn_ID	USER_ID	Status	atom #(H-D)	atom #(H-A)	CPU time (s)

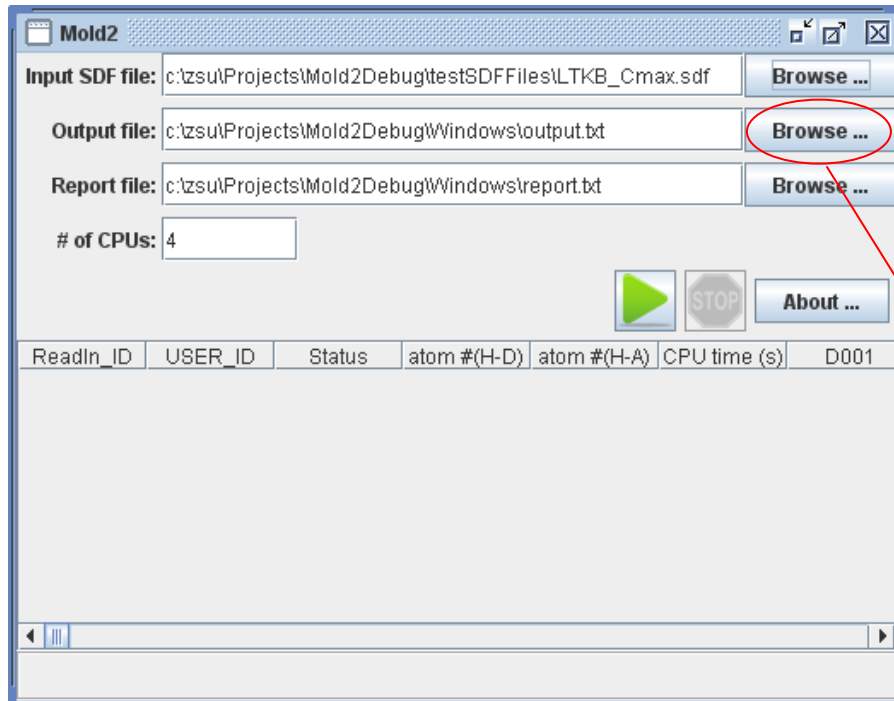
# Choosing an Input File

Click the Browse button and select a .sdf or a .mol file

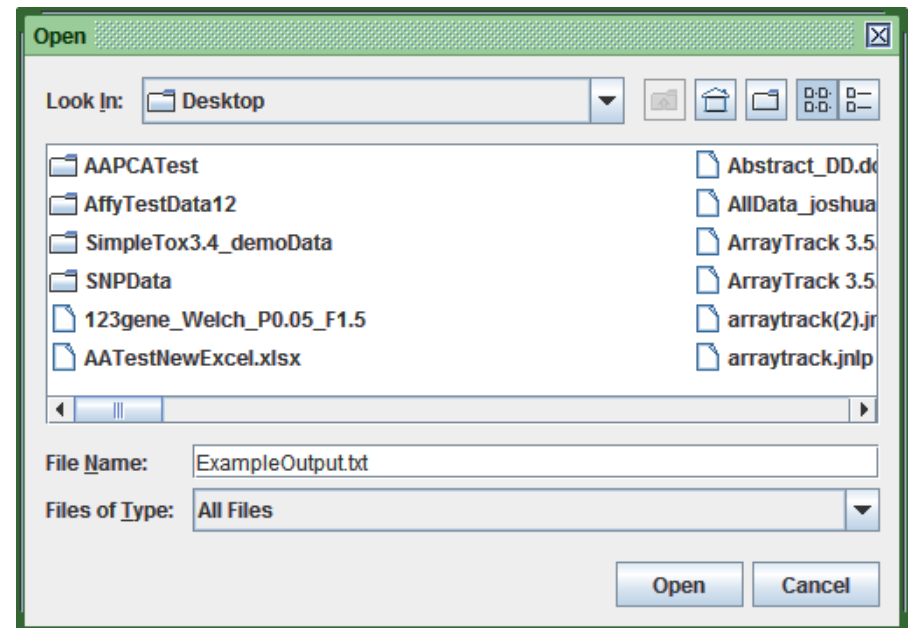
After selecting a file, you will see your selected file in the "Input SDF file" text box



