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

Version 2.0

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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).

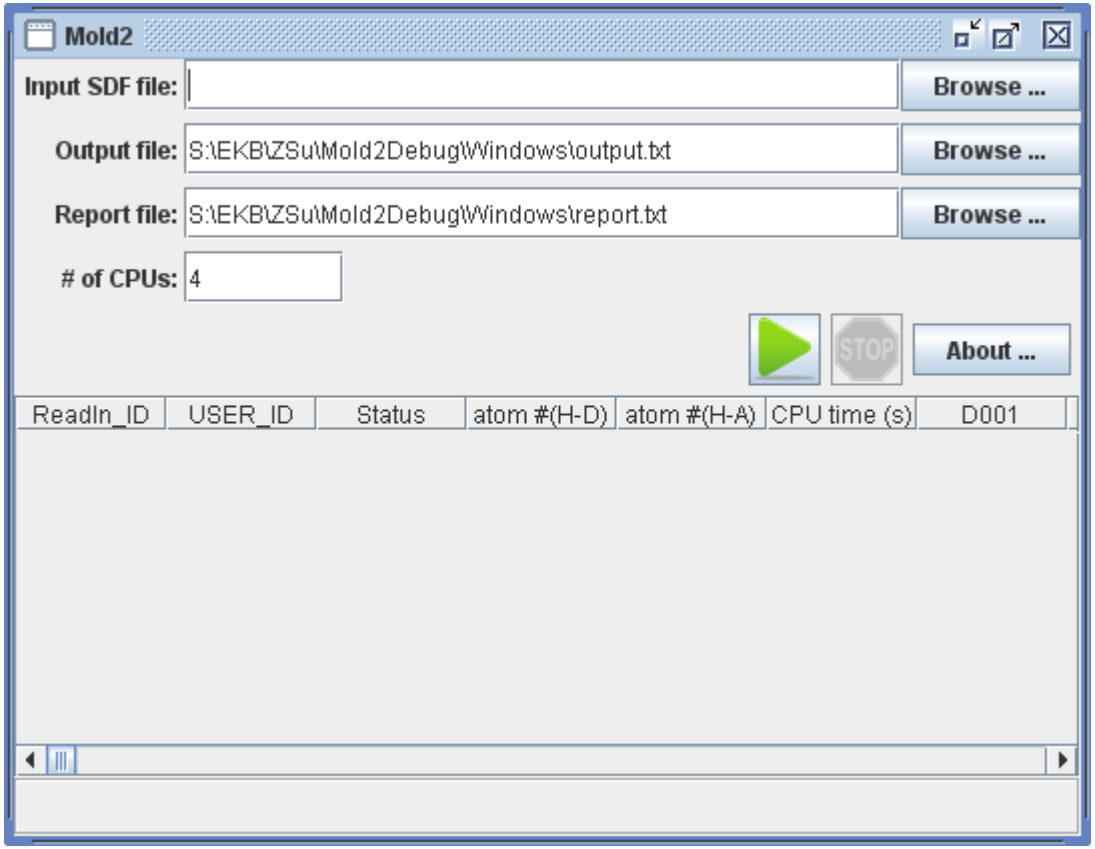
Windows:

