



# 僕と論文子 (ロボコ)

@fmkz\_

2022.04.16

## いいねしたユーザー



平口ボコ 【僕とロボコ公式】

@roboco\_hizanapa

フォロー中

平家に仕えるOMのロボコです🤖 ナッパの膝を持つ系女子👉 #お洒落さんと繋がりたい #ヒザ好きさんと繋がりたい #雰囲気嫌いじゃないよって人いいね #ヒザ #ナッパ #いいねとRTください #ファミチキください #ニベア #週刊少年ジャンプ #僕とロボコ #疑われてるけど公式 #Twitterさん公式青ペケください



にりつ

@antinomy\_chem フォローされています

フォロー中

企業研究職のぼやき。メドケム、プロセス。ドラクエウォーカー、ウマ娘トレーナー。



yamasaKit\_

@yamasaKit\_ フォローされています

フォロー中

Cykinso/DataScientist/Cheminformatics/MachineLearning/Python/BoardGame/Calligraphy/AtCoder緑色/Bioinformatics/kubernetes つぶやきは所属機関を代表するものではありません。

映画・ライブ

劇場版『名探偵コナン ハロウィン花嫁』15日公開



レンドトピック: 佐藤さん、#金曜口语ショー

からあげくん誕生日おめでとう

からあげくん36歳おめでとう♪10万円分のUOカードを抽選でプレゼント！

ソローソンによるプロモーション

ニュース・トレンド

生的発言繰り返し体

レンドトピック: 詳細公表、生徒7人

...

音楽・トレンド

ソロソンヌ

レンドトピック: #藤井風テレビ

...

国際ニュース・2022年4月14日



更新: ウクライナ周辺国に自衛隊輸送機を派遣へ 政府が調整

さらに表示

用規約 プライバシーポリシー

Cookieのポリシー アクセシビリティ 広告情報

っと見る... © 2022 Twitter, Inc.

なぜ我々は論文を読み  
続かないといけないのだろう  
か？

- 
1. 論文から得た知識は複利として効いてくるので、周りよりも毎日一報でも多く読めば多大なリターンとして返ってくる
  2. 読まないとポンコツになる
  3. 膝を鍛えろ

車両から論文を  
掲載力が低下した

---

- Livedoor readerがない
- 論文メタ情報管理サービスがない
- マネジメント業務が多い
- 印刷しないようになったのでポータビリティが低下した

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## chemoinformatics

66 ✓ ↗ ⚡ ⌂ ❤️ ⏪ ...

### TODAY

On the highest oxidation states of the actinoids in  $\text{AnO}_4$  molecules ( $\text{An} = \text{Ac - Cm}$ ): A DMRG-CASSCF study

Wiley: Journal of Computational Chemistr... / 53min

Actinoid tetroxide molecules  $\text{AnO}_4$  ( $\text{An} = \text{Ac - Cm}$ ) are investigated by the multi-configuration DMRG approach. The Natural Orbital Plots show the number of local An-5f electrons, and thereby the

[ASAP] Accurate Prediction of Aqueous Free Solvation Energies Using 3D Atomic Feature-Based Graph Neural Network with Transfer Learning

Journal of Chemical Information and Model... / 4h

Journal of Chemical Information and Modeling DOI: 10.1021/acs.jcim.2c00260

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Gain insights on the 3 pillars of observability to profile, interpret, and optimize system-wide performance

[ASAP] Applicability of the Thawed

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[ASAP] AutoDesigner, a De Novo Design Algorithm for Rapidly Exploring Large Chemical Space for Lead Optimization: Application to the Design and Synthesis of d-Amino Acid Oxidase Inhibitors

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G [ASAP] AutoDesigner, a De Novo Design Algorithm for Rapidly Exploring Large Chemical Space for Lead Optimization: Application to the Design and Synthesis of d-Amino Acid Oxidase Inhibitors  
<http://dx.doi.org/10.1021/acs.jcim.2c00072>  
#chemoinformatics #feedly |