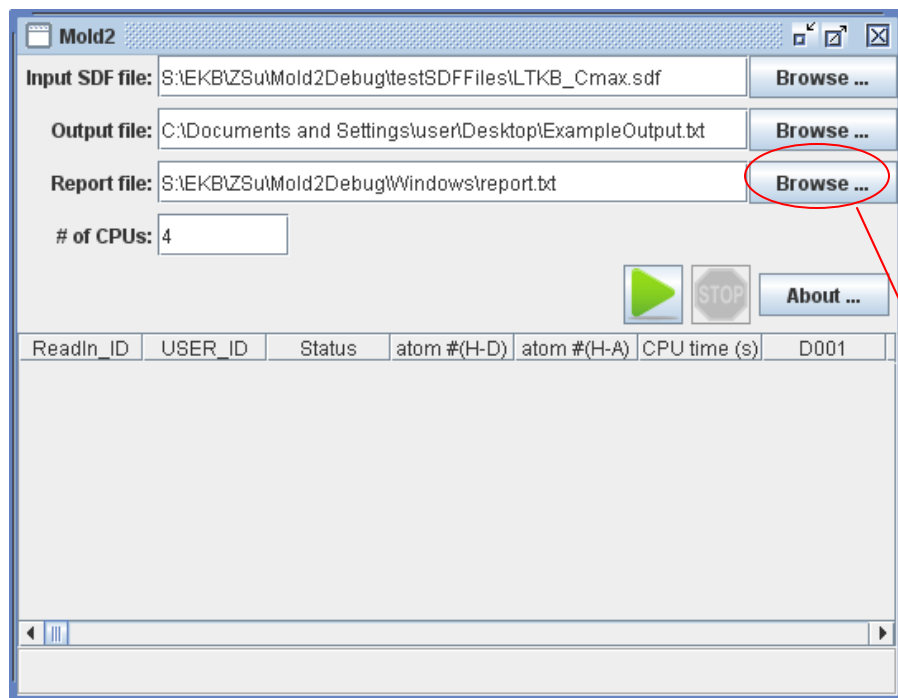
# Choosing an Output File



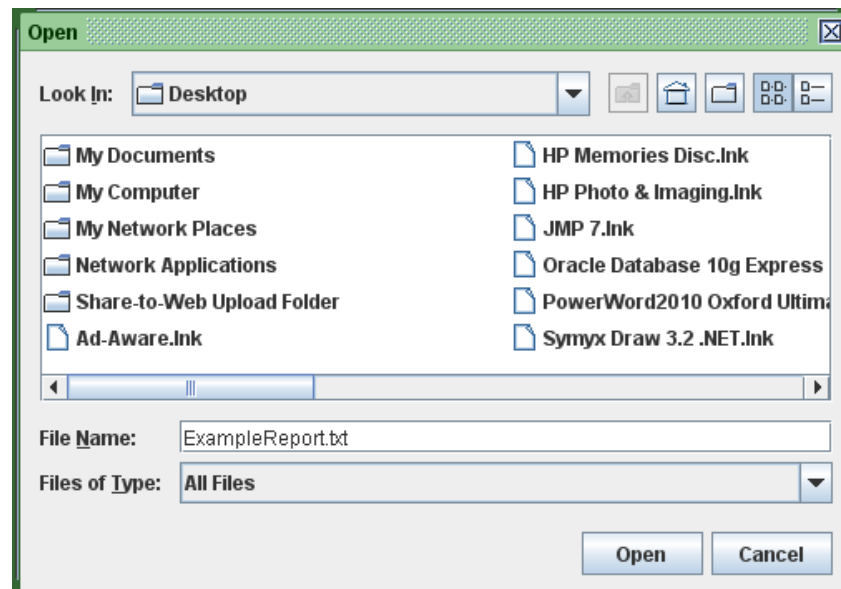
Choose a directory and type in a filename for your output file; it is recommended to save it with a .txt extension