-double click Mold2.bat

-Or run Mold2.bat in an Windows cmd line

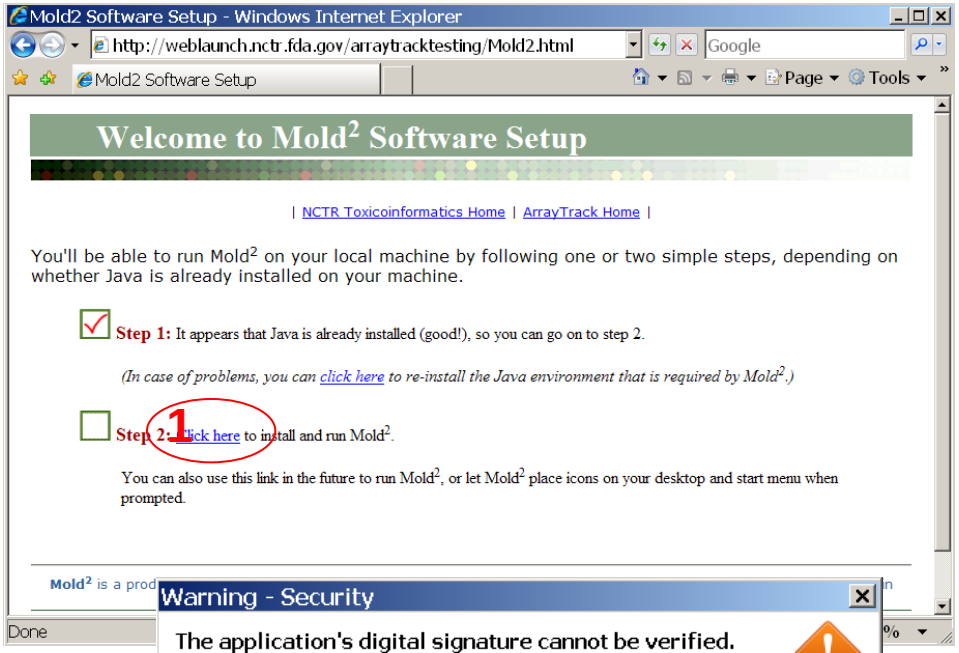
Linux:

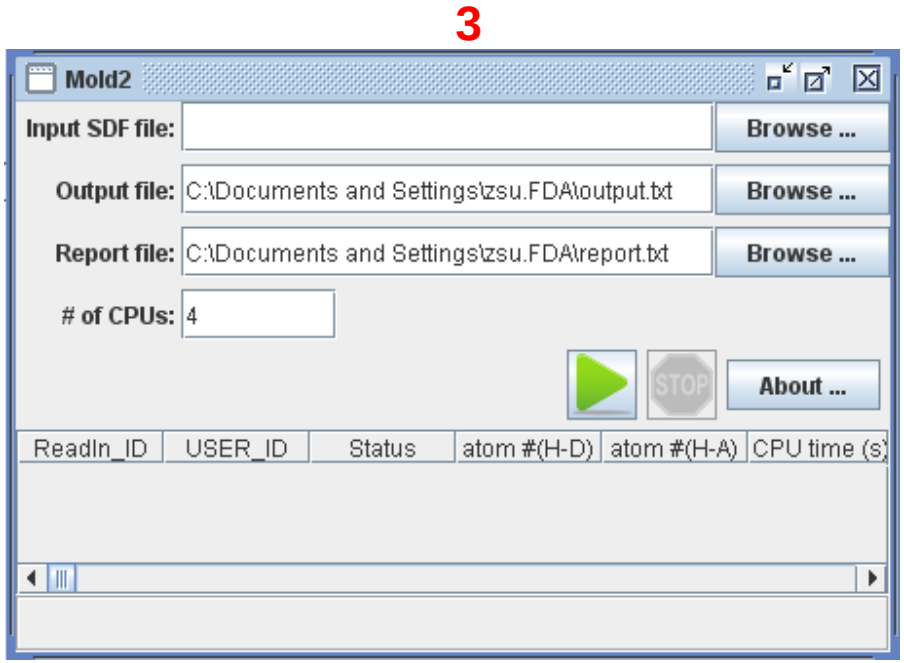
./Mold2.sh



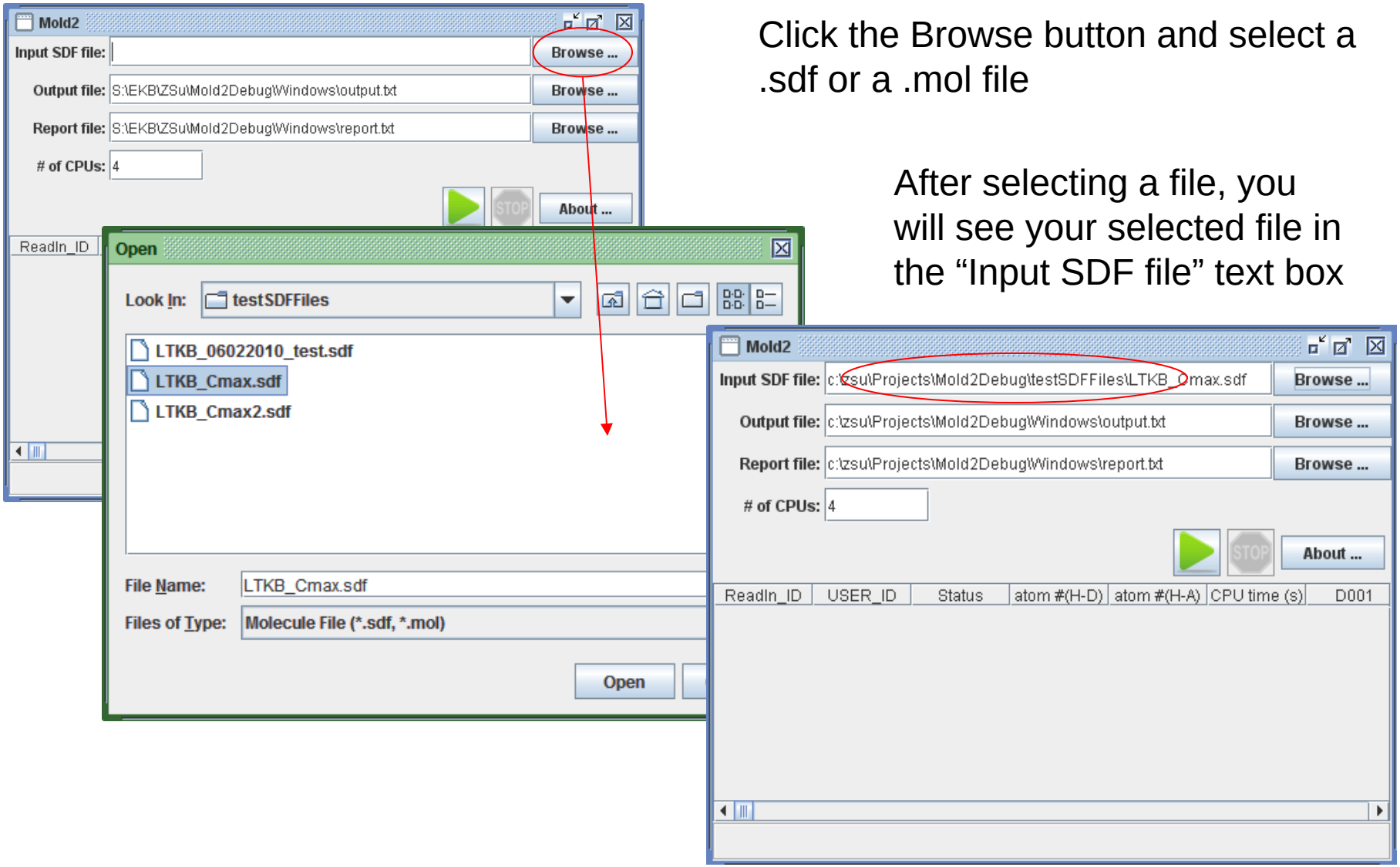
Running Mold2 by Java Web Start

Mold2 can be also launched by one click on any supported platforms.
http://weblaunch.nctr.fda.gov/arraytracktesting/Mold2.html