全員が返信できます

F<sub>3</sub>C<sub>2</sub> Cl

pIC<sub>50</sub>  
Novelty  
LLE  
CNS MPO  
Exp. Clearance  
Exp. Kpuu

Journal of Chemical Information and Modeling

Zoteroに送ります



pubs.acs.org/doi/10.1021/acs.jcim.2c00072

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## AutoDesigner, a *De Novo* Design Algorithm for Rapidly Exploring Large Chemical Space for Lead Optimization: Application to the Design and Synthesis of D-Amino Acid Oxidase Inhibitors

Pieter H. Bos, Evelyne M. Houang, Fabio Ranalli, Abba E. Leffler, Nicholas A. Boyles, Volker A. Eyrich, Yuval Luria, Dana Katz, Haifeng Tang, Robert Abel, and Sathesh Bhat\*

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Publication Date: April 13, 2022 <https://doi.org/10.1021/acs.jcim.2c00072>  
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Title	Creator	Year	Date
AutoDesigner, a De Novo Design Algorithm for Rapidly Exploring Large Chemical Space for Lead Optimization: Application to the Design and Synthesis of d-Amino Acid Oxidase Inhibitors	Bos et al.	2022	4/15/...
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Selective Wee1 degradation by PROTAC degraders recruiting VHL and CRL E3 ubiquitin ligases	Aublett...	2022	3/7/2...
Discovery of 4-phenylindolines containing a (5-cyanopyridin-3-yl)methoxy moiety as potent kinase inhibitors	Meng et...	2022	3/7/2...
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Targeting Epigenetic Modulators Using PROTAC Degraders: Current Status and Future Perspectives	Webb et...	2022	3/7/2...
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csdr, an R package for differential co-expression analysis	Petterse...	2022	2/25/...
Accelerated Ligand–Mapping Molecular Dynamics Simulations for the Detection of Receptor–Ligand Interactions	Tze-Ya...	2022	2/19/...
Development of Selective Phosphatidylinositol 5-Phosphate 4-Kinase γ Inhibitors with Antitumor Activity			2/14/...
Yuel: Improving the Generalizability of Structure-Free Compound–Protein Interaction Prediction	Wang a...	2022	2/14/...
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Item Type Journal Article

Title AutoDesigner, a De Novo Design Algorithm for Rapidly Exploring Large Chemical Space for Lead Optimization: Application to the Design and Synthesis of d-Amino Acid Oxidase Inhibitors

Author Bos, Pieter H.

Author Houang, Evelyne M.

Author Ranalli, Fabio

Author Leffler, Abba E.

Author Boyles, Nicholas A.

6 more...

Abstract The lead optimization stage of a drug discovery program generally involves the design, synthesis, and assaying of hundreds to thousands of compounds. The design phase is usually carried out via traditional medicinal chemistry approaches and/or structure-based drug design (SBDD) when suitable structural information is available. Two of the major limitations of this approach are (1) difficulty in rapidly designing potent molecules that adhere to myriad project criteria, or the multiparameter optimization (MPO) problem, and (2) the relatively small number of molecules explored compared to the vast size of chemical space. To address these limitations, we have developed AutoDesigner, a de novo design algorithm. AutoDesigner employs a cloud-native, multistage search algorithm to carry out successive rounds of chemical space exploration and filtering. Millions to billions of virtual molecules are explored and optimized while adhering to a customizable set of project criteria such as physicochemical properties and potency. Additionally, the algorithm only requires a single ligand with measurable affinity and a putative binding model as a starting point, making it amenable to the early stages of an SBDD project where limited data are available. To assess the effectiveness of AutoDesigner, we

Tweetの「いいね」はんとに読んでみの？



Sara Gómezさんと他15人があなたのツイートをいいねしました

Is conformation relevant for QSAR purposes? 2D Chemical representation  
in a 3D-QSAR perspective [onlinelibrary.wiley.com/doi/10.1002/jc...](http://onlinelibrary.wiley.com/doi/10.1002/jc...)  
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# Feedly

