CDT-CARD
Centrum Rozwoju Terapii
Chorób Cywilizacyjnych i Związanych z Wiekiem

Laboratorium Bioinformatyki i Analiz in silico

Prof. dr hab. Aleksander Mendyk
dr Jakub Szlęk

Fundusze Europejskie
Inteligentny Rozwój

Rzeczpospolita Polska

UNIWERSYTET JAGIELLOŃSKI
COLLEGIUM MEDICUM
W KRAKOWIE

Unia Europejska
Europejski Fundusz
Rozwoju Regionalnego

LBA – czym dysponujemy?

HARDWARE

- 2 serwery HPC
  - 1,5 TB RAM
  - 2x Xeon Gold
  - Nvidia RTX 6000
- 17 stacji roboczych PC
- macierz dyskowa 60 TB

> 1000 wątków obliczeniowych

SOFTWARE

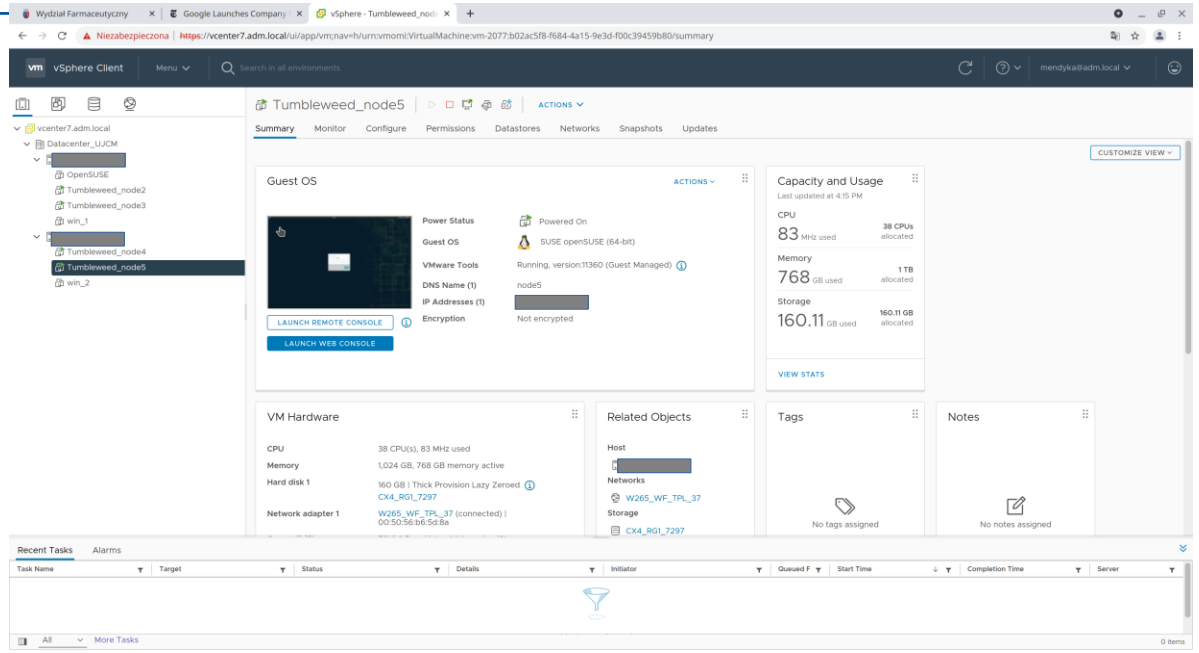
- Linux / Windows
- VMWare / Proxmox
- R / Python / Java
- H2O / mljar
- dso /PySR
- Tensorflow
- Orca, Psi4, Gromacs

METODY

- statystyka
- AI/ML (Deep learning)
- informatyka chemiczna
- analiza obrazu
- GPU computing

ŚRODOWISKO “NA ŻYCZENIE”

LBA – czym dysponujemy?