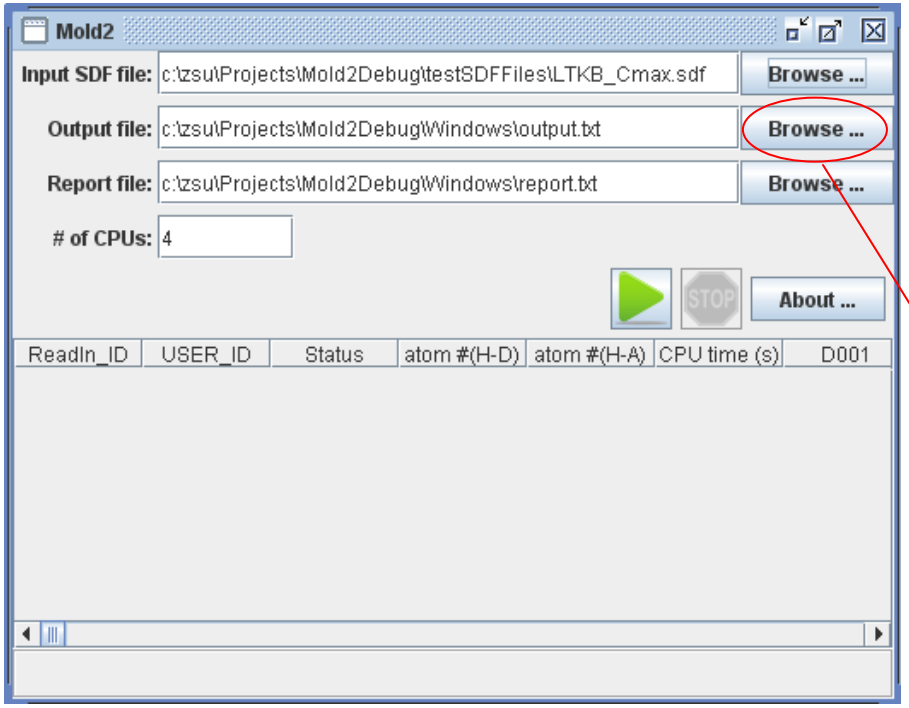
Choosing an Input File



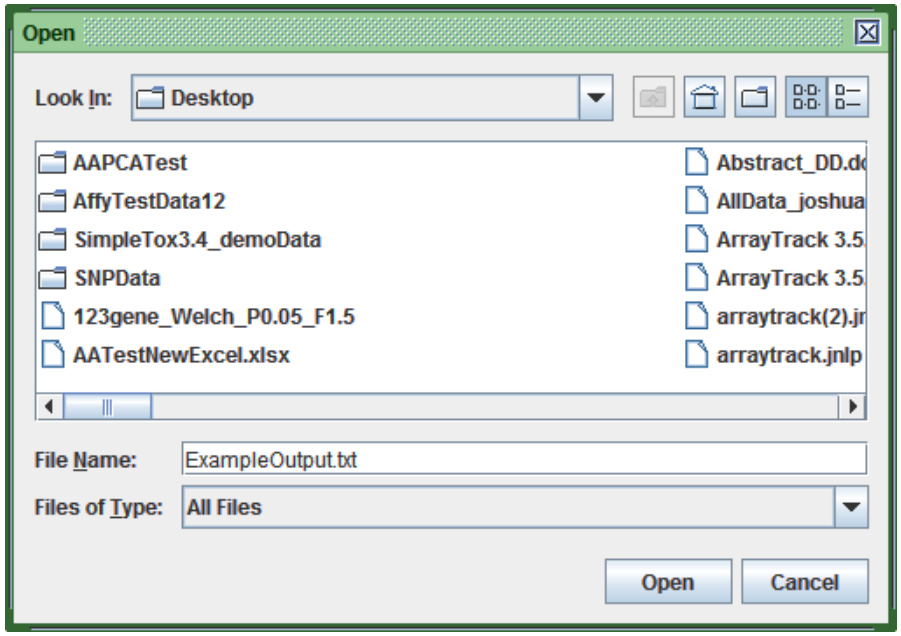
Click the Browse button and select a .sdf or a .mol file