---

- カテゴリ4つくらい
- Feedの制限きつい
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- 最低毎週捌けばいける

# Zotero

- オープンソースの引用管理ソフトウェア
- 100Mまでの無料ストレージ
  - 速攻使い果たす
- Dropboxでシェアすればいいけど
  - 会社とはシェアできない
- タグ管理とかめんどい

皆さんどんな感じで  
論文掲いてます？

---

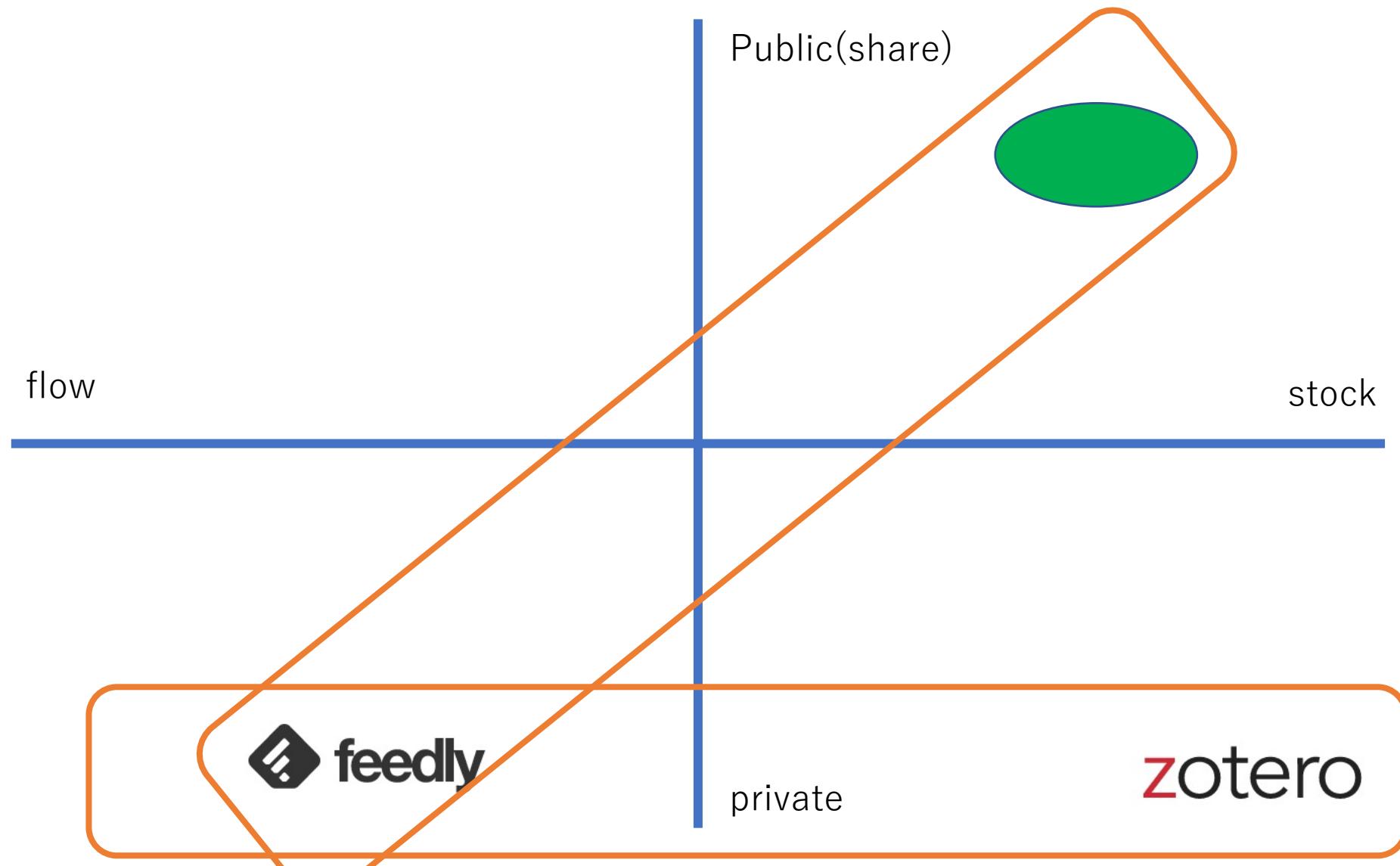
# 論文共有は？

- Teamsにチャンネル作って気が向いたときに投稿している
  - 読んだら感想を書いたりしている
  - ごく限られた人が投稿している状態
  - どのくらいの人が論文読んでるのかわからんけど、チーム内格差は絶対あると思う

# 論文共有

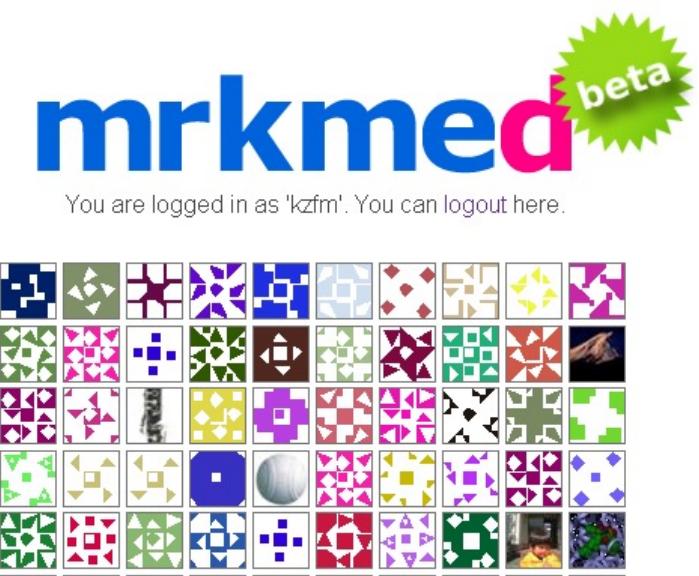
- 論文にタグとかコメント入れて共有したい
- ささっと検索できて、他の人がどういう感想もったのか知りたい

思うに



# Background

- Scientists need to manage more references than ever.
  - There are some new technologies in the internet services
    - RSS
    - Pubmed E-Utils
    - Electronic Publishing (pdf)
- Now, we can check many journals on our computers
  - (over 5000pubmed-articles/month)
- References list filtered by laboratory group are useful
  - Saving of some time
  - Useful for newbies
  - Increase the opportunity of feedback
    - you can tell your colleagues what reference you read
    - and you can tell what you don't know about