Użytkownik 1

Internet

VPN/SSH

Medyczna 7

2 serwery HPC

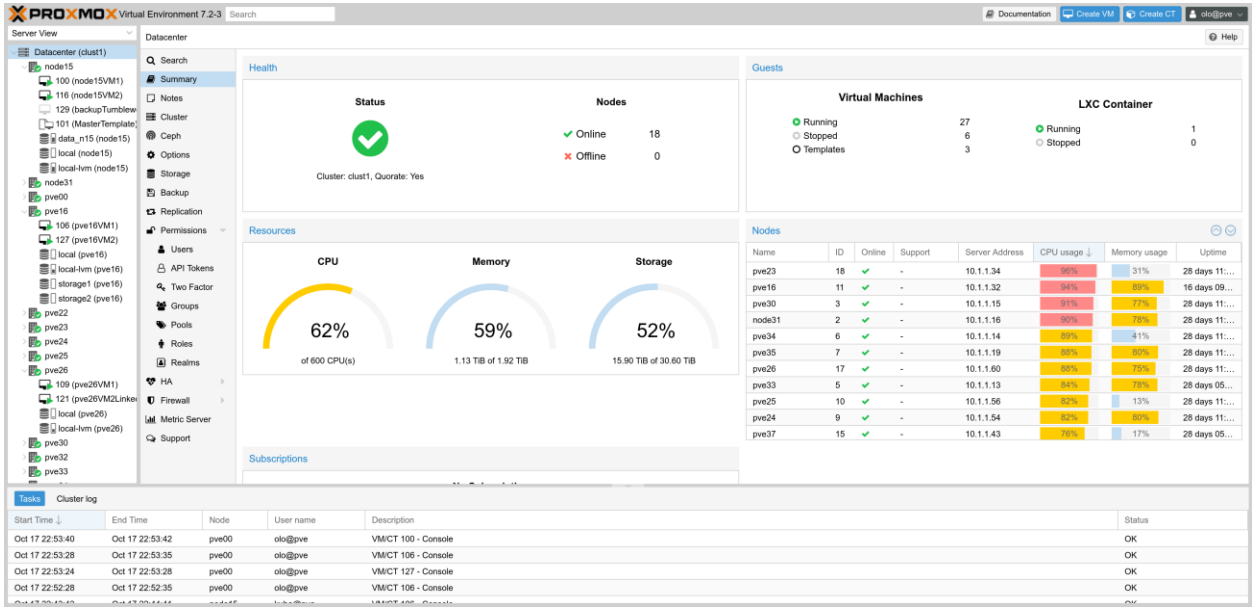
Medyczna 9

17 PC

VPN/SSH

Użytkownik 2

LBA – czym dysponujemy?



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Użytkownik 2

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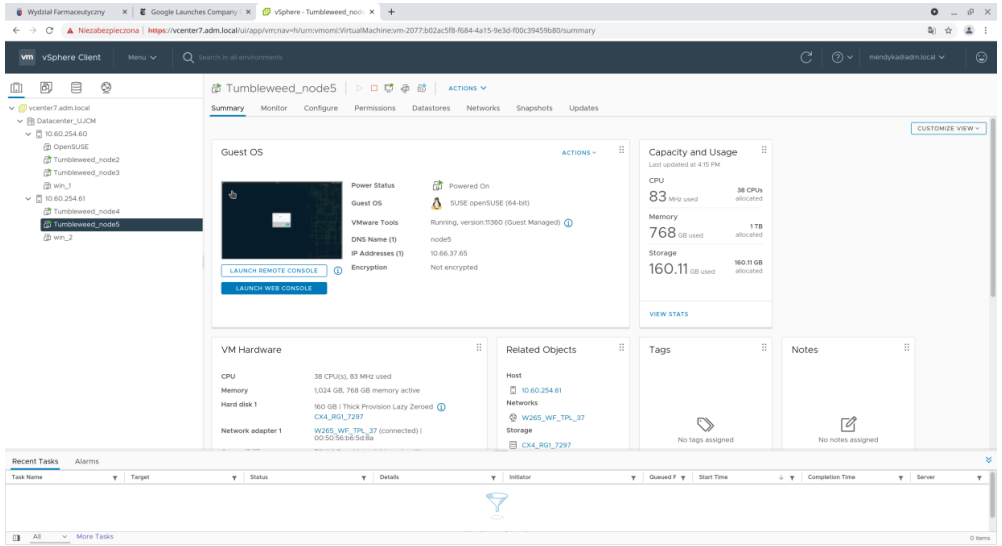
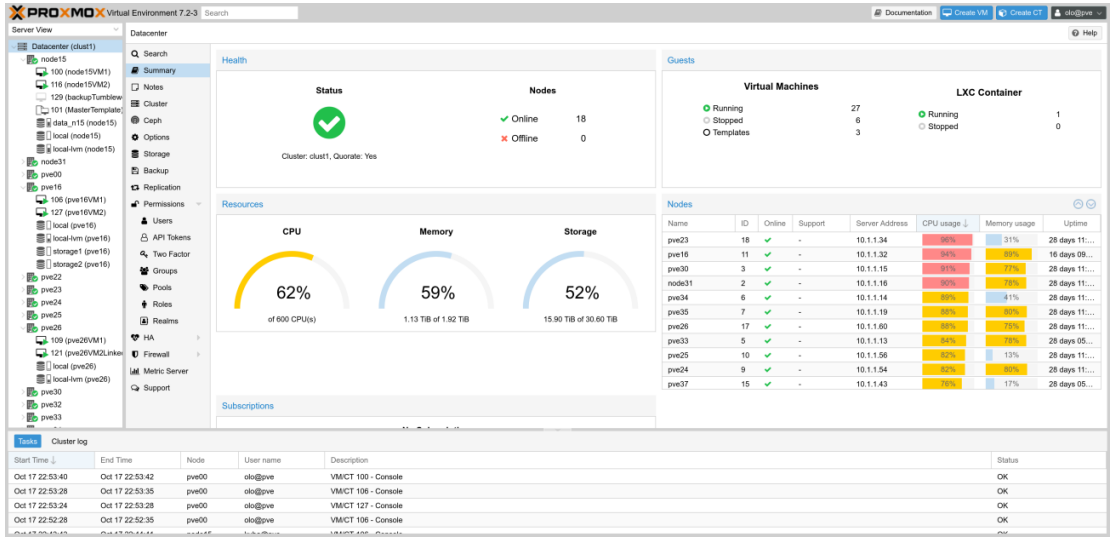
Więcej informacji dostępnych pod adresem:

www.cdt-card.cm-uj.krakow.pl/
www.linkedin.com/showcase/cdt-card/

VMware



Proxmox



bash

rozproszenie

>10 000 jobs (randomForest, Cubist)

80 wątków (Orca, AutoML)

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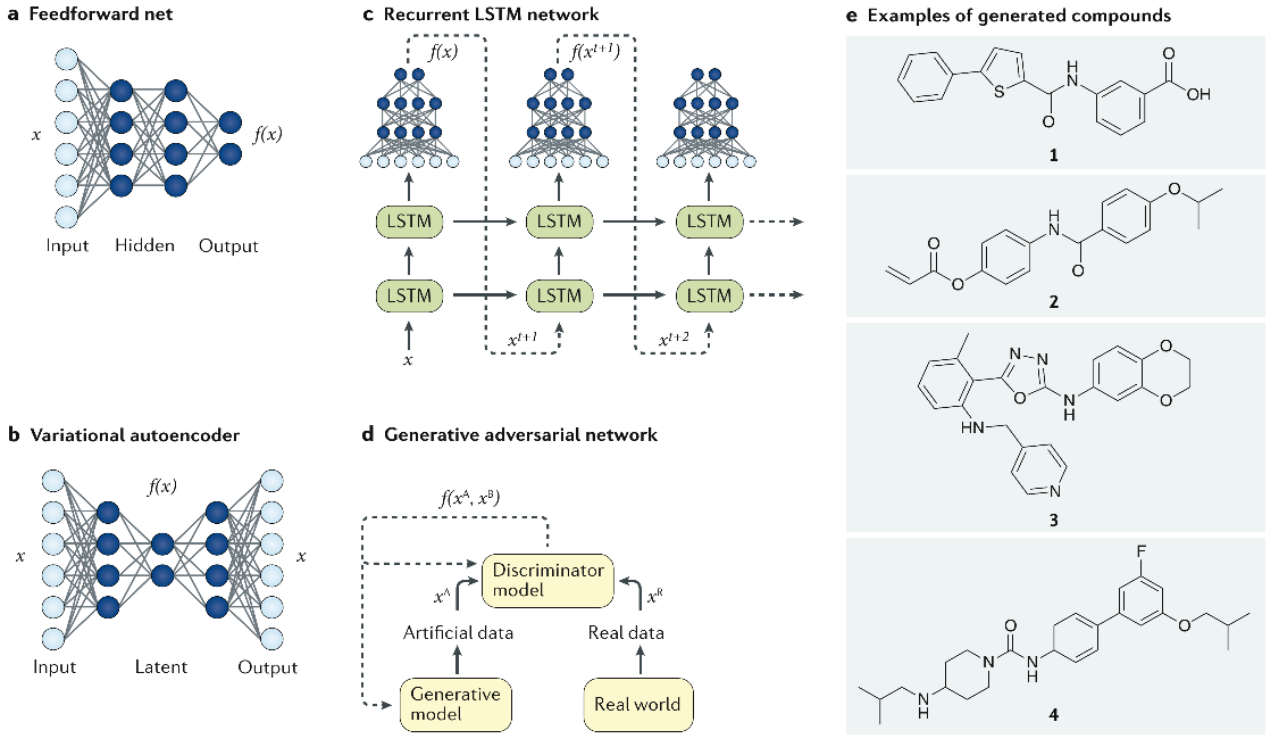
QSAR: AI/ML

LBA – co robimy?



