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## Name

spectral-analyzer

## Overview

吸収スペクトルを様々な手法で解析するツールです。

# Requirement

- Docker Desktop (Windows10, macOS)
- Windows10の場合 https://qiita.com/zaki-lknr/items/db99909ba1eb27803456
- macOSの場合
  https://docs.docker.jp/docker-for-mac/install.html

## Install

- \$ cd spectral-analyzer
- \$ docker-compose up -d --build

## Usage

http://127.0.0.1:8000/

# Description

## Preprocessing

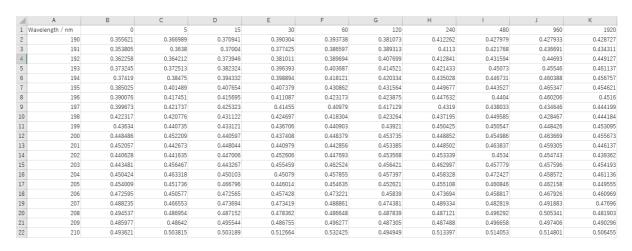
- 吸収スペクトルのバッファー補正
- 吸収スペクトルの任意の波長のゼロ点補正
- アップロードデータ例 (csv形式)

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|    | A               | В        | С        | D        | E        | F        | G        | Н        | 1        | J        | K        | L,       |
|----|-----------------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| 1  | Wavelength / nm | buffer   | 0        | 5        | 15       | 30       | 60       | 120      | 240      | 480      | 960      | 1920     |
| 2  | 190             | 1.046234 | 1.414688 | 1.425613 | 1.429367 | 1.449005 | 1.452179 | 1.438812 | 1.47023  | 1.485291 | 1.484497 | 1.483887 |
| 3  | 191             | 1.12204  | 1.488678 | 1.49823  | 1.504272 | 1.511932 | 1.520844 | 1.522858 | 1.545074 | 1.554886 | 1.569061 | 1.565277 |
| 4  | 192             | 1.26265  | 1.637741 | 1.639252 | 1.648788 | 1.656128 | 1.664551 | 1.681854 | 1.687225 | 1.705322 | 1.71991  | 1.720703 |
| 5  | 193             | 1.390762 | 1.77684  | 1.775665 | 1.785278 | 1.799622 | 1.806656 | 1.816788 | 1.823929 | 1.85257  | 1.856552 | 1.860825 |
| 6  | 194             | 1.510468 | 1.897491 | 1.907608 | 1.916992 | 1.921829 | 1.940796 | 1.942307 | 1.95723  | 1.968277 | 1.981186 | 1.976151 |
| 7  | 195             | 1.620224 | 2.018082 | 2.034103 | 2.04007  | 2.04007  | 2.063293 | 2.063293 | 2.081635 | 2.074829 | 2.095901 | 2.083771 |
| 8  | 196             | 1.725677 | 2.128586 | 2.155518 | 2.153564 | 2.149231 | 2.161057 | 2.161057 | 2.185043 | 2.177155 | 2.196213 | 2.186203 |
| 9  | 197             | 1.822495 | 2.235001 | 2.256622 | 2.26001  | 2.249512 | 2.244492 | 2.251129 | 2.266129 | 2.271606 | 2.267471 | 2.27562  |