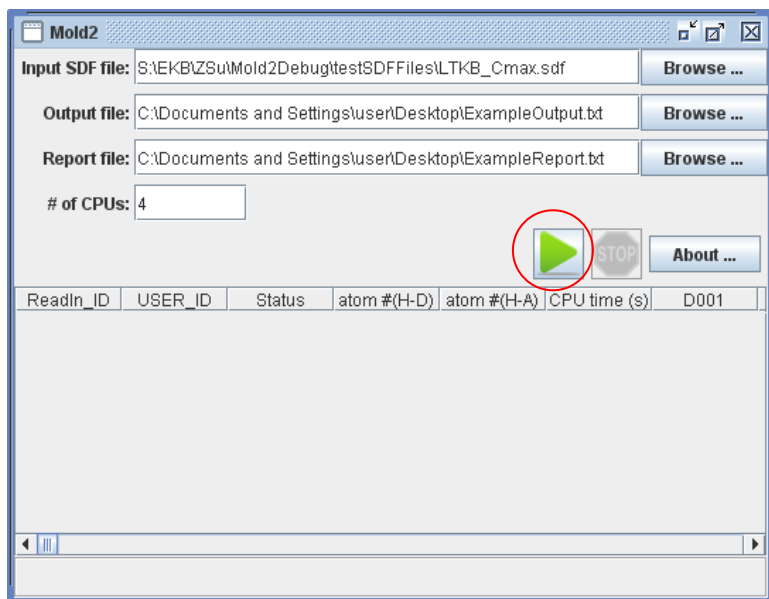
# Choosing a Report File



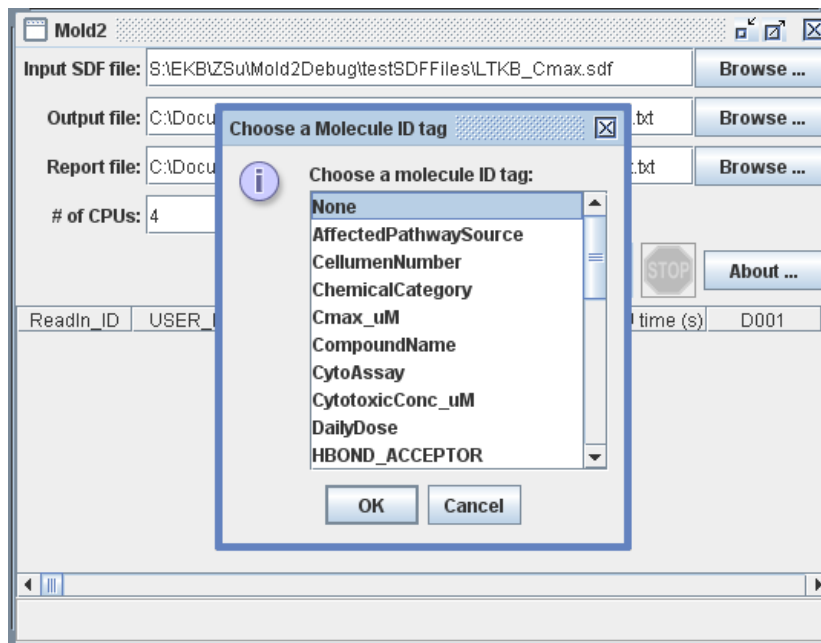
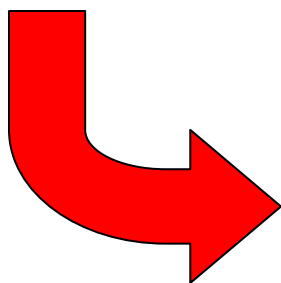
Choose a directory and type in a filename for your report file; it is recommended to save it with a .txt extension



