



Showcase to Illustrate how the web-server iATC_Deep-mISF is working

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Introduction- In 2020, a very powerful web-server predictor has been established for identifying the Anatomical Therapeutic Chemicals [1], in which a same chemical may occur in two or more classes and hence needs to be marked with the multi-label approach [2].

The web-server predictor is called “iATC_Deep-mISF”, where “Deep” means the web-server has been further improved by the “Deep Learning” technique [3-6], and “m” means the capacity able to deal with the multi-label systems. To learn how the web-server is working, please do the following.

Step 1: Click the link at http://www.jci-bioinfo.cn/iATC_Deep-mISF/, the top page of the iATC_Deep-mISF web-server will appear on your computer screen, as shown in **Fig.1**. Click on the **Read Me** button to see a brief introduction about the predictor.

GJSFR-G Classification: FOR Code: 100499, 080505



Strictly as per the compliance and regulations of:



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Short Title: Anatomical Therapeutic Chemicals

Kuo-Chen Chou

INTRODUCTION

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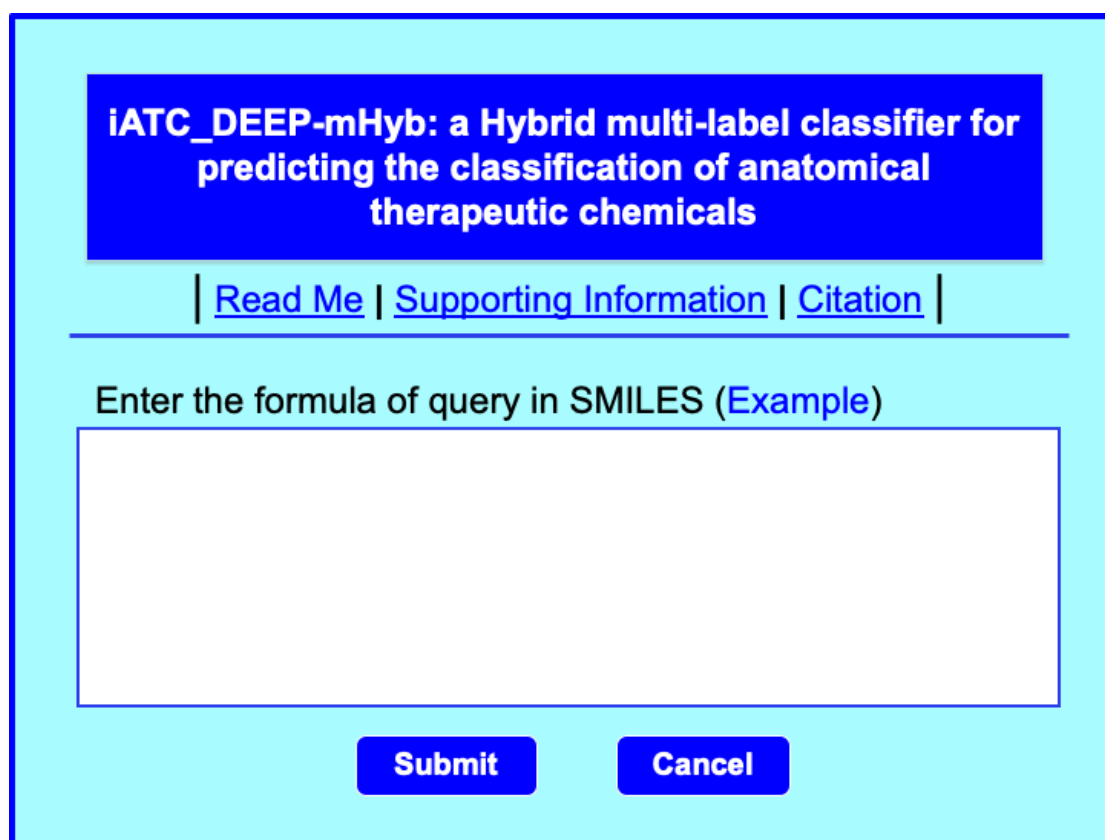


Figure 1

Step 2: Either type or copy/paste the Anatomical Therapeutic Chemicals into the input box at the center of **Fig. 1**. The input sample should be in the FASTA format. For the examples of FASTA format, click the [Example](#) button right above the input box.

