Checking cards of Models

Page 1 backlink Tag

"Identifier": "eos1579"

JSON


```
{
    "Identifier": "eos1579",
    "Input": [
        "Compound"
    ],
    "Mode": "Pretrained",
    "GitHub": "https://github.com/ersilia-os/eos1579",
    "Publication": "https://doi.org/10.1038/s41589-022-01110-7",
    "Source Code": "https://github.com/the-ahuja-
lab/Metabokiller",
    "License": "Non-commercial",
    "Output": [
        "Probability"
    ],
    "Description": "Carcinogenicity is a result of several
potential effects on  cells. This model predicts the
carcinogenic potential of a small molecule based on their
potential to induce cellular proliferation, genomic instability,
oxidative stress, anti-apoptotic responses and epigenetic
alterations. Metabokiller uses the Chemical Checker signaturizer
to featurize the molecules, and the Lime package to provide
interpretable results. Using Metabokiller, the authors screened
a panel of human metabolites and experimentally demonstrated two
of the predicted carcinogenic metabolites induced carcinogenic
transformations in yeast and human cells.\n",
    "Status": "Ready",
    "Slug": "metabokiller",
    "Title": "Carcinogenic potential of metabolites and small
molecules",
    "Tag": [
        "Toxicity",
        "Cancer",
        "Metabolism"
    ],
```

```
    "Input Shape": "Single",
    "Interpretation": "Probability that the molecule has each of
the specified carcinogenic properties",
    "Task": [
        "Classification"
    ],
    "Contributor": "brosular",
    "Output Shape": "List",
    "Output Type": [
        "Float"
    ],
    "DockerHub": "https://hub.docker.com/r/ersiliaos/eos1579",
    "Docker Architecture": [
        "AMD64",
        "ARM64"
    ],
    "S3": "https://ersilia-models-zipped.s3.eu-central-
1.amazonaws.com/eos1579.zip",
    "Deployment": "Local",
    "Repository": {
        "label": "GitHub",
        "url": "https://github.com/ersilia-os/eos1579"
    },
    "Code": "$ ersilia serve metabokiller\n$ ersilia api -i
'CCCOCCC'\n$ ersilia close",
    "Date": "2022-08-30",
    "Calculation": "https://github.com/brosular"
}
```


"Identifier": "eos157v"

JSON


```
{
    "Identifier": "eos157v",
    "Input": [
        "Compound"
    ],
    "Mode": "Pretrained",
    "GitHub": "https://github.com/ersilia-os/eos157v",
    "Publication":
"https://papers.nips.cc/paper/2020/hash/94aef38441efa3380a3bed3f
af1f9d5d-Abstract.html",
    "Source Code": "https://github.com/tencent-ailab/grover",
    "License": "MIT",
```

```
    "Output": [
        "Other value"
    ],
    "Description": "Model based on experimental and calculated
hydration free energy of small molecules in water, the FreeSolv
dataset from MoleculeNet. Hydration free energies are relevant
to understand the binding interaction between a molecule (in
solution) into its binding site.  This model has been trained
using the GROVER transformer (see eos7w6n or grover-embedding
for a detail of the molecular featurization step with GROVER).
\n",
    "Status": "Ready",
    "Slug": "grover-freesolv",
    "Title": "Hydration free energy of small molecules in
water",
    "Tag": [
        "MoleculeNet",
        "Chemical graph model",
        "Quantum properties"
    ],
    "Input Shape": "Single",
    "Interpretation": "Calculated Hydration Free energy in
kcal/mol",
    "Task": [
        "Regression"
    ],
    "Contributor": "Amna-28",
    "Output Shape": "Single",
    "Output Type": [
        "Float"
    ],
    "DockerHub": "https://hub.docker.com/r/ersiliaos/eos157v",
    "Docker Architecture": [
        "AMD64",
        "ARM64"
    ],
    "S3": "https://ersilia-models-zipped.s3.eu-central-
1.amazonaws.com/eos157v.zip",
    "BiomodelAnn": "Yes",
    "Deployment": "Local",
    "Repository": {
        "label": "GitHub",
        "url": "https://github.com/ersilia-os/eos157v"
    },
    "Code": "$ ersilia serve grover-freesolv\n$ ersilia api -i
'CCCOCCC'\n$ ersilia close",
```

```
    "Date": "2022-07-13",
    "Calculation": "https://github.com/Amna-28"
}
```