# Choosing an ID Tag



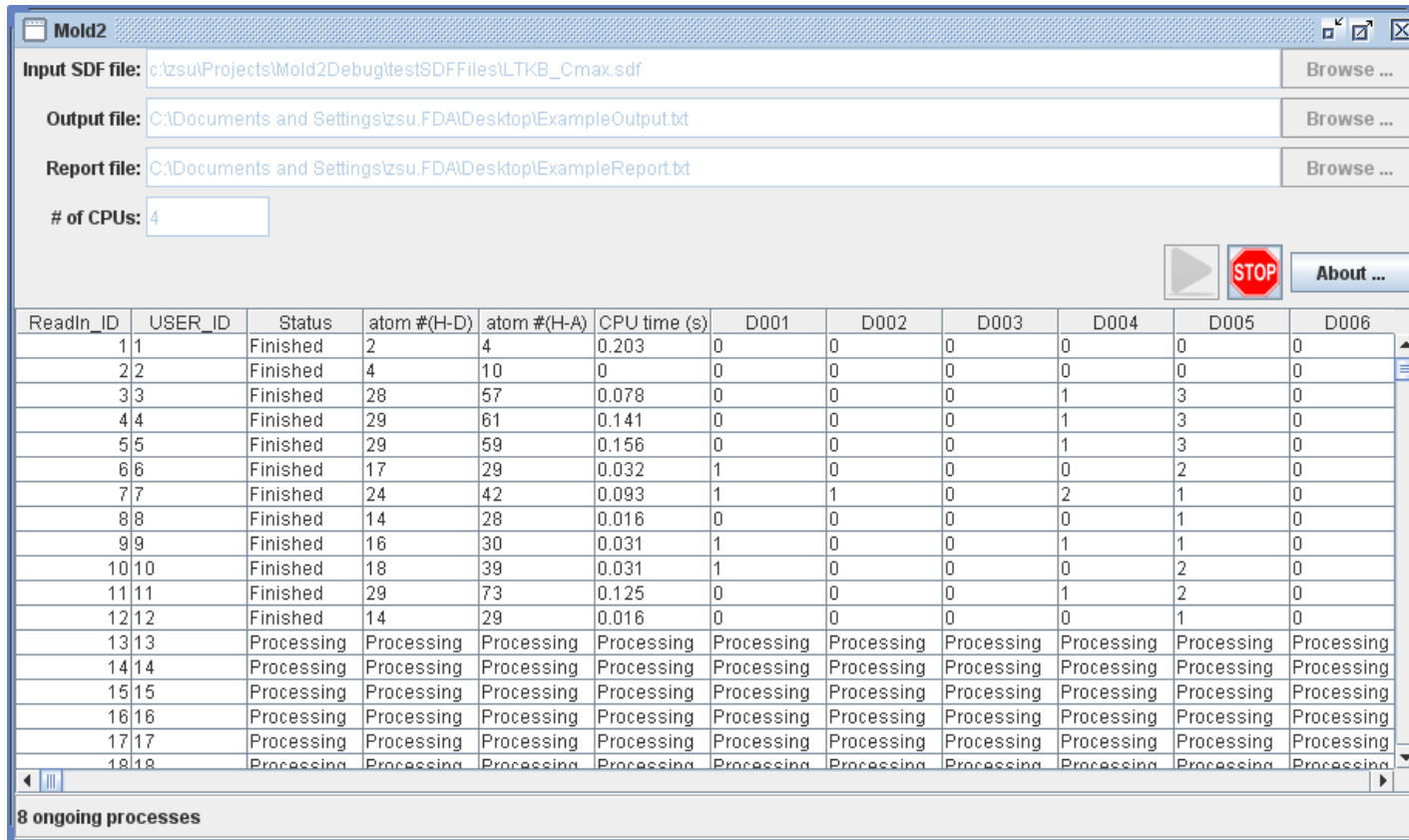
After selecting Input, Output and Report files, click the green arrow button to run the analysis. An option pane is shown for users to choose a structure ID tag. Available ID tags are listed in a ListBox. “None” means have no an ID tag will be used.





# Performing Analysis

The progress of calculation can be monitored from the table view. There are four statuses: Loaded (chemical structure is loaded from the input file), processing (perform calculation), Finished (calculation is finished), and Saved (the descriptors are written into the output file)



The screenshot shows the Mold2 software interface. At the top, there are fields for 'Input SDF file', 'Output file', and 'Report file', each with a 'Browse ...' button. Below these is a field for '# of CPUs' set to 4. A play button, a red 'STOP' button, and an 'About ...' button are also visible. The main part of the interface is a table with the following columns: ReadIn\_ID, USER\_ID, Status, atom #(H-D), atom #(H-A), CPU time (s), D001, D002, D003, D004, D005, and D006. The table shows 18 rows of data. Rows 1-12 are 'Finished', rows 13-17 are 'Processing', and row 18 is 'Processing'. The status of the processes is also shown at the bottom of the window as '8 ongoing processes'.

ReadIn_ID	USER_ID	Status	atom #(H-D)	atom #(H-A)	CPU time (s)	D001	D002	D003	D004	D005	D006
1	1	Finished	2	4	0.203	0	0	0	0	0	0
2	2	Finished	4	10	0	0	0	0	0	0	0
3	3	Finished	28	57	0.078	0	0	0	1	3	0
4	4	Finished	29	61	0.141	0	0	0	1	3	0
5	5	Finished	29	59	0.156	0	0	0	1	3	0
6	6	Finished	17	29	0.032	1	0	0	0	2	0
7	7	Finished	24	42	0.093	1	1	0	2	1	0
8	8	Finished	14	28	0.016	0	0	0	0	1	0
9	9	Finished	16	30	0.031	1	0	0	1	1	0
10	10	Finished	18	39	0.031	1	0	0	0	2	0
11	11	Finished	29	73	0.125	0	0	0	1	2	0
12	12	Finished	14	29	0.016	0	0	0	0	1	0
13	13	Processing	Processing	Processing	Processing	Processing	Processing	Processing	Processing	Processing	Processing
14	14	Processing	Processing	Processing	Processing	Processing	Processing	Processing	Processing	Processing	Processing
15	15	Processing	Processing	Processing	Processing	Processing	Processing	Processing	Processing	Processing	Processing
16	16	Processing	Processing	Processing	Processing	Processing	Processing	Processing	Processing	Processing	Processing
17	17	Processing	Processing	Processing	Processing	Processing	Processing	Processing	Processing	Processing	Processing
18	18	Processing	Processing	Processing	Processing	Processing	Processing	Processing	Processing	Processing	Processing

8 ongoing processes