Step 3: Click on the [Submit](#) button to see the predicted result. For instance, if you use the four samples in the [Example](#) window as the input, after 10 seconds or so, you will see a new screen (**Fig. 2**) occurring. On its upper part

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are listed the names of the samples (1) to (14) covered by the current predictor. On its lower part are the predicted results: the query compound-1 of example-1 corresponds to “3, 5, 9” the query compound-2 corresponds to “3,” and so forth. All these results are perfectly consistent with experimental observations.

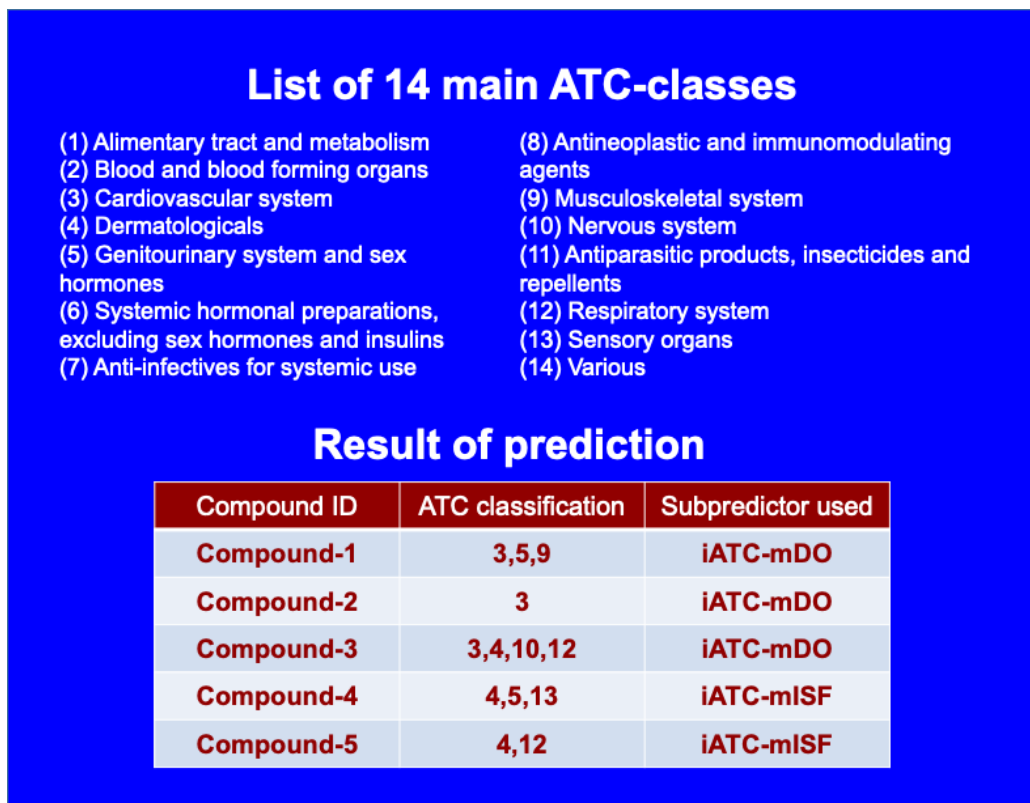


Figure 2

Step 4: As shown on the lower panel of **Fig. 2**, you may also choose the batch prediction by entering your e-mail address and your desired batch input file (in FASTA format of course) via the [Browse](#) button. To see the sample of batch input file, click on the button [Batch-example](#). After clicking the button [Batch-submit](#), you will see “Your batch job is under computation; once the results are available, you will be notified by e-mail.”

Step 5: Click on the [Citation](#) button to find the papers that have played the key role in developing the current predictor of iATC_Deep-mISF.

Step 6: Click the Supporting Information button to download the Supporting Informations mentioned in this paper.

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