웹기반의 단일세포 RNA-seq 데이터 자동분석 서비스 SCODA™를 이용한 종양/조직 미세환경 연구

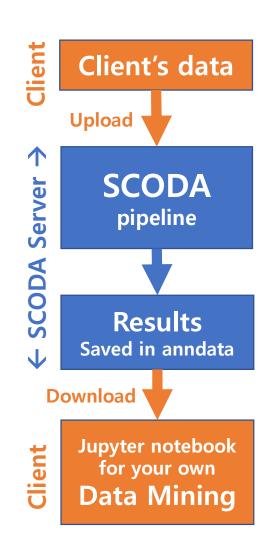
윤석현

㈜ 엠엘비아이랩 (MLBI Lab) 단국대학교 전자전기공학부 단국대학교 대학원 인공지능융합학과

SCODA?

- Web-based, Fully-automated, all-in-one computing service for Single-Cell (transcript)Omics Data Analysis (single-cell RNA-seq)
- ☐ It is useful for
 - In-vivo tissue/tumor micro-environment (TME) study.
 - O Immune cell profiling in many diseases, e.g., autoimmune disease & cancer

How SCODA works?



(1) Simply upload your data

- 1. Compressed 10x mtx files + optional meta_data.csv
- 2. Compressed CSV file + optional meta_data.csv
- 3. Compressed h5ad file (including meta data in obs field)

(2) Automated pipeline analyzes your data

- 1. Celltype annotation (HiCAT, MIT license)
- 2. DEG & GSA/GSEA (GSEApy, MIT license)
- 3. Cell-cell interaction (CellPhoneDB, MIT license)
- 4. Tumor cell identification (InferCNV, BSD-3c + icnv_addon)
- **❖** We use proven & standardized analysis tools
- **❖** The pipeline can be tailored with optional settings

(3) Once it is done, you can download the result

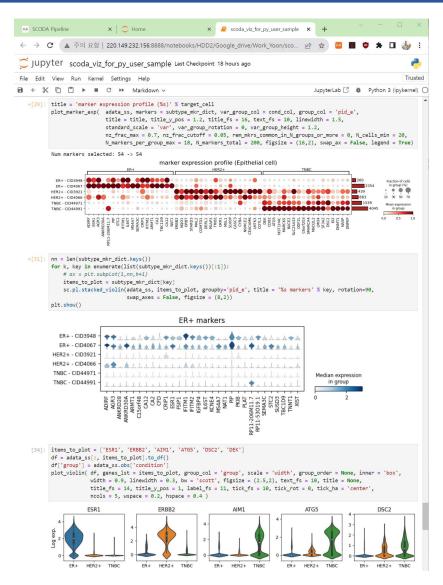
- 1. Saved in Anndata formatted h5ad file (tar.gz compressed)
- 2. It contains all the analysis results and the count matrix itself

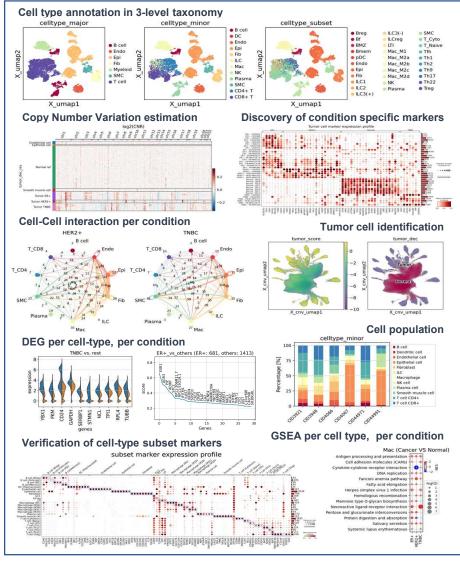
(4) Explore the results by yourself on your web browser

- 1. We provide "jupyter notebook" with example codes
- 2. You can freely use SCODA-viz & SCANpy (free open SW)
- 3. With a little bit of programming, you can get deeper insight into the single-cell RNA-seq data you uploaded
- 4. We offer free workshop for data mining (upon request)

3

Visualization & data mining





Using SCODA

- □ SCODA homepage: https://mlbi-lab.net
- ☐ MLBI lab company homepage: https://mlbi-lab.com

Why SCODA?

