getSDF -f|s|i input.csv [--id=molecule_id] [-o output.sdf][--header]

-f|s|i input.csv	Name of CSV file containing a list of molecules identified by their names(- f), smiles(-s) or InChI(-i). Must contain the molecule information (name, SMILES or InChI) in the first column.
--id=molecule_id	Name of the field where the unique id will be added to output.sdf file
-o output.sdf	Name of SDFile containing the results of the operation
--header	The first line of the list will be considered a list header and therefore be ignored

Examples of use:

getSDF -f input.csv -o output.sdf

This will build a new sdf using the provided names of each molecule.

getSDF -s input.csv -o output.sdf

This will build a new sdf using the provided smiles of each molecule.

getSDF -s input.csv -o output.sdf --id=name

This will build a new SDFile using the provided InChi of each molecule and labeled the molecule with the field given on column 'name'.

viewSDF [-f file.sdf] [-o output.html[[--name=name]

-f file.sdf	Name of a SDFile containing one or more molecules
-o output.html	Name of a file in HTML formal containing the results of the visualization
--name=name	Assign to each image file the name given by the field. If no name is specified the command assigns an id generated as molecule0001... etc

addInchi [-f file.sdf] [-o output.sdf]

-f file.sdf	Name of a SDFile containing one or more molecules
-o output.sdf	Name of a SDFile containing the results: the same input.sdf but including new fields for InChi and InChiKey

addDataToSDF -f file.sdf -d data.csv --id=molecule_id [-o output.sdf]

-f file.sdf	Name of a SDFile containing one or more molecules
-d data.csv	Must contain tab separated info and a single line header
--id=molecule_id	Specified the unique id which is used for the matching. Must be present in the SDFile and in the CSV file
-o output.sdf	Name of a SDFile containing the results of adding CSV data to the SDF file. The output file will include all molecules present in the original SDFile.

addSDFToData -f file.sdf -d data.csv --id=molecule_id [-o output.sdf]

-f file.sdf	Name of a SDFile containing one or more molecules.
-d data.csv	Must contain tab separated info and a single line header
--id=molecule_id	Specified the unique id which is used for the matching. Must be present in the SDFile and in the CSV file
-o output.sdf	Name of a SDFile containing the results of adding SDF information to the CSV data. The output file will include only molecules present in the data.csv

extractData -f file.sdf –-name|--field=activ|--table

-f file.sdf	Name of a SDFile containing one or more molecules
--name	Prints in screen the molecule names
--field=activ	Prints in screen information about the specified field
--table	Prints in screen all the properties of the SDFile, separated by tabs and with a header

Examples of use:

extractData -f file.sdf –field=smiles

This will show an extraction of the smiles of each the molecule

extractData -f file.sdf –-name

This show an extraction of the different names of each the molecule

extractData -f file.sdf –table

This command will show all data of file.sdf formatted as a table

join -a fileA.csv -b fileB.csv --id molecule_id [-o output.csv] [--soft]

-a fileA.csv -b fileB.csv	Names of the CSV files you want to join
--id molecule_id	Name of the column which is used as common key to join the csv files
-o output.csv	Name of the CSV file resulting of join fileA with fileB
--soft	Used for InChiKey based comparisons. The last 3 chars are discarded. This makes the comparison insensitive to the charge of the compound and the InChi software version