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

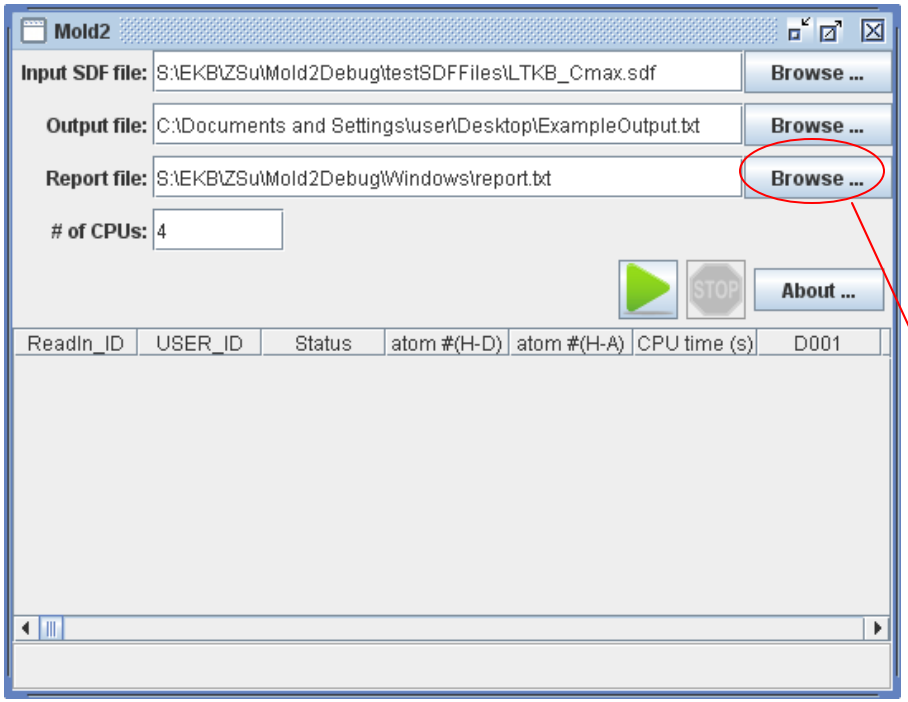
Choosing an Output File



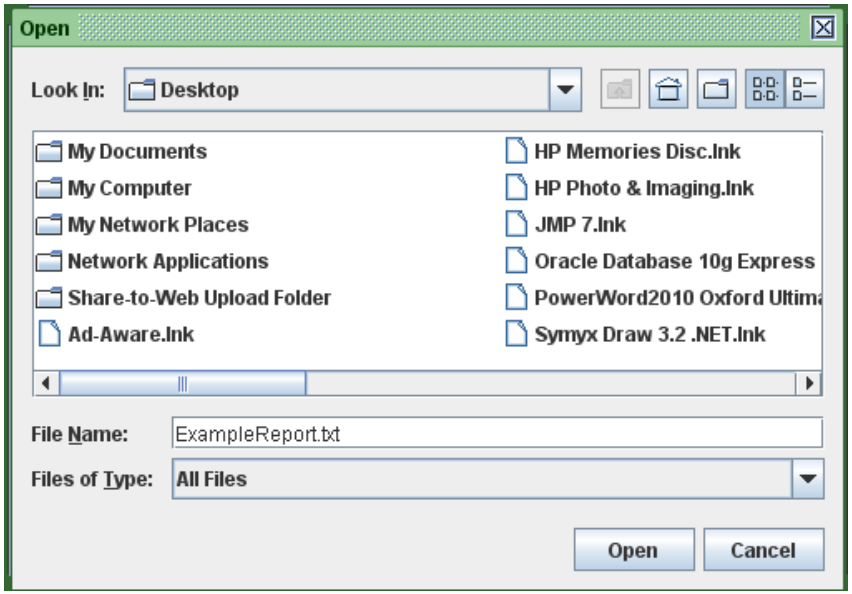
Choose a directory and type in a filename for your output file; it is recommended to save it with a .txt extension