| 10 | 198             | 1.905243 | 2.340393 | 2.338409 | 2.348557 | 2.342407 | 2.335754 | 2.340012 | 2.354172 | 2.365906 | 2.34404  | 2.358353 |
| 11 | 199             | 1.973846 | 2.423019 | 2.426971 | 2.419159 | 2.423019 | 2.426956 | 2.424561 | 2.436005 | 2.435471 | 2.432602 | 2.435867 |
| 12 | 200             | 2.037308 | 2.498627 | 2.501907 | 2.490097 | 2.487183 | 2.497894 | 2.502548 | 2.497894 | 2.503372 | 2.511307 | 2.501907 |
| 13 | 201             | 2.095764 | 2.560654 | 2.550827 | 2.556    | 2.54921  | 2.550827 | 2.560654 | 2.556    | 2.570679 | 2.565399 | 2.550827 |
| 14 | 202             | 2.149765 | 2.603226 | 2.60379  | 2.608963 | 2.614838 | 2.609665 | 2.614838 | 2.614838 | 2.614243 | 2.614838 | 2.598053 |
| 15 | 203             | 2.205948 | 2.662262 | 2.674805 | 2.661407 | 2.673874 | 2.680679 | 2.673874 | 2.680679 | 2.674805 | 2.673874 | 2.669067 |
| 16 | 204             | 2.258362 | 2.721619 | 2.73407  | 2.720657 | 2.721619 | 2.728424 | 2.727264 | 2.728424 | 2.741867 | 2.727264 | 2.728424 |
| 17 | 205             | 2.301987 | 2.768829 | 2.766113 | 2.780975 | 2.760468 | 2.768829 | 2.766113 | 2.768829 | 2.773911 | 2.774475 | 2.760468 |
| 18 | 206             | 2.338577 | 2.824005 | 2.801544 | 2.823334 | 2.808472 | 2.824005 | 2.808472 | 2.824005 | 2.808472 | 2.816833 | 2.808472 |
| 19 | 207             | 2.375946 | 2.877014 | 2.854889 | 2.861832 | 2.861832 | 2.877014 | 2.861832 | 2.877014 | 2.869843 | 2.878159 | 2.861832 |
| 20 | 208             | 2.409363 | 2.916733 | 2.908707 | 2.908707 | 2.900192 | 2.908218 | 2.908707 | 2.908218 | 2.916733 | 2.925034 | 2.900192 |
| 21 | 209             | 2.434845 | 2.933655 | 2.933655 | 2.942581 | 2.934067 | 2.943329 | 2.933655 | 2.934067 | 2.942581 | 2.942581 | 2.934067 |
| 22 | 210             | 2.451462 | 2.957916 | 2.967667 | 2.966843 | 2.976593 | 2.996094 | 2.957916 | 2.976593 | 2.976593 | 2.976593 | 2.966843 |
| 23 | 211             | 2.457199 | 3.002792 | 3.012543 | 2.992386 | 3.002136 | 3.002457 | 2.982483 | 3.012543 | 3.023575 | 3.012543 | 2.982483 |
| 24 | 212             | 2.450562 | 3.026306 | 3.015884 | 3.038605 | 3.015884 | 3.005997 | 3.005997 | 3.015884 | 3.037338 | 3.015884 | 2.995575 |

