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

dockerを起動後 http://127.0.0.1:8000/ をクリック

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)

	A	B	C	D	E	F	G	H	I	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)

	A	B	C	D	E	F	G	H	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

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)

	A	B	C	D	E	F	G	H	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

ICA (Independent Component Analysis)

- 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	B	C	D	E	F	G	H	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