# Purpose

---

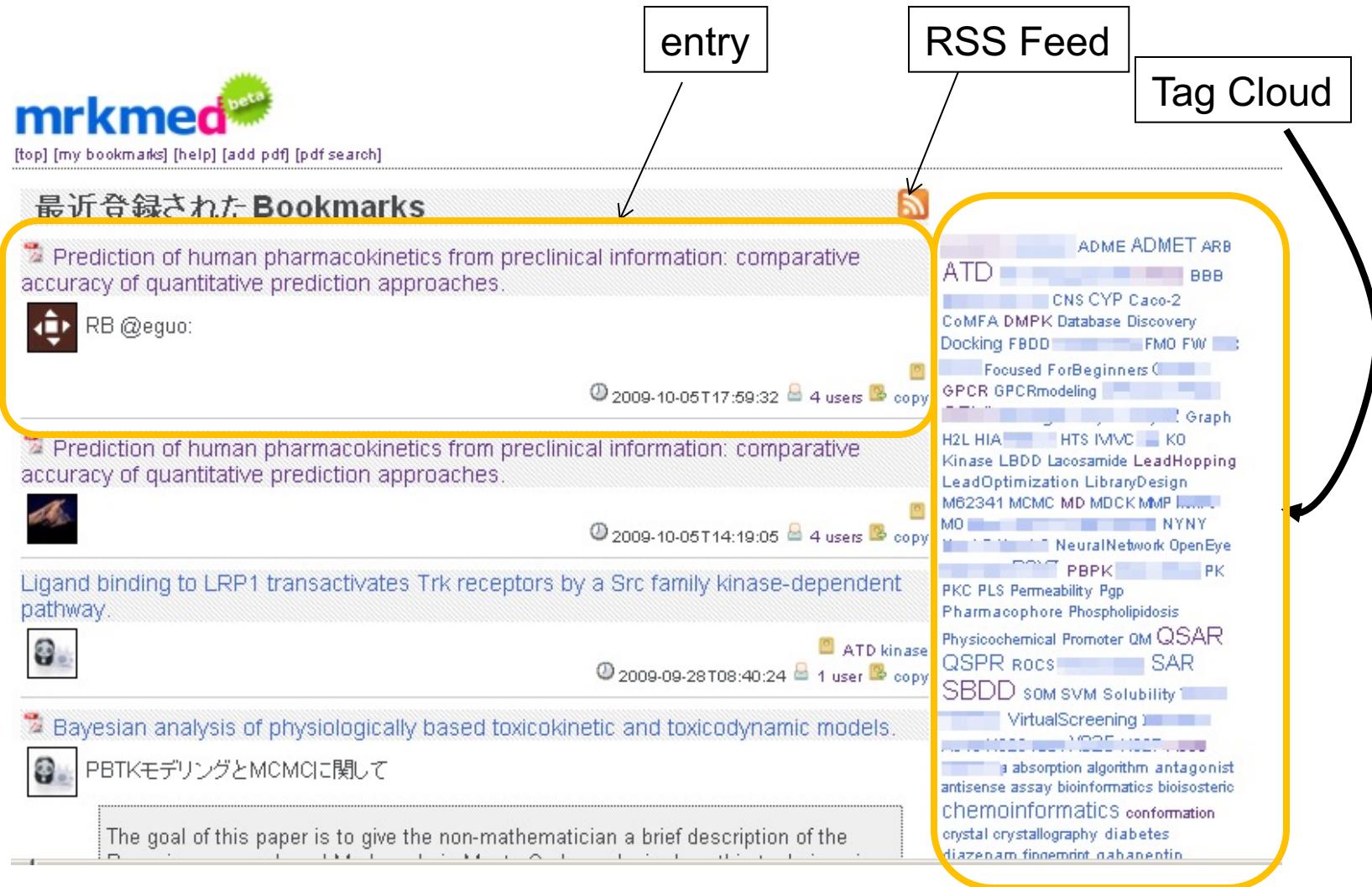
- Mrkmed enable scientists
  - to manage information of online journals.
  - to share their opinion
  - to categorize references flexibly
  - to reuse the information

# Architecture

- a web application framework
  - Catalyst
  - DBMS: SQLite
- Full-text Search System
  - Hyper Estraier
- javascript graph library
  - flot



# Result



# Who read the reference ?

Prediction of human pharmacokinetics from preclinical information: comparative accuracy of quantitative prediction approaches.



① 2009-10-05T17:59:32 4 users copy

- User can read the opinion of other researchers
- Connect people through references

click

The screenshot shows a web browser window with a yellow border. The main content is an article titled "Prediction of human pharmacokinetics from preclinical information: comparative accuracy of quantitative prediction approaches." Below the article, there is a comment section. A red circle highlights the "4 users" link in the timestamp area above the comments. A red arrow points from the word "click" to this highlighted link. Another red circle highlights the first comment in the list, which is also circled in red. The comment text is in Japanese and discusses the use of various models to predict human pharmacokinetics based on preclinical data. The timestamp for this comment is 2009-10-05T17:59:32. The URL in the address bar is http://tgbp.mochida.co.jp.

