

[Article Navigation](#)

iATC-mISF: a multi-label classifier for predicting the classes of anatomical therapeutic chemicals

Xiang Cheng, Shu-Guang Zhao, Xuan Xiao , Kuo-Chen Chou

Bioinformatics (2017) 33 (3): 341-346. DOI: <https://doi.org/10.1093/bioinformatics/btw644>

Published: 14 October 2016 **Article history** ▼

A correction has been published: [Bioinformatics btx387](#).

 Views ▼  Cite  Permissions  Share ▼

Abstract

Motivation: Given a compound, can we predict which anatomical therapeutic chemical (ATC) class/classes it belongs to? It is a challenging problem since the information thus obtained can be used to deduce its possible active ingredients, as well as its therapeutic, pharmacological and chemical properties. And hence the pace of drug development could be substantially expedited. But this problem is by no means an easy one. Particularly, some drugs or compounds may belong to two or more ATC classes.

Sk

Results: To address it, a multi-label classifier, called **iATC-mISF**, was developed by incorporating the information of chemical-chemical interaction, the information of

the structural similarity, and the information of the fingerprintal similarity. Rigorous cross-validations showed that the proposed predictor achieved remarkably higher prediction quality than its cohorts for the same purpose, particularly in the absolute true rate, the most important and harsh metrics for the multi-label systems.

Availability and Implementation: The web-server for **iATC-mISF** is accessible at <http://www.jci-bioinfo.cn/iATC-mISF>. Furthermore, to maximize the convenience for most experimental scientists, a step-by-step guide was provided, by which users can easily get their desired results without needing to go through the complicated mathematical equations. Their inclusion in this article is just for the integrity of the new method and stimulating more powerful methods to deal with various multi-label systems in biology.

Contact: xxiao@gordonlifescience.org

Supplementary information: [Supplementary data](#) are available at *Bioinformatics* online.

Issue Section: [Sequence analysis](#)

© The Authors 2016. Published by Oxford University Press. All rights reserved. For Permissions, please e-mail: journals.permissions@oup.com

You do not currently have access to this article.

Comments

0 Comments

Sign in

Don't already have an Oxford Academic account? [Register](#)

[Skip to Main Content](#)

Oxford Academic account

Sign in via your Institution

Email address / Username [?]

Password

Sign In

[Forgot password?](#)

[Don't have an account?](#)

[Sign in](#)

Purchase

[Subscription prices and ordering](#)

Short-term Access

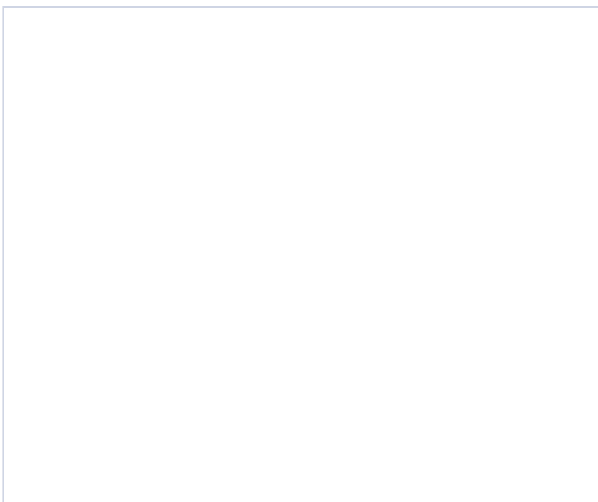
iATC-mISF: a multi-label classifier for predicting the classes of anatomical therapeutic chemicals -
24 Hours access

EUR €33.00

GBP £26.00

USD \$42.00

[Buy](#)



[Skip to Main Content](#)

[View Metrics](#)



Email alerts

[New issue alert](#)

[Advance article alerts](#)

[Article activity alert](#)

[Receive exclusive offers and updates
from Oxford Academic](#)

Related articles in

[Web of Science](#)

[Google Scholar](#)

Citing articles via

[Web of Science \(4\)](#)

[Google Scholar](#)

[CrossRef](#)

Latest | **Most Read** | **Most Cited**

Analysis and prediction of protein folding energy changes upon mutation by element specific persistent homology

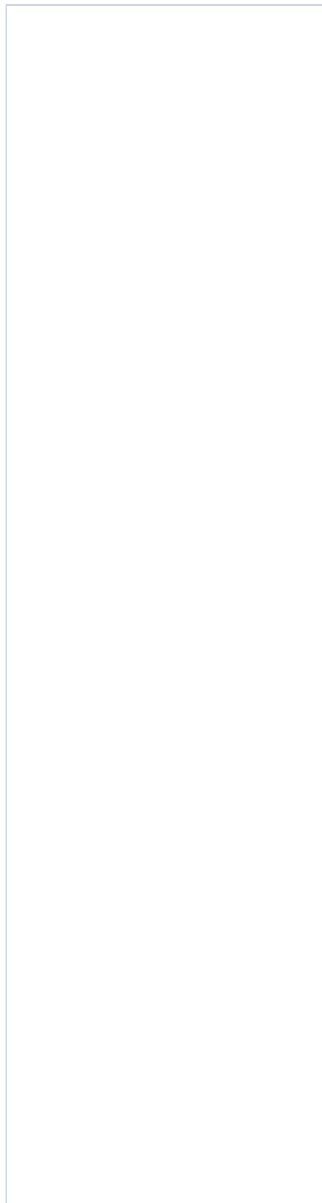
proFIA: A data preprocessing workflow for Flow Injection Analysis coupled to High-Resolution

[Skip to Main Content](#)
Mass Spectrometry

A robust DF-REML framework for variance components estimation in genetic studies

SVmine improves structural variation detection by integrative mining of predictions from multiple algorithms

Cancer Hallmarks Analytics Tool (CHAT): A text mining approach to organise and evaluate scientific literature on cancer



[About Bioinformatics](#)

[Editorial Board](#)

[Author Guidelines](#)

[Purchase](#)

[Recommend to your Library](#)

[Advertising and Corporate Services](#)

[Facebook](#)[Journals Career Network](#)[Twitter](#)

Online ISSN 1460-2059

Print ISSN 1367-4803

Copyright © 2017 Oxford University Press

[About Us](#)[Contact Us](#)[Careers](#)[Help](#)[Access & Purchase](#)[Rights & Permissions](#)[Open Access](#)**Resources**[Authors](#)[Librarians](#)[Societies](#)[Sponsors & Advertisers](#)[Press & Media](#)[Agents](#)**Connect**[Join Our Mailing List](#)[OUPblog](#)[Twitter](#)[Facebook](#)[YouTube](#)[Tumblr](#)**Explore**[Shop OUP Academic](#)[Oxford Dictionaries](#)[Oxford Index](#)[Epigeum](#)[OUP Worldwide](#)[University of Oxford](#)

Oxford University Press is a department of the University of Oxford. It furthers the University's objective of excellence in research, scholarship, and education by publishing worldwide

OXFORD
UNIVERSITY PRESS

