

Gut Rhythm Prediction Report (Sample)

Drug name: **ABC**

Short name: abc Drug CAS number: 123456-78-9 SIDER_ID: CID12345678 Dates of experiment: 01-01-2001

Summary

Sitagliptin is likely to induce Decreased appetite, Gastrointestinal pain, Skin disorder, Dermatitis, Diarrhoea, Constipation, Anaphylactic shock, Rash, Musculoskeletal discomfort and Abdominal pain.

Sitagliptin is unlikely to induce Rhinitis, Oedema peripheral, Hepatitis, Alopecia, Agitation, Leukopenia and Tinnitus.

Prediction models performance and Probability

All prediction models for each adverse drug reaction (ADR) are separately trained models using the AEON models (<u>www.aeon-toolkit.org</u>). The best trained models were selected to create this prediction report. Every model has an accuracy at over 0.68 and the area under the receiver operating characteristic curve (AUROC) at over 0.68 to secure an acceptable overall accuracy of the trained prediction model used for this prediction report.



Positively-correlated ADR table

| ADR | AEON model | Accuracy | AUROC | Precision(c0) | Precision(c1) | Probability |
|----------------------------|------------|----------|-------|---------------|---------------|-------------|
| Decreased appetite | ict | 0.900 | 0.900 | 0.900 | 0.900 | 1.000 |
| Gastrointestinal pain | ict | 0.900 | 0.900 | 0.900 | 0.900 | 1.000 |
| Skin disorder | cnn | 0.900 | 0.900 | 0.900 | 0.900 | 0.991 |
| Dermatitis | fcn | 0.900 | 0.900 | 0.900 | 0.900 | 0.947 |
| Diarrhoea | ict | 0.900 | 0.900 | 0.900 | 0.900 | 0.867 |
| Constipation | cnn | 0.800 | 0.800 | 0.800 | 0.800 | 0.863 |
| Anaphylactic shock | ict | 0.800 | 0.800 | 0.800 | 0.800 | 0.828 |
| Rash | cnn | 0.800 | 0.800 | 0.800 | 0.800 | 0.788 |
| Musculoskeletal discomfort | cnn | 0.800 | 0.800 | 0.800 | 0.800 | 0.696 |
| Abdominal pain | ict | 0.800 | 0.800 | 0.800 | 0.800 | 0.593 |

A precision value at over 0.8 for positively-correlated predictions for each ADR was used as the final gate to predict if Sitagliptin could potentially induce that ADR. Probability value sorted in the order the highest probability to the lowest (0.5).



Negatively-correlated ADR table

| ADR | AEON model | Accuracy | AUROC | Precision(c0) | Precision(c1) | Probability |
|-------------------|------------|----------|-------|---------------|---------------|-------------|
| Rhinitis | fcn | 0.900 | 0.900 | 0.900 | 0.900 | 0.399 |
| Oedema peripheral | cnn | 0.900 | 0.900 | 0.900 | 0.900 | 0.379 |
| Hepatitis | fcn | 0.900 | 0.900 | 0.900 | 0.900 | 0.183 |
| Alopecia | cnn | 0.800 | 0.800 | 0.800 | 0.800 | 0.073 |
| Agitation | cnn | 0.800 | 0.800 | 0.800 | 0.800 | 0.031 |
| Leukopenia | cnn | 0.800 | 0.800 | 0.800 | 0.800 | 0.000 |
| Tinnitus | ict | 0.800 | 0.800 | 0.800 | 0.800 | 0.000 |

A precision value at over 0.8 for negatively-correlated predictions for each ADR was used as the final gate to predict that Sitagliptin will <u>NOT</u> induce that ADR.



| Accuracy | Overall accuracy of drug being correctly predicted |
|---------------|--|
| AUROC | Area under the receiver operating characteristic (AUROC) - the |
| | model's ability to discriminate between positively-correlated |
| | and negatively-correlated class |
| Precision(c1) | how often an ML model is correct when predicting the |
| | positively-correlated side effect