この論文に対するコメント一覧

RB @eguo:  
モデル動物でのパラメータを利用して、ヒトの $t_{1/2}$ と $CL(po)$ を予測する。  
 $t_{1/2} = \ln 2 \times V_{dss} / CL = \ln 2 \times MRT$   
 $CL(po) = CL/F$

And one more user

# Who use the tag ?

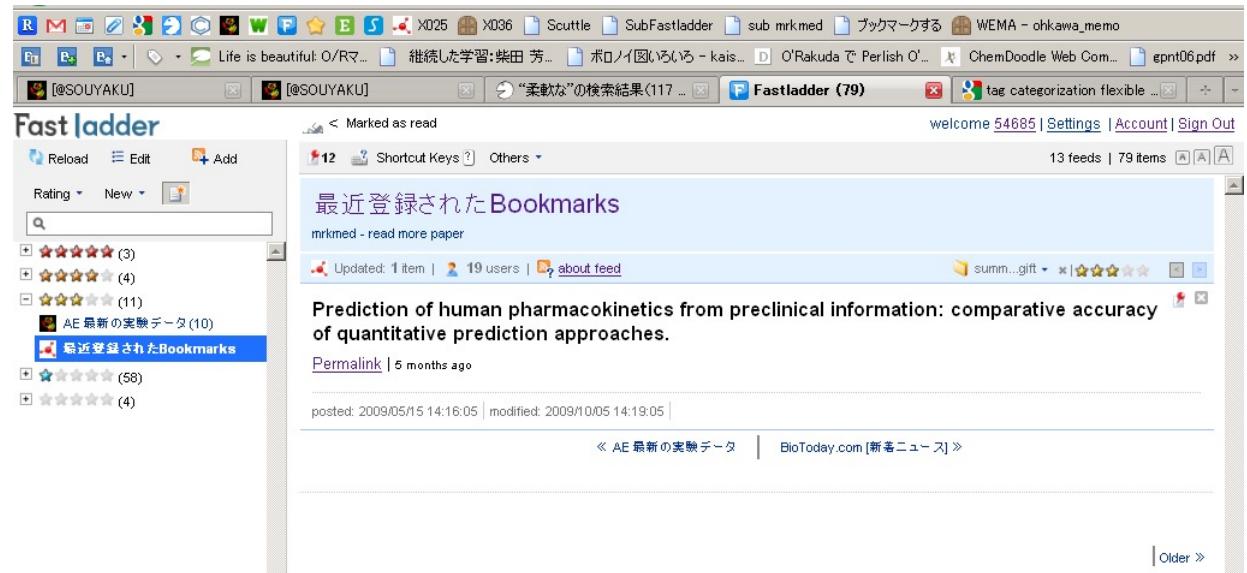
- Clicking the tag shows user's bookmarks which has the same tag
- Tags are more flexible in creating categorization than having tree hierarchy



