

S3 storage

Aws s3 storage service is used to store all uploaded and result files.

Account: adam.a@feynmanlabs.com

MongoDB

We are using mongodb as database service, it is hosted in a container in DGX

Url

cellvera.dyndns.org:5099

One Signal

One signal notifications service is used to send notifications from backend to frontend.

Frontend

Provides the UI that users can interact with our platform by. Developed using react and hosted on the dgx. It only interacts with the backend.

Git repo

<http://cellvera.dyndns.org:6969/root/Frontend>

Url

<https://app.prepaire.com:5067/>

Dependencies

Backend - one signal

Backend

Provides all the endpoints that frontend interacts with (endpoints to all modules of prepare, for example frontend doesn't call drug-drug interaction directly, it calls the backend and backend calls drug-drug interaction). Developed using python and hosted on the dgx.

Git repo

<http://cellvera.dyndns.org:6969/root/Backend>

Url

cellvera.dyndns.org:5098

Dependencies

Mongodb - one signal - s3

Drugs

Part of the backend, drugs are imported from drugbank and other databases, stored in mongodb.

Input

Name of the drug or part of it

Output

Drug details

Dependencies

Mongodb - backend

Natural products

Part of the backend, natural products are imported from ISDB and other databases, stored in mongodb.

Input

Name of the natural product or part of it

Output

Natural product details

Dependencies

Mongodb - backend

Xdl

Part of the backend, xdl records are added to mongodb.

Input

Drug name

Output

Xdl instructions

Dependencies

Mongodb - backend

Proteins

Part of the backend, proteins are imported from uniprot and other databases, stored in mongodb.

Input

name of the protein or part of it and name of the organism or part of it

Output

Protein details

Dependencies

Mongodb - backend

Map

Part of the backend, list countries, cities, diseases, events, news are loaded into mongodb

Input

Name of the disease or part of it

Output

List of diseases and events - disease details and statistics

Dependencies

Mongodb - backend

Map update

Currently it is a part of the backend, triggered by a cron job twice a day to update diseases and news data.

Git repo

<http://cellvera.dyndns.org:6969/habib/gra-map-update>

Dependencies

Mongodb - backend

<https://raw.githubusercontent.com/owid/covid-19-data/master/public/data/owid-covid-data.csv>
(covid)

<https://raw.githubusercontent.com/owid/monkeypox/main/owid-monkeypox-data.csv>
(monkeypox)

<https://newsdata.io/api> (news)

Warfarin dose

Currently it is a part of the backend, it calculates dose of warfarin based on personal attributes

Git repo

<http://cellvera.dyndns.org:6969/fouad.azar/warfarin-dosing>

Input

Height, weight, age, smoker, race, INR, DVT_PE, dna sequence

Output

Warfarin dose

Maintenance dose

Currently it is a part of the backend, it calculates the maintenance dose of multiple drugs based on personal attributes.

Input

Drug, weight, height, geo, age, gender

Output

Maintenance dose

Chat

Chatbot trained on some documents

Input

Any question or query

Output

Answer to the question

Dependencies

Backend

<https://chatthing.ai/app/bots> (Preoaire's Concierge bot)

Bio chat

Chatbot trained on some documents

Input

Any question or query

Output

Answer to the question

Dependencies

Backend

<https://chatthing.ai/app/bots> (BioBot bot)

Forecast

<https://partslab.sanger.ac.uk/FORECasT> an instance of it is deployed on the dgx.

Url

cellvera.dyndns.org:5095

Input

Sequence & pam index

Output

Some drawing

Codon optimization

Automates codon optimization of a gene to the species of your choice

<https://www.idtdna.com/CodonOpt>

Dependencies

Idtdna api

Oligo analyzer

Identifies oligonucleotide properties, including melting temperature, hairpins, dimers and mismatches <https://www.idtdna.com/calc/analyzer>

Dependencies

Idtdna api

gRNA

Select from predesigned Alt-R CRISPR-Cas9 guide RNAs (gRNAs, such as crRNA and sgRNA) targeting human, mouse, rat, zebrafish, or C. elegans gene targets.

Generate CRISPR-Cas9 guide RNAs (gRNAs, such as crRNA and sgRNA) targeting any sequence from any species. Currently, analysis of off-target effects against human, mouse, rat, zebrafish, or C. elegans genes are available.