QSAR

↓

revQSAR

Schneider P, Walters WP, Plowright AT, Sieroka N, Listgarten J, Goodnow RA Jr, Fisher J, Jansen JM, Duca JS, Rush TS, Zentgraf M, Hill JE, Krutoholow E, Kohler M, Blaney J, Funatsu K, Luebkemann C, Schneider G. Rethinking drug design in the artificial intelligence era. Nat Rev Drug Discov. 2020 May;19(5):353-364. doi: 10.1038/s41573-019-0050-3. Epub 2019 Dec 4. PMID: 31801986.

QSAR: AI/ML

Curated Database and Preliminary AutoML QSAR Model for 5-HT1A Receptor

by Natalia Czub, Adam Pacławski *, Jakub Szlęk and Aleksander Mendyk

Department of Pharmaceutical Technology and Biopharmaceutics, Jagiellonian University Medical College, 30-688 Kraków, Poland

* Author to whom correspondence should be addressed.

Pharmaceutics **2021**, *13*(10), 1711; https://doi.org/10.3390/pharmaceutics13101711

molecular informatics
models – molecules – systems

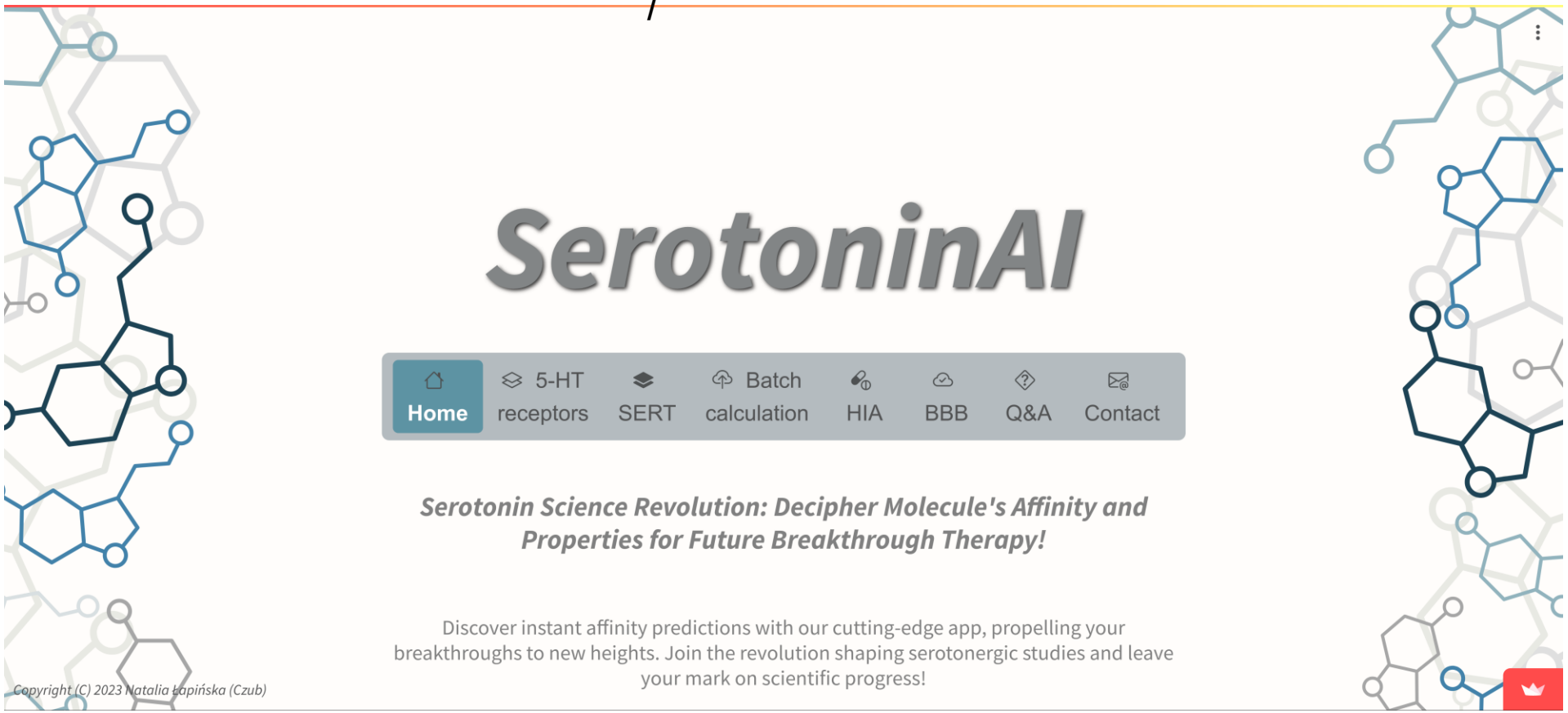
Research Article

Application of automated machine learning in the identification of multi-target-directed ligands blocking PDE4B, PDE8A, and TRPA1 with potential use in the treatment of asthma and COPD