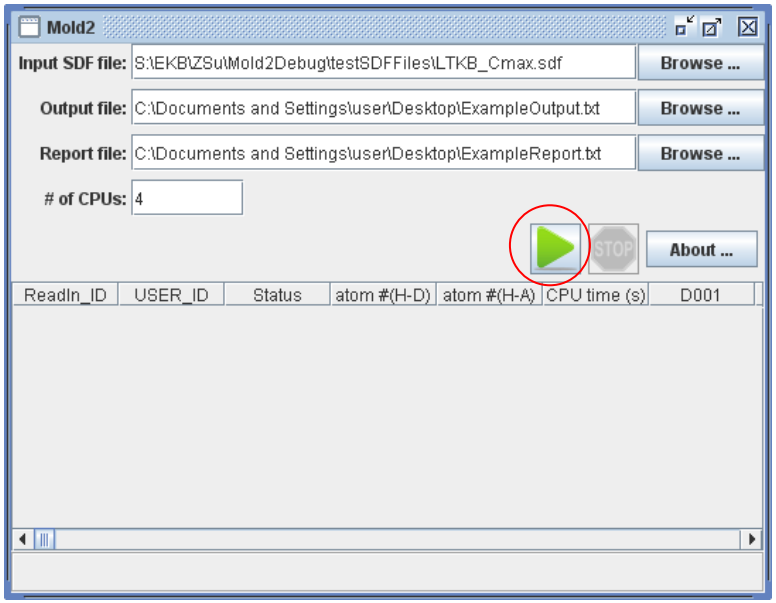
Choosing a Report File



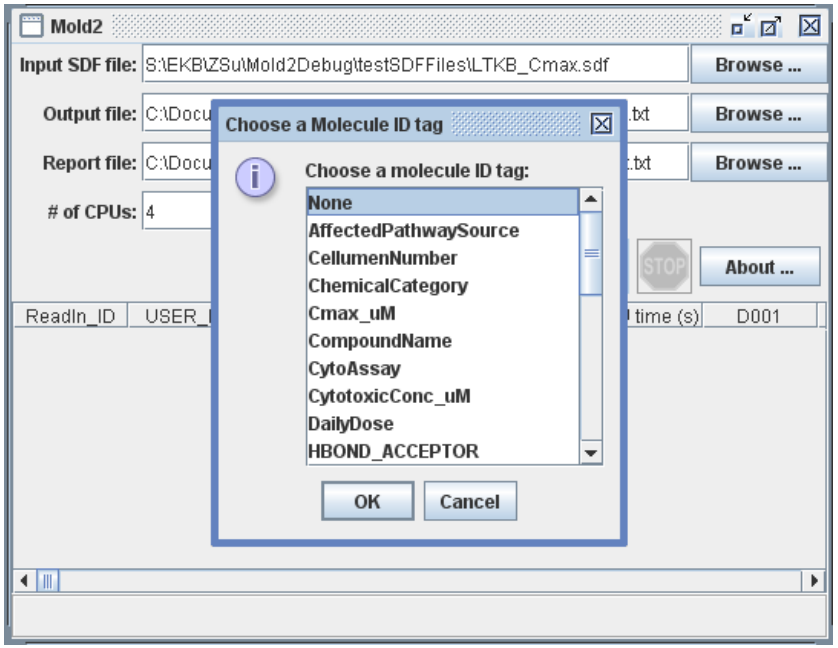
Choose a directory and type in a filename for your report file; it is recommended to save it with a .txt extension