"Identifier": "eos18ie"

JSON


```
{
    "Identifier": "eos18ie",
    "Input": [
        "Compound"
    ],
    "Mode": "Pretrained",
    "GitHub": "https://github.com/ersilia-os/eos18ie",
    "Publication": "https://www.nature.com/articles/s41586-023-06887-8",
    "Source Code": "https://github.com/felixjwong/antibioticsai",
    "License": "MIT",
    "Output": [
        "Probability"
    ],
    "Description": "The authors use a large dataset (>30k) to train an explainable graph-based model to identify potential antibiotics with low cytotoxicity. The model uses a substructure-based approach to explore the chemical space. Using this method, they were able to screen 283 compounds and identify a candidate active against methicillin-resistant S. aureus (MRSA) and vancomycin-resistant enterococci.\n",
    "Status": "Ready",
    "Slug": "antibiotics-ai",
    "Title": "Substructure-based search of novel antibiotics",
    "Tag": [
        "Cytotoxicity",
        "Antimicrobial activity",
        "ESKAPE"
    ],
    "Input Shape": "Single",
    "Interpretation": "Probability off growth inhibition (80% cut off at 50uM)",
    "Task": [
        "Classification"
    ],
    "Contributor": "Richiio",
    "Output Shape": "Single",
```

```
    "Output Type": [
        "Float"
    ],
    "DockerHub": "https://hub.docker.com/r/ersiliaos/eos18ie",
    "Docker Architecture": [
        "AMD64",
        "ARM64"
    ],
    "S3": "https://ersilia-models-zipped.s3.eu-central-
1.amazonaws.com/eos18ie.zip",
    "BiomodelAnn": "Yes",
    "Deployment": "Local",
    "Repository": {
        "label": "GitHub",
        "url": "https://github.com/ersilia-os/eos18ie"
    },
    "Code": "$ ersilia serve antibiotics-ai\n$ ersilia api -i
'CCCOCCC'\n$ ersilia close",
    "Date": "2024-01-26",
    "Calculation": "https://github.com/Richiio"
}
```


"Identifier": "eos1af5"

JSON


```
{
    "Identifier": "eos1af5",
    "Input": [
        "Compound"
    ],
    "Mode": "Pretrained",
    "GitHub": "https://github.com/ersilia-os/eos1af5",
    "Publication":
"https://pubs.acs.org/doi/10.1021/acs.jcim.0c01344",
    "Source Code":
"https://github.com/josejimenezluna/molgrad/",
    "License": "AGPL-3.0",
    "Output": [
        "Experimental value"
    ],
    "Description": "By combining a Message-Passing Graph Neural
Network (MPGNN) and a Forward fully connected Neural Network
(FNN) with an integrated gradients explainable artificial
intelligence (XAI) method, the authors developed MolGrad and
tested it on a number of ADME predictive tasks. MolGrad
```

```
incorporates explainable features to facilitate interpretation
of the predictions.\u00a0 This model has been trained using
experimental data on the permeability of molecules across Caco2
cell membranes (Papp, cm s-1)\n",
    "Status": "Ready",
    "Slug": "molgrad-caco2",
    "Title": "Coloring molecules for Caco-2 cell permeability",
    "Tag": [
        "Permeability",
        "ADME",
        "Papp",
        "Chemical graph model"
    ],
    "Input Shape": "Single",
    "Interpretation": "Log 10 of the Passive permeability in cm
s-1",
    "Task": [
        "Regression"
    ],
    "Contributor": "miquelduranfrigola",
    "Output Shape": "Single",
    "Output Type": [
        "Float"
    ],
    "DockerHub": "https://hub.docker.com/r/ersiliaos/eos1af5",
    "Docker Architecture": [
        "AMD64"
    ],
    "S3": "https://ersilia-models-zipped.s3.eu-central-
1.amazonaws.com/eos1af5.zip",
    "BiomodelAnn": "Yes",
    "Deployment": "Local",
    "Repository": {
        "label": "GitHub",
        "url": "https://github.com/ersilia-os/eos1af5"
    },
    "Code": "$ ersilia serve molgrad-caco2\n$ ersilia api -i
'CCCOCCC'\n$ ersilia close",
    "Date": "2021-10-19",
    "Calculation": "https://github.com/miquelduranfrigola"
}
```