Alicja Gawalska, Natalia Czub, Michał Sapa, Marcin Kołaczkowski, Adam Bucki, Aleksander Mendyk

QSAR: AI/ML

https://serotoninai.streamlit.app/



QSPR: AI/ML

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Artificial Intelligence-Based Quantitative Structure–Property Relationship Model for Predicting Human Intestinal Absorption of Compounds with Serotonergic Activity

Natalia Czub, Jakub Szlęk, Adam Pacławski*, Klaudia Klimończyk, Matteo Puccetti, and Aleksander Mendyk

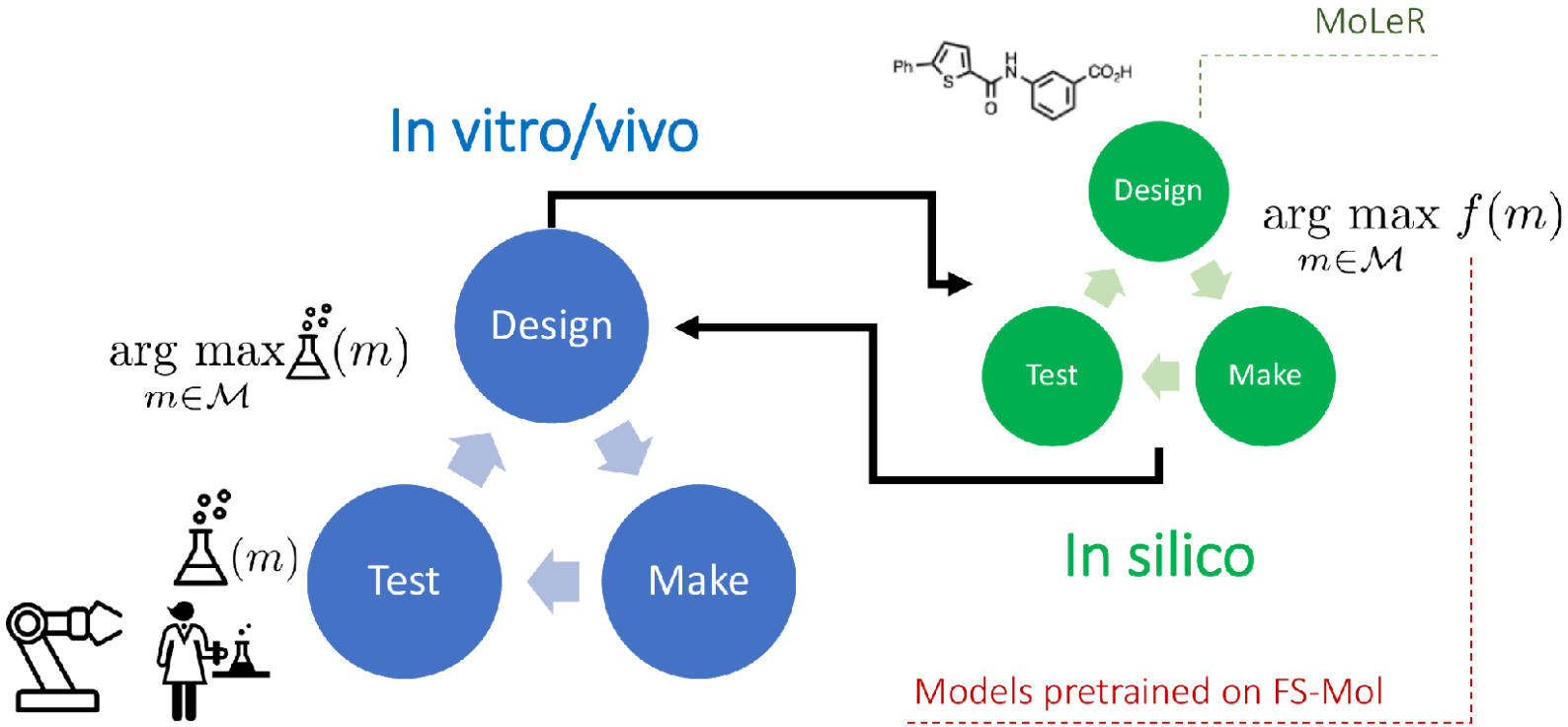
Cite this: *Mol. Pharmaceutics* 2023, 20, 5, 2545–2555
Publication Date: April 18, 2023
https://doi.org/10.1021/acs.molpharmaceut.2c01117