Assess on- and off-targeting potential of protospacer designs of your own or from publications before ordering guide RNAs (gRNAs, such as crRNA and sgRNA) that are synthesized using our Alt-R gRNA modifications.

https://www.idtdna.com/site/order/designtool/index/CRISPR_PREDESIGN

Dependencies

Idtdna api

Genes

Currently it is a part of the backend, you can search for genes by disease and get sequences of the genes by ensabl id.

Input

Disease name

Output

Related genes + sequence

Dependencies

<http://mygeneset.info>

<https://rest.ensembl.org>

Search engine

Currently it is a part of the backend.

- Related publications from pubmed and xrxiv to the drugs, natural products, and proteins are uploaded into mongodb.
- Mondo graph integrated with ncbi taxa is loaded into mongodb.
- Drugs with scores related to diseases generated by a model are loaded into mongodb.

We answer the queries based on the above listed data and pubmed api.

Git repo

<http://cellvera.dyndns.org:6969/jeanmarcbillod/search-engine-prepaire>

Input

Search query

Output

Corrections of the input, related drugs, related natural products, related proteins with organisms

Dependencies

Mongodb - pubmed api

Docking

To draw a drug associated with a protein we are using the docking module. Docking app receives a request from the backend to do the docking process, then the processing starts, when it is finished it uploads the resulting file to s3 and sends to backend the resulting file name and affinity.

Git repo

<http://cellvera.dyndns.org:6969/jeanmarcbillod/docking-prepaire>

Url

cellvera.dyndns.org:5050

Input

Drugbank id or drug smiles - pdb id or pdb file

Output

Pdb file represents the docking result - affinity

Dependencies

Backend - s3

Alphafold

To draw a protein we can use Alphafold. Alphafold app receives a request from the backend to do the folding process, then the processing starts, when it is finished it uploads the resulting file to s3 and sends to backend the resulting file name.

Git repo

<http://cellvera.dyndns.org:6969/jeanmarcbillod/alphafold-prepaire>

Url

cellvera.dyndns.org:5003

Input

Protein sequence

Output

Pdb file represents the folding result

Dependencies

Backend - s3

Esmfold

Currently it is a part of the backend. To draw a protein we can use Esmfold (sequence must be less than 400 chars)

Input

Protein sequence

Output

Pdb file represents the folding result

Dependencies

Backend - s3

<https://api.esmatlas.com/foldSequence/v1/pdb>

Emboss

To preprocess a sequence we use emboss (I don't know what type of processing it is)

Git repo

<http://cellvera.dyndns.org:6969/habib/emboss>

Url

cellvera.dyndns.org:5096

Input

sequence

Output

Processed sequence

Dependencies

Backend

https://www.ebi.ac.uk/Tools/services/rest/emboss_backtranseq

Drug-drug interaction

To predict the interactions between 2 drugs we use the drug-drug interaction module.

Git repo

<http://cellvera.dyndns.org:6969/root/ds-docker-drug-drug-interaction>

Url

cellvera.dyndns.org:5083

Input

Smiles of 2 drugs

Output

Interactions between the 2 drugs

Toxicity

To predict the toxicity of a drug we use the toxicity module.

Git repo

<http://cellvera.dyndns.org:6969/root/ds-docker-toxicity>

Url

<http://cellvera.dyndns.org:5062>

Input

Smiles of a drugs

Output

Toxicity object

Solubility

To predict the solubility of a drug we use the solubility module.

Git repo

<http://cellvera.dyndns.org:6969/root/ds-docker-solubility>

Url

<http://cellvera.dyndns.org:5061>

Input

Smiles of a drugs

Output

Solubility value

drug-protein pec50

To predict the pec50 between a drug and a protein we use the pec50 module.

Git repo

<http://cellvera.dyndns.org:6969/root/ds-docker-drug-protein-interaction>

Url

cellvera.dyndns.org:5081

Input

Smiles of a drug and sequence of a protein

Output

pec50 value

Drug-protein KD

To predict the kd between a drug and a protein we use the kd module.

Git repo

<http://cellvera.dyndns.org:6969/jeanmarcbillod/ds-docker-drug-protein-kd>

Url

cellvera.dyndns.org:5088

Input

Smiles of a drug and sequence of a protein

Output

Kd value

Drug-Synergy

To predict the synergy between 2 drugs we use the drug-synergy module.

Git repo

<http://cellvera.dyndns.org:6969/habib/drugsynergy>

Url

cellvera.dyndns.org:5085

Input

Smiles of 2 drugs

Output

Synergy between the 2 drugs