"Identifier": "eos1amn"

Plain Text

```
Model exists in catalog but not on https://www.ersilia.io/model-hub or docker hub
```

"Identifier": "eos1amr"

JSON


```
{
    "Identifier": "eos1amr",
    "Input": [
        "Compound"
    ],
    "Mode": "Pretrained",
    "GitHub": "https://github.com/ersilia-os/eos1amr",
    "Publication": "https://papers.nips.cc/paper/2020/hash/94aef38441efa3380a3bed3faf1f9d5d-Abstract.html",
    "Source Code": "https://github.com/tencent-ailab/grover",
    "License": "MIT",
    "Output": [
        "Probability"
    ],
    "Description": "This model predicts the Blood-Brain Barrier (BBB) penetration potential of small molecules using as training data the curated MoleculeNet benchmark containing 2000 experimental data points. It has been trained using the GROVER transformer (see eos7w6n or grover-embedding for a detail of the molecular featurization step with GROVER). \n",
    "Status": "Ready",
    "Slug": "grover-bbbp",
    "Title": "Blood-brain barrier penetration",
    "Tag": [
        "Permeability",
        "MoleculeNet",
        "Chemical graph model",
        "Alzheimer"
    ],
    "Input Shape": "Single",
    "Interpretation": "Probability that a molecule crosses the blood brain barrier",
    "Task": [
        "Classification"
```

```
    ],
    "Contributor": "Amna-28",
    "Output Shape": "Single",
    "Output Type": [
        "Float"
    ],
    "DockerHub": "https://hub.docker.com/r/ersiliaos/eos1amr",
    "Docker Architecture": [
        "AMD64",
        "ARM64"
    ],
    "S3": "https://ersilia-models-zipped.s3.eu-central-
1.amazonaws.com/eos1amr.zip",
    "BiomodelAnn": "Yes",
    "Deployment": "Local",
    "Repository": {
        "label": "GitHub",
        "url": "https://github.com/ersilia-os/eos1amr"
    },
    "Code": "$ ersilia serve grover-bbbp\n$ ersilia api -i
'CCCOCCC'\n$ ersilia close",
    "Date": "2021-06-04",
    "Calculation": "https://github.com/Amna-28"
}
```


"Identifier": "eos1bba"

Plain Text

```
Model exists in catalog but not on https://www.ersilia.io/model-
hub or docker hub
```

"Identifier": "eos1d7r"

JSON


```
{
    "Identifier": "eos1d7r",
    "Input": [
        "Compound"
    ],
    "Mode": "Online",
    "GitHub": "https://github.com/ersilia-os/eos1d7r",
    "Publication":
```

```
"https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3606195/",
    "Source Code": "https://pypi.org/project/smallworld-api/",
    "License": "MIT",
    "Output": [
        "Compound"
    ],
    "Description": "Small World is an index of chemical space
containing more than 230B molecular substructures. Here we use
the Small World API to post a query to the SmallWorld server. We
sample 100 molecules within a distance of 10 specifically for
the ZINC map, not the entire SmallWorld domain. Please check
other small-world models available in our hub.\n",
    "Repository": {
        "label": "GitHub",
        "url": "https://github.com/ersilia-os/eos1d7r"
    },
    "Status": "Ready",
    "Slug": "small-world-zinc",
    "Title": "Small World Zinc search",
    "Tag": [
        "Similarity"
    ],
    "Input Shape": "Single",
    "Code": "$ ersilia serve small-world-zinc\n$ ersilia api -i
'CCCOCCC'\n$ ersilia close",
    "Interpretation": "List of 100 nearest neighbors",
    "Task": [
        "Similarity"
    ],
    "Contributor": "miquelduranfrigola",
    "Date": "2023-11-02",
    "Calculation": "https://github.com/miquelduranfrigola",
    "Output Shape": "List",
    "Output Type": [
        "String"
    ],
    "DockerHub": "https://hub.docker.com/r/ersiliaos/eos1d7r",
    "Docker Architecture": [
        "AMD64",
        "ARM64"
    ],
    "S3": "https://ersilia-models-zipped.s3.eu-central-
1.amazonaws.com/eos1d7r.zip",
    "Deployment": "Local"
}
```

