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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 <u>Read Me</u> button to see a brief introduction about the predictor.

GJSFR-G Classification: FOR Code: 100499, 080505



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

Short Title: Anatomical Therapeutic Chemicals

Kuo-Chen Chou

Introduction

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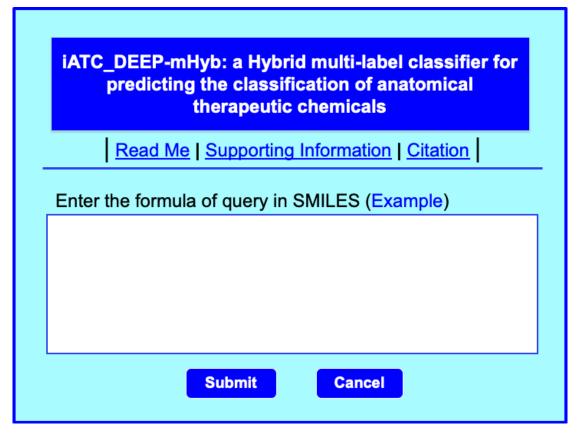


Figure 1

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 $\underline{\text{Example}}$ button right above the input box.

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

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.

List of 14 main ATC-classes (1) Alimentary tract and metabolism (8) Antineoplastic and immunomodulating (2) Blood and blood forming organs (3) Cardiovascular system (9) Musculoskeletal system (4) Dermatologicals (10) Nervous system (5) Genitourinary system and sex (11) Antiparasitic products, insecticides and (6) Systemic hormonal preparations, (12) Respiratory system excluding sex hormones and insulins (13) Sensory organs (7) Anti-infectives for systemic use (14) Various **Result of prediction** ATC classification Compound ID Subpredictor used Compound-1 3,5,9 iATC-mDO Compound-2 iATC-mDO 3,4,10,12 Compound-3 iATC-mDO Compound-4 4,5,13 iATC-mISF Compound-5 4,12 iATC-mISF

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 <u>Browse</u> button. To see the sample of batch input file, click on the button <u>Batch-example</u>. After clicking the button <u>Batch-submit</u>, 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 <u>Citation</u> 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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