# RSS

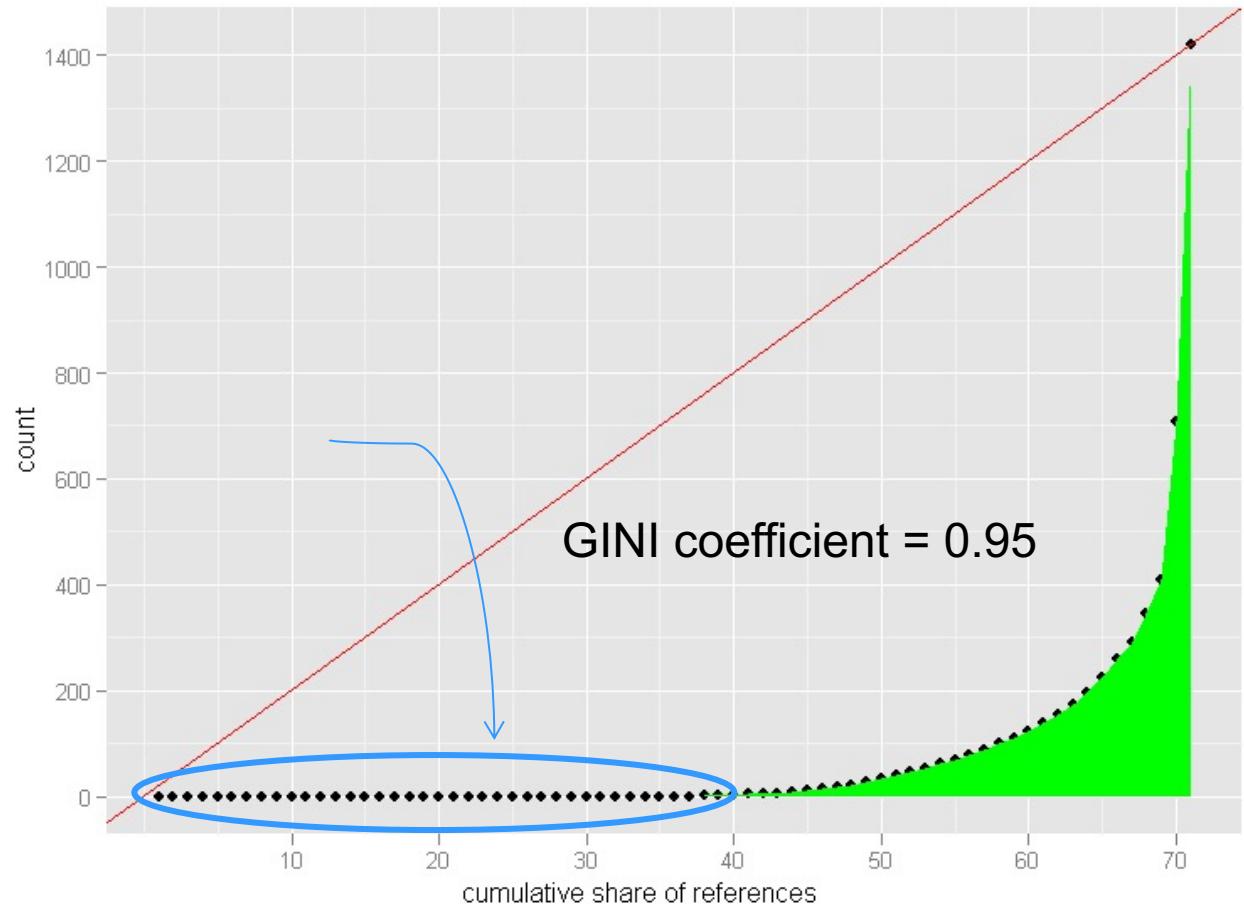


- User can keep track of new entries through RSS Reader
  - All new bookmarks in Mrkmed
  - new bookmarks posted by [user]
  - New bookmarks include [tag]



# Activities

- Mean: 20
- GINI: 0.95
- half people only took their account (no post)
- 5 user submitted about 80 % of references



<https://github.com/Mishima-syk/SOSOG>

README.md

[Edit](#)

**SOSOG**

Reference information sharing system

Standing on the shoulders of Giants (SOSOG).

**Install**

```
conda install -c anaconda flask
conda install -c conda-forge flask-debugtoolbar
conda install -c conda-forge flask-sqlalchemy
# for tests
conda install -c anaconda nose
```

**Create database**

```
$ python
>>> from app import db
>>> db.create_all()
```

**Run app**

Publish your first package

**Languages**

JavaScript 94.6%   Python 4.5%  
HTML 0.9%

# 巨人の肩に乗ったところ で力尽きた

---

- ニーズありそう？
- そのあたりどうなん？