"Identifier": "eos1mxi"

JSON


```
{
    "Identifier": "eos1mxi",
    "Input": [
        "Compound"
    ],
    "Mode": "Pretrained",
    "GitHub": "https://github.com/ersilia-os/eos1mxi",
    "Publication":
"https://pubs.acs.org/doi/abs/10.1021/acs.jcim.0c01127",
    "Source Code": "https://github.com/XinhaoLi74/SmilesPE",
    "License": "Apache-2.0",
    "Output": [
        "Compound"
    ],
    "Description": "The Smiles Pair Encoding method generates
smiles substring tokens based on high-frequency token pairs from
large chemical datasets. This method is well-suited for both
QSAR activities as well as generative models. The model provided
here has been pretrained using ChEMBL.\n",
    "Status": "Ready",
    "Slug": "smiles-pe",
    "Title": "SmilesPE: tokenizer algorithm for SMILES,
DeepSMILES, and SELFIES",
    "Tag": [
        "Chemical language model",
        "Chemical notation",
        "ChEMBL"
    ],
    "Input Shape": "Single",
    "Interpretation": "A data-driven tokenization method for
SMILES-based deep learning models in cheminformatics,
demonstrating high performance in molecular generation and QSAR
prediction tasks compared to atom-level tokenization",
    "Task": [
        "Generative"
    ],
    "Contributor": "Richiio",
    "Output Shape": "Flexible List",
    "Output Type": [
        "String"
    ],
```

```
    "DockerHub": "https://hub.docker.com/r/ersiliaos/eos1mxi",
    "Docker Architecture": [
        "AMD64",
        "ARM64"
    ],
    "S3": "https://ersilia-models-zipped.s3.eu-central-
1.amazonaws.com/eos1mxi.zip",
    "Deployment": "Local",
    "Repository": {
        "label": "GitHub",
        "url": "https://github.com/ersilia-os/eos1mxi"
    },
    "Code": "$ ersilia serve smiles-pe\n$ ersilia api -i
'CCCOCCC'\n$ ersilia close",
    "Date": "2023-08-02",
    "Calculation": "https://github.com/Richiio"
}
```


"Identifier": "eos1n4b"

JSON


```
{
    "Identifier": "eos1n4b",
    "Input": [
        "Compound"
    ],
    "Mode": "Pretrained",
    "GitHub": "https://github.com/ersilia-os/eos1n4b",
    "Publication":
"https://onlinelibrary.wiley.com/doi/10.1002/minf.202000105",
    "Source Code": "https://github.com/jwxia2014/HDAC3i-Finder",
    "License": "GPL-3.0",
    "Output": [
        "Score"
    ],
    "Description": "The model predicts the inhibitory potential
of small molecules against Histone deacetylase 3 (HDAC3), a
relevant human target for cancer, inflammation,
neurodegenerative diseases and diabetes. The authors have used a
dataset of 1098 compounds from ChEMBL and validated the model
using the benchmark MUBD-HDAC3\n",
    "Repository": {
        "label": "GitHub",
        "url": "https://github.com/ersilia-os/eos1n4b"
```

```
    },
    "Status": "Ready",
    "Slug": "hdac3-inh",
    "Title": "Identifying HDAC3 inhibitors",
    "Tag": [
        "Cancer",
        "ChEMBL"
    ],
    "Input Shape": "Single",
    "Code": "$ ersilia serve hdac3-inh\n$ ersilia api -i
'CCCOCCC'\n$ ersilia close",
    "Interpretation": "Probability that the molecule is a HDAC3
inhibitor",
    "Task": [
        "Classification"
    ],
    "Contributor": "Richiio",
    "Date": "2023-12-14",
    "Calculation": "https://github.com/Richiio",
    "Output Shape": "Single",
    "Output Type": [
        "Float"
    ],
    "DockerHub": "https://hub.docker.com/r/ersiliaos/eos1n4b",
    "Docker Architecture": [
        "AMD64"
    ],
    "S3": "https://ersilia-models-zipped.s3.eu-central-
1.amazonaws.com/eos1n4b.zip",
    "Deployment": "Local"
}
```