Molecular Pharmaceutics

PDF (4 MB) | SI Supporting Info (3) »

SUBJECTS: Absorption, Biological databases, Molecular modeling, Molecules, Permeability

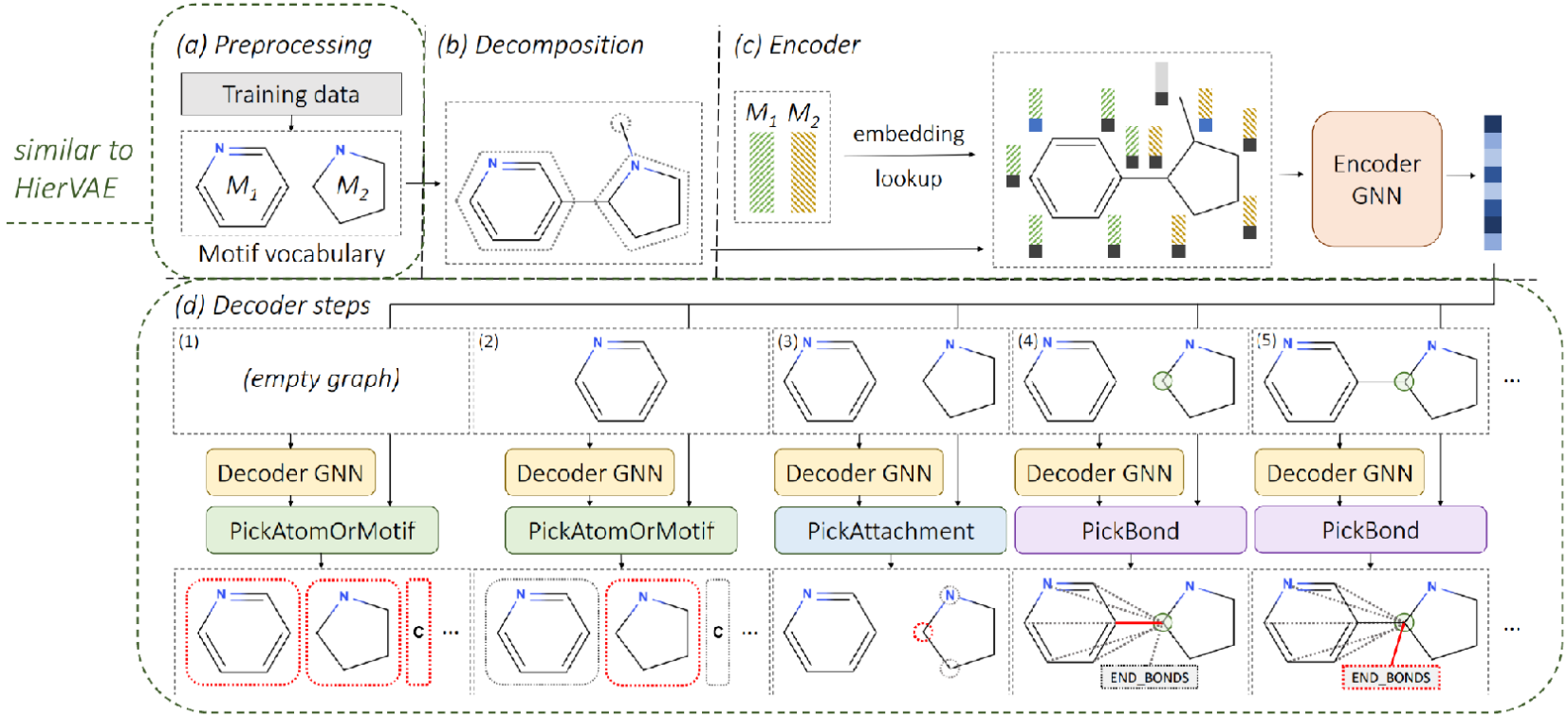
Modele generatywne



https://github.com/kmaziarz

https://www.microsoft.com/en-us/research/blog/moler-creating-a-path-to-more-efficient-drug-design/

