Running TEST from the command prompt

To run TEST from the command line, run the following at the command prompt:

java –Xmx512m -cp "test.jar" ToxPredictor.Application.runTEST_From_Command_Line inputFile fileType outputFile endpointNumber methodNumber

where

inputFile = input file name such as “chemicals.sdf” or “chemicals.smi”. These files should be in the same folder as the .jar files or you need to specify the file path.

For **fileType**, choose a number option from the following table:

fileType	Option
1	SDF file
2	SMILES text file

outputFile = output file name such as “results.txt”. This file will be created in the same folder unless you specify a filepath.

For **endpointNumber**, choose a number option from the following table:

endpointNumber	Option
1	Fathead minnow LC50 (96 hr)
2	Daphnia magna LC50 (48 hr)
3	T. pyriformis IGC50 (48 hr)
4	Oral rat LD50
5	Bioaccumulation factor
6	Developmental Toxicity
7	Mutagenicity
20	Normal boiling point
21	Vapor pressure at 25°C
22	Melting point
23	Flash point
24	Density
25	Surface tension at 25°C
26	Thermal conductivity at 25°C
27	Viscosity at 25°C
28	Water solubility at 25°C
99	Molecular Descriptors

For **methodNumber**, choose a number option from the following table:

methodNumber	Option
1	Hierarchical clustering
2	FDA
3	Single model
4	Nearest neighbor
5	Group contribution
10	Consensus
-1	N/A (no QSAR method is needed to just calculate molecular descriptors)

Examples

Example 1. To run the consensus method for the T. pyriformis IGC50 (48 hr) endpoint for SDF input use the following

> java -Xmx512m -cp "test.jar" ToxPredictor.Application.runTEST_From_Command_Line "Sample_MDL_SDfile.sdf" 1 "resultsIGC50.txt" 3 10

Example 2. To run the group contribution method for flash point for smiles input use the following:

> java -Xmx512m -cp "test.jar" ToxPredictor.Application.runTEST_From_Command_Line "chemicals.smi" 2 "resultsFP.txt" 23 5

Example 3. To just calculate molecular descriptors from chemicals for SDF input use the following:

> java -Xmx512m -cp "test.jar" ToxPredictor.Application.runTEST_From_Command_Line "Sample_MDL_SDfile.sdf" 1 "descriptors.txt" 99 -1

Example 4. To run the hierarchical clustering method for the fathead minnow LC50 (96 hr) endpoint for SDF input use the following:

> java -Xmx512m -cp "test.jar" ToxPredictor.Application.runTEST_From_Command_Line "Sample_MDL_SDfile.sdf" 1 "FHM_LC50_Hiearchical_Clustering_Method.txt" 1 1

The commands for the above examples are provided in 4 .bat files which can be run by double clicking on them in Microsoft Windows.

Running TEST from Java

Create a method to create an instance of the runTEST_From_Command_Line class as follows:

```
void runFromJava() {
      ToxPredictor.Application.runTEST_From_Command_Line r=new
ToxPredictor.Application.runTEST_From_Command_Line();

      String inputFilePath="Sample_MDL_SDfile.sdf";
      String outputFilePath="results.txt";
      int iFileType=runTEST_From_Command_Line.numFileTypeSDF;
      int iEndpoint=runTEST_From_Command_Line.ChoiceFHM_LC50;
      int iMethod=runTEST_From_Command_Line.ChoiceHierarchicalMethod;

      r.go(inputFilePath,outputFilePath,iFileType,iEndpoint,iMethod);

}
```

Note: once the data files for a given endpoint are loaded, successive calls to the go method should be faster.