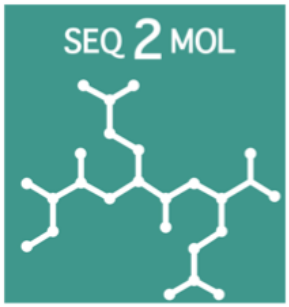


# SEQ2MOL: From Amino acid Sequence to Molecular Graph

(Version 1.1)

Jesus A Beltran, Gabriel Del Rio, Carlos A Brizuela

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# Introduction

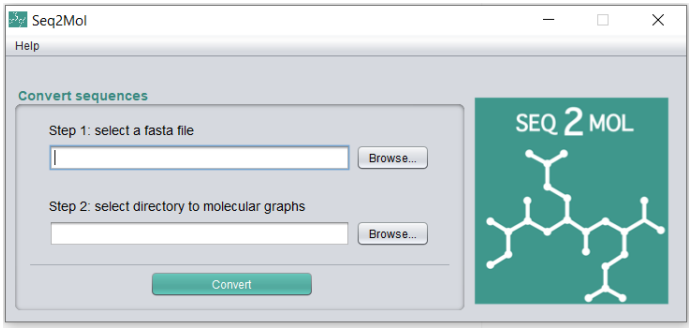
SEQ2Mol is a toolbox designed to read amino acids sequences in Fasta file format and convert them into molecular graphs. Then, each molecular graph is stored into a Molfile format (V2000). Molfile [1] is supported by Elsevier MDL, this file allows to efficiently communicate the chemical information.

## Instructions to run SEQ2MOL

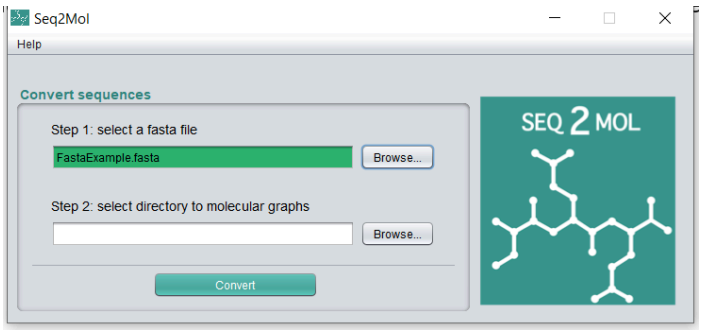
SEQ2MOL could be executed in two ways: By using a GUI or by command line.

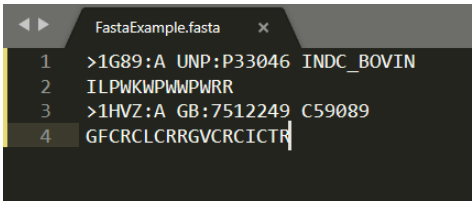
To launch SEQ2MOl in graphical mode, please follow the steps below.

1. You should run SEQ2MOL using: java -jar "Seq2Mol.jar". Then, the following screen is displayed:

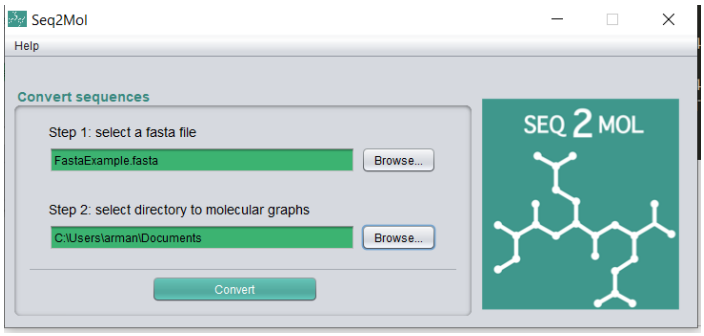



2. You should choose a Fasta file where amino acid sequences are stored. For example:

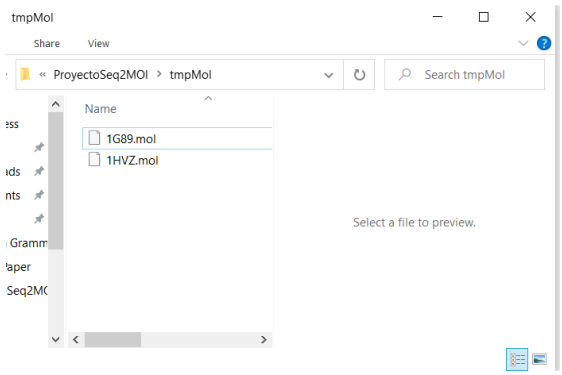


3. Select the directory where you want to store the mol files. Each file stored a molecular graph.




4. Click on the convert button. Then a message is displayed and the directory where the mol file is open. For example:




To launch SEQ2MOl in command line mode, type as follows:

- java -jar “Seq2Mol.jar” fastafile outputdirectory

## References


- [1] MDL (2005). CT file format. MDL Information Systems Inc, 14600 Catalina St., San Leandro, CA 94577.