Bio/Medical background



SCODA

with SCODA-viz tool

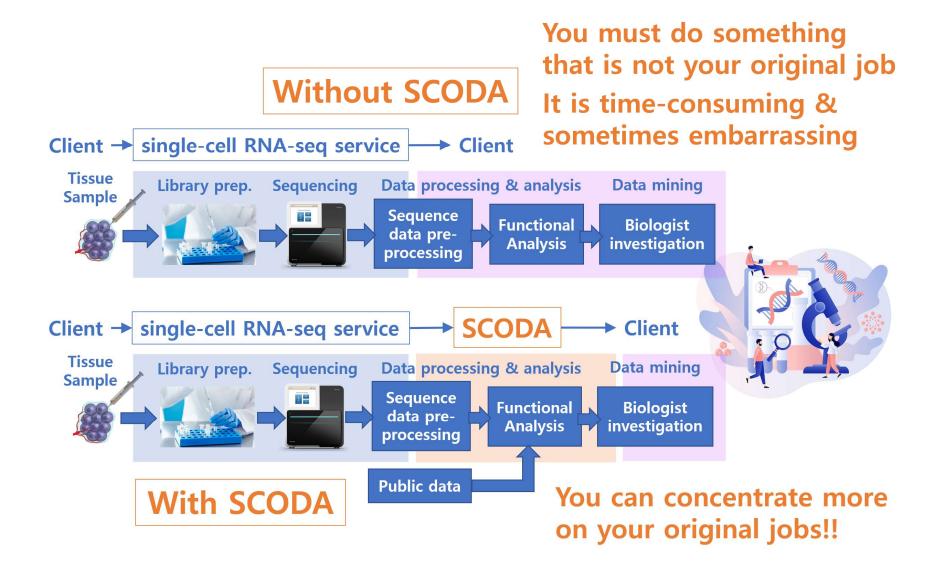


Little bit of programming skill (Free Training workshop available)



Single-cell RNA-seq 데이터 분석 전문가

Why SCODA?



Related papers

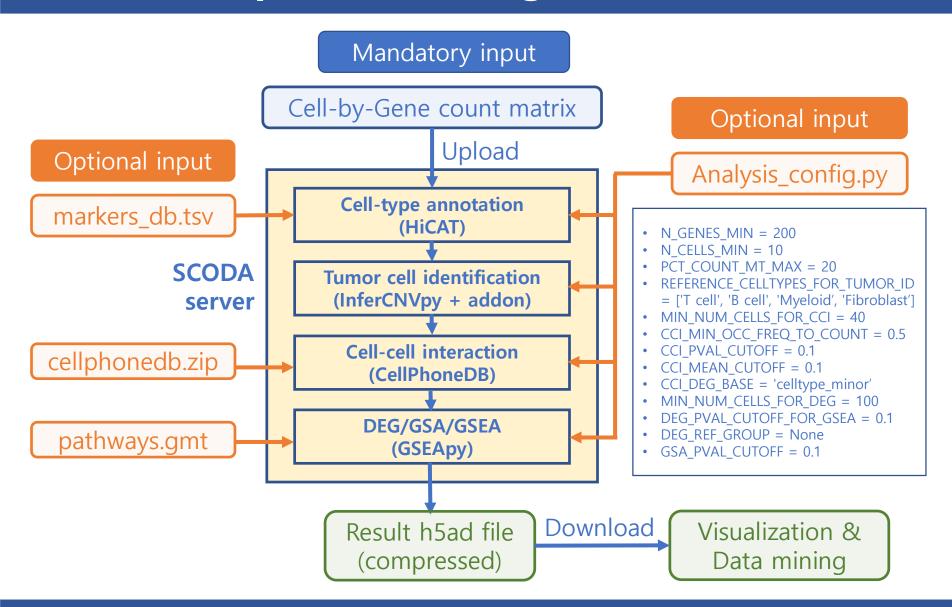
□ HiCAT

O Hierarchical cell-type identifier accurately distinguishes immune-cell subtypes enabling precise profiling of tissue microenvironment with single-cell RNA-sequencing, **Briefings in bioinformatics**, **March 2023**

☐ Studies using SCODA

- Colon-Targeted eNAMPT-Specific Peptide Systems for Treatment of DSS-Induced Acute and Chronic Colitis in Mouse, Antioxidants, Nov. 2022
- O Integrative analysis of ulcerative colitis progression using singlecell RNA-seq and microbiome, **Communications Biology, in revision**
- A Retrospective View on Triple Negative Breast Cancer Microenvironment: Novel Markers, Interactions, and Mechanisms of Tumor-Associated Components using public Single-cell RNA Seq Datasets, Cancers, submitted

SCODA Optional configuration



SCODA?

□ SCODA is useful for

- In-vivo tissue/tumor micro-environment (TME) study.
- Immune cell profiling in many diseases, e.g., autoimmune disease & cancer
- O Discovery of diagnostic/prognostic markers
- O Discovery of druggable targets and its biological mechanism around pathological tissue
- Exploring drug response and mechanism of action

☐ But not suitable yet for

- Studies with cell line
- Differentiation study

Summary

- **□** SCODA utilizes proven open-source software
 - O HiCAT (MIT license) for cell type annotation
 - O CellPhoneDB (MIT license) for inferring cell-cell interaction
 - InferCNVpy (BSC-3clause) for CNV estimation
 - O GSEApy (BSC-3clause) for gene set enrichment analysis
- □ SCODA-viz package and example jupyter notebook freely available for visualization and data mining
 - With a little bit of programming skill, you can create any kind of plots you want. (Free training workshop available upon request)
- ☐ It accelerate your research with single-cell RNA-seq experiment, saving your time and the cost.
 - Use SCODA first to get insight into the tissue of your interest.
 - Then, plan biological experiment to verify your hypothesis.

Service & Cost

Pricing

- 유효 셀 당 ₩20 (unassigned 포함, 2024년 6월 30일 까지)
- 자동 결제 시스템 구축 중 (3월 중 오픈 예정)

□ Our primary concern is client's satisfaction

- 동일 데이터에 대해 (optional configuration 변경하여) 추가 결재 없이 재분석 가능 (6개월 이내 8회)
- 3시간 무료 training workshop (주피터 노트북 사용법, 데이터 시각화 관련 내용)

□ Suggestion & request

- SCODA 데모 페이지에서 먼저 보유하고 계신 데이터를 테스트 해보신 후 (대체적으로 예상되는 결과를 미리 보시고) Full Service 요청하면 좋을 듯 합니다.
- SCODA 데모 분석 결과에 대한 문의/의견/Bug report 등 환영 합니다.
- 가능한 한 의견들 반영하여 당분간 지속적으로 업그레이드 할 예정입니다.

■ Any inquiries?

- **O** 070-7766-5841
- inquiry@mlbi-lab.com

Thank you

Input data formatting (1) 10x_mtx

1. 압축된 예제 데이터셋을 알집으로 열어 보면

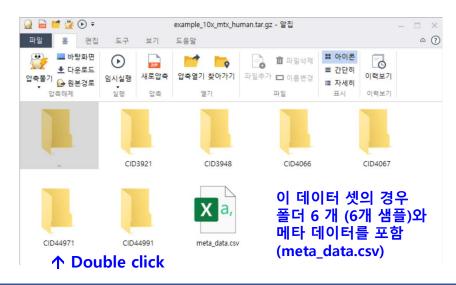


3. 각 데이터 폴더를 더블 클릭해서 열면

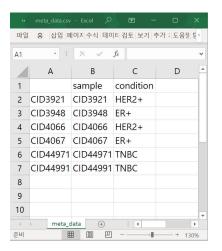


CellRanger로 생성된 3개 파일을 포함

2. 메인 폴더를 더블 클릭해서 열면



4. meta_data.csv 파일을 엑셀로 열어 보면



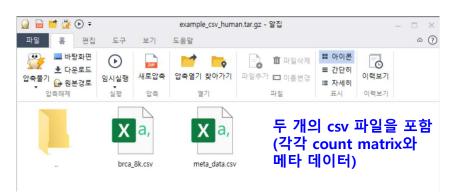
- 1열: 인덱스 열 2열: sample (name) 3열: condition
- 인덱스 열의 각 인덱스는 폴 더 명과 일치해야 함.
- Sample name과 인덱스가 동일할 필요는 없음.
- Condition 열의 조건들을 대상으로 DEG, GSEA, cellcell interaction 비교가 수 행됨

Input data formatting (2) csv format

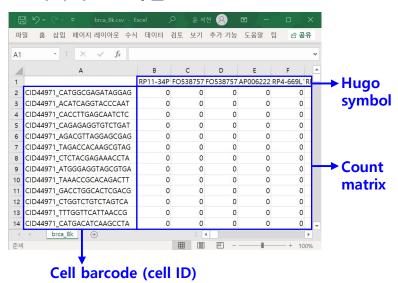
1. 압축된 예제 데이터셋을 알집으로 열어 보면



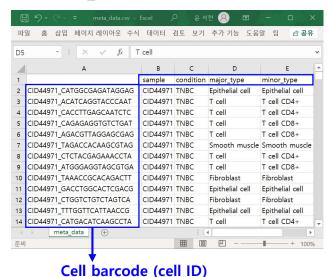
2. 메인 폴더를 더블 클릭해서 열면



3. 데이터 csv 파일



4. meta data.csv 파일



GSEA, cell-cell

1열: 인덱스 열

3열: condition

4열~: optional items

• Count 데이터 파일

과 메타 데이터 파일

의 인덱스 열은 일치

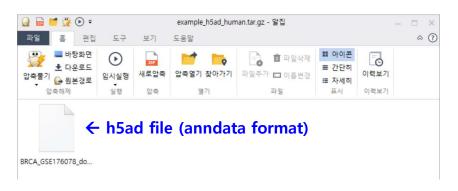
2열: sample

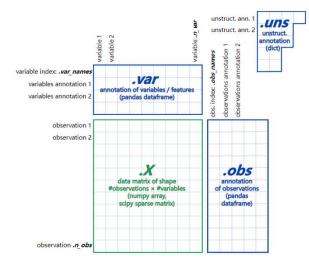
해야 함.

• Condition 열의 조건 들을 대상으로 DEG. interaction 비교가 수행됨

Input data formatting (3) h5ad format

1. 압축된 예제 데이터셋을 알집으로 열어 보면





https://anndata.readthedocs.io/en/latest/

2. h5ad file contents

```
adata_t = sc.read_h5ad(file_h5ad)
adata_t

AnnData object with n_obs × n_vars = 12000 × 29733
   obs: 'Patient', 'Percent_mito', 'nCount_RNA', 'nFeature_RNA', 'Celltype_Major', 'Celltype_Minor', 'Celltype_Subset', 'subtype', 'gene_module', 'Calls', 'normal_cell_call', 'CNA_value', 'sample', 'condition'
   var: 'gene_ids'
```

- AnnData contains "sample" and "condition" columns to run DEG/GSEA. DEG/GSEA will not be performed if the obs field does not contain both "sample" and "condition" column.
- If the "sample" column exists in the obs field, cell-cell interaction will be performed per-sample the same as in the above.