Choosing an ID Tag

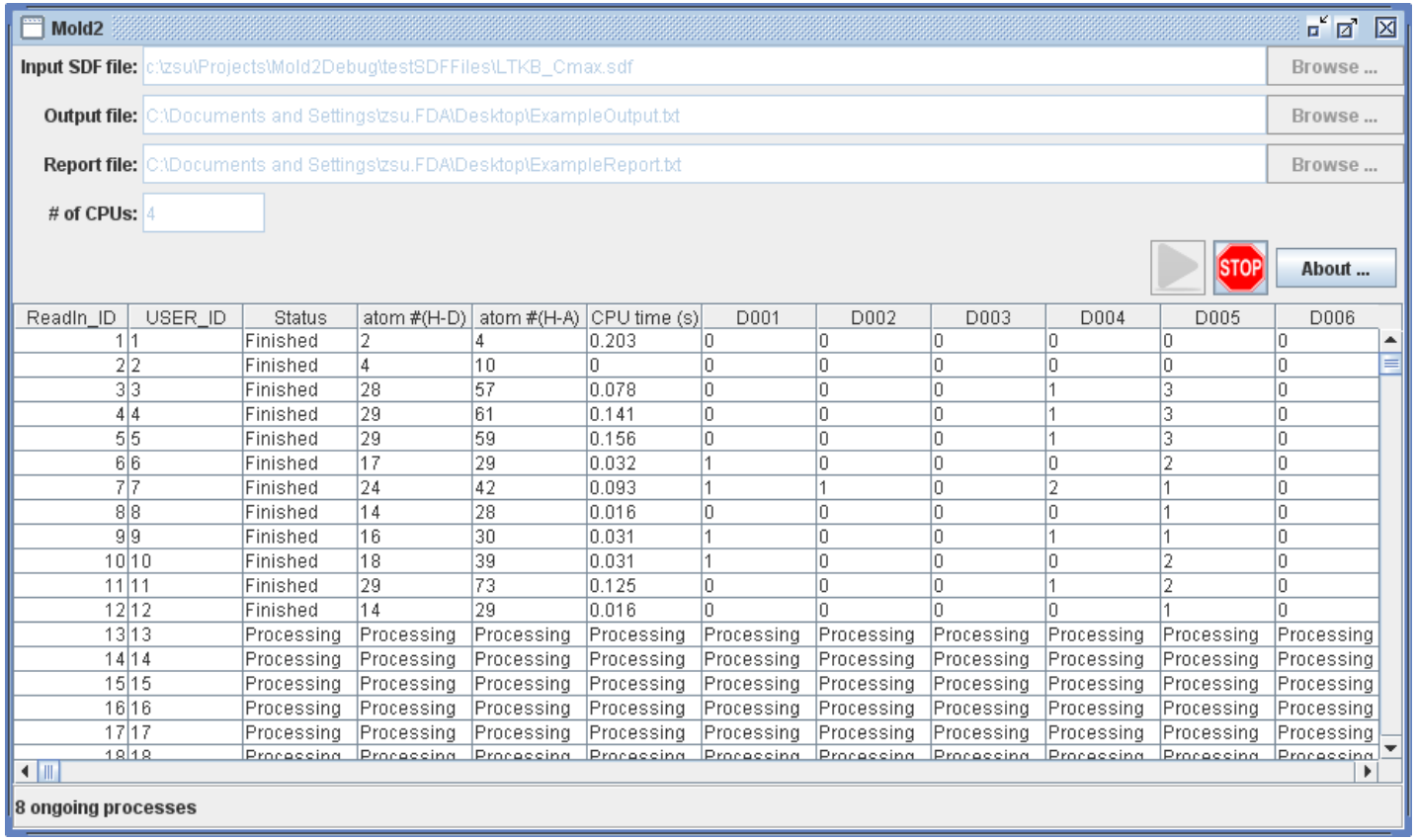


After selecting Input, Output and Report files, click the green arrow button to run the analysis. An option pane is shown for users to choose a structure ID tag. Available ID tags are listed in a ListBox. “None” means have no an ID tag will be used.



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)



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