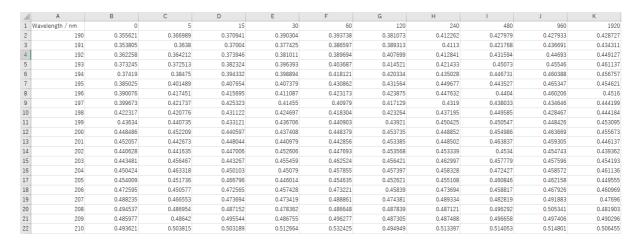
#### Difference

- 吸収スペクトルの差吸収スペクトルの算出
- アップロードデータ例 (csv形式)



#### **Derivatives**

- 吸収スペクトルの微分変換
- 微分スペクトルのスムージング
- アップロードデータ例 (csv形式)



#### ICA (Independent Component Analysis)

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- スペクトルの独立成分分析
- アップロードデータ例 (csv形式)

|    | A               | В        | С        | D        | E        | F        | G        | Н        | T I      | J        | K        |
|----|-----------------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| 1  | Wavelength / nm | 0        | 5        | 15       | 30       | 60       | 120      | 240      | 480      | 960      | 1920     |
| 2  | 190             | 0.355621 | 0.366989 | 0.370941 | 0.390304 | 0.393738 | 0.381073 | 0.412262 | 0.427979 | 0.427933 | 0.428727 |
| 3  | 191             | 0.353805 | 0.3638   | 0.37004  | 0.377425 | 0.386597 | 0.389313 | 0.4113   | 0.421768 | 0.436691 | 0.434311 |
| 4  | 192             | 0.362258 | 0.364212 | 0.373946 | 0.381011 | 0.389694 | 0.407699 | 0.412841 | 0.431594 | 0.44693  | 0.449127 |
| 5  | 193             | 0.373245 | 0.372513 | 0.382324 | 0.396393 | 0.403687 | 0.414521 | 0.421433 | 0.45073  | 0.45546  | 0.461137 |
| 6  | 194             | 0.37419  | 0.38475  | 0.394332 | 0.398894 | 0.418121 | 0.420334 | 0.435028 | 0.446731 | 0.460388 | 0.456757 |
| 7  | 195             | 0.385025 | 0.401489 | 0.407654 | 0.407379 | 0.430862 | 0.431564 | 0.449677 | 0.443527 | 0.465347 | 0.454621 |
| 8  | 196             | 0.390076 | 0.417451 | 0.415695 | 0.411087 | 0.423173 | 0.423875 | 0.447632 | 0.4404   | 0.460206 | 0.4516   |
| 9  | 197             | 0.399673 | 0.421737 | 0.425323 | 0.41455  | 0.40979  | 0.417129 | 0.4319   | 0.438033 | 0.434646 | 0.444199 |
| 10 | 198             | 0.422317 | 0.420776 | 0.431122 | 0.424697 | 0.418304 | 0.423264 | 0.437195 | 0.449585 | 0.428467 | 0.444184 |
| 11 | 199             | 0.43634  | 0.440735 | 0.433121 | 0.436706 | 0.440903 | 0.43921  | 0.450425 | 0.450547 | 0.448426 | 0.453095 |
| 12 | 200             | 0.448486 | 0.452209 | 0.440597 | 0.437408 | 0.448379 | 0.453735 | 0.448852 | 0.454986 | 0.463669 | 0.455673 |
| 13 | 201             | 0.452057 | 0.442673 | 0.448044 | 0.440979 | 0.442856 | 0.453385 | 0.448502 | 0.463837 | 0.459305 | 0.446137 |
| 14 | 202             | 0.440628 | 0.441635 | 0.447006 | 0.452606 | 0.447693 | 0.453568 | 0.453339 | 0.4534   | 0.454743 | 0.439362 |
| 15 | 203             | 0.443481 | 0.456467 | 0.443267 | 0.455459 | 0.462524 | 0.456421 | 0.462997 | 0.457779 | 0.457596 | 0.454193 |
| 16 | 204             | 0.450424 | 0.463318 | 0.450103 | 0.45079  | 0.457855 | 0.457397 | 0.458328 | 0.472427 | 0.458572 | 0.461136 |
| 17 | 205             | 0.454009 | 0.451736 | 0.466796 | 0.446014 | 0.454635 | 0.452621 | 0.455108 | 0.460846 | 0.462158 | 0.449555 |
| 18 | 206             | 0.472595 | 0.450577 | 0.472565 | 0.457428 | 0.473221 | 0.45839  | 0.473694 | 0.458817 | 0.467926 | 0.460969 |
| 19 | 207             | 0.488235 | 0.466553 | 0.473694 | 0.473419 | 0.488861 | 0.474381 | 0.489334 | 0.482819 | 0.491883 | 0.47696  |
| 20 | 208             | 0.494537 | 0.486954 | 0.487152 | 0.478362 | 0.486648 | 0.487839 | 0.487121 | 0.496292 | 0.505341 | 0.481903 |
| 21 | 209             | 0.485977 | 0.48642  | 0.495544 | 0.486755 | 0.496277 | 0.487305 | 0.487488 | 0.496658 | 0.497406 | 0.490296 |
| 22 | 210             | 0.493621 | 0.503815 | 0.503189 | 0.512664 | 0.532425 | 0.494949 | 0.513397 | 0.514053 | 0.514801 | 0.506455 |