Modele generatywne

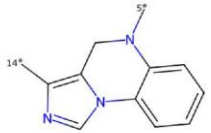


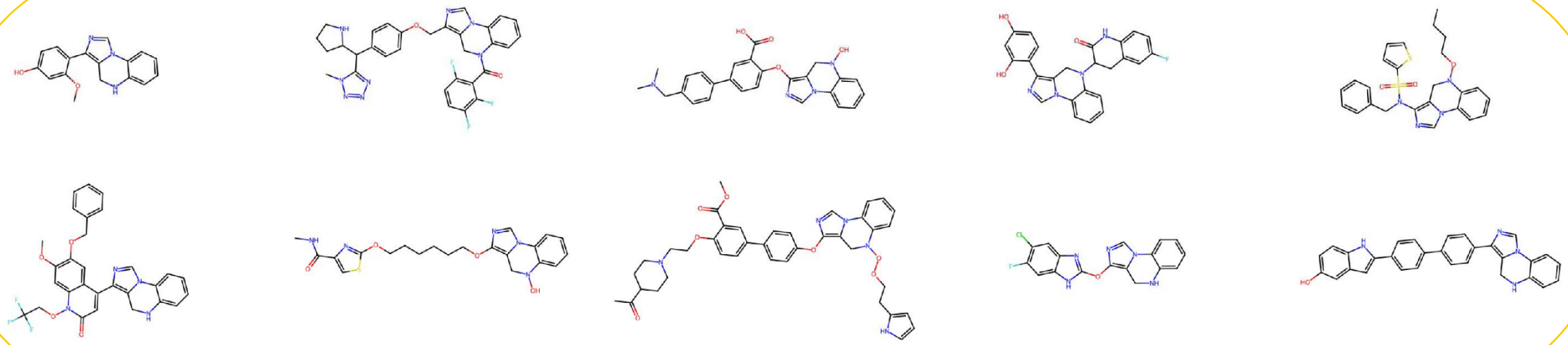
decoder steps independent given encoder output → can start from scaffold

https://github.com/kmaziarz

https://www.microsoft.com/en-us/research/blog/moler-creating-a-path-to-more-efficient-drug-design/

Modele generatywne





Wygenerowane cząsteczki na podstawie dostrojonego (fine-tuned) modelu

AI/ML → modele surogatowe

nature

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NEWS | 14 November 2023

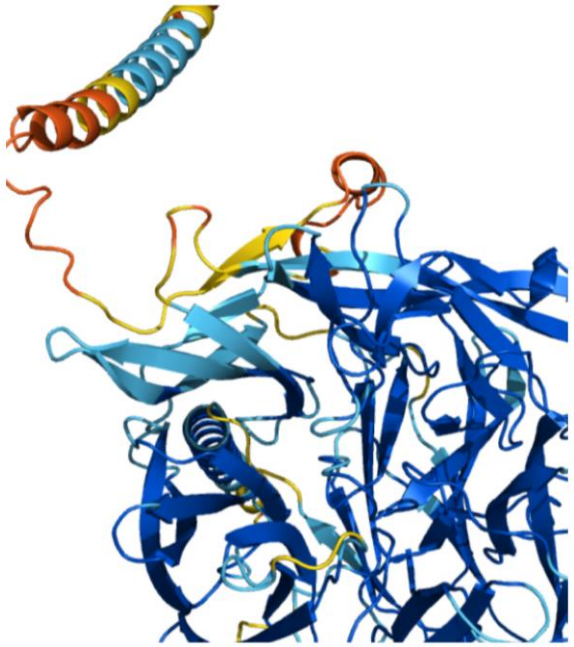
DeepMind AI accurately forecasts weather – on a desktop computer

The machine-learning model takes less than a minute to predict future weather worldwide more precisely than other approaches.

Carissa Wong

AlphaFold is an AI system developed by DeepMind that predicts a protein's 3D structure from its amino acid sequence. It regularly achieves accuracy competitive with experiment.

DeepMind and EMBL's European Bioinformatics Institute (EMBL-EBI) have partnered to create AlphaFold DB to make these predictions freely available to the scientific community. The latest database release contains over 200 million entries, providing broad coverage of UniProt (the standard repository of protein sequences and annotations). We provide individual downloads for the human proteome and for the proteomes of 47 other key organisms important in research and global health. We also provide a download for the manually curated subset of UniProt (Swiss-Prot).



Q8I3H7: May protect the malaria parasite against attack by the immune system. Mean pLDDT 85.57.

View protein

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AI/ML → surogatowy model matematyczny

1728 pacjentów wirtualnych

X1 – Age [years]

X2 – Gender [1 = woman; 0 = man]

X3 - Body_mass [kg]

X4 – Height [cm]

X5 – Doses [mg]

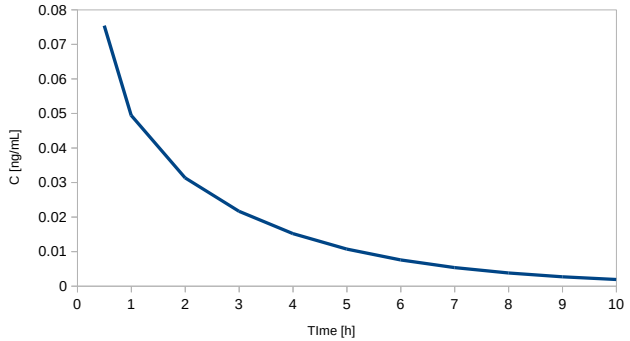
X6 – Administration_time [h]

X7 - Infusion_duration [h]

X8 - PK_sample_time [h]

X9 – Concentration [mg/h]

PBPK



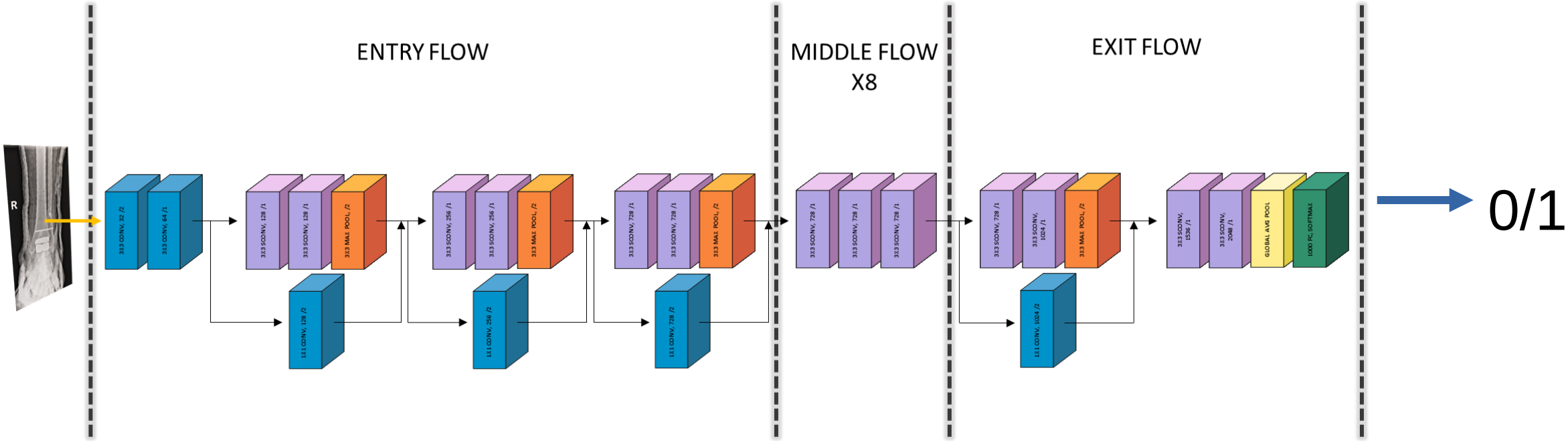
↓ DoE

Baza danych

↓ Symbolic Regression (dso)

$$X9 = \exp(-0.282*X8)*\exp(\exp(X8*(-1.78+X2)))*(\ln(X1)*(\exp(-7.99)*X5))$$

AI/ML → analiza obrazu



Automatyzacja procesu określania poprawności projekcji zdjęć rentgenowskich stawu skokowego przy użyciu konwolucyjnych sieci neuronowych

Piotr Gabryś, Natalia Czub, Aleksander Mendyk, Grzegorz Tatoń

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AI/ML → własne oprogramowanie

```
import numpy as np
import pandas as pd
import sys
import autokeras as ak
from configparser import ConfigParser
from sklearn.metrics import mean_squared_error, r2_score
# ----------------------------------------
config = ConfigParser(allow_no_value=True)
config.read('config.ini')
# ----------------------------------------
train_file_path = config['USERCONFIG']['train_dataset']
```

- Python
- R
- bash

AI/ML → modelowanie i optymalizacja

- postać leku i technologia wytwarzania
- QSAR/QSPR
- PK/PD
- korelacja in vitro in vivo (IVIVC / IVIVR)
- ekstrapolacja in vitro in vivo (IVIVE)
- proteomika i metabolomika
- analiza obrazu
- prace doktorskie, magisterskie, koło naukowe

modelowanie oparte na danych

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www.**linkedin.com/showcase/cdt-card/**

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dr Jakub Szlęk, j.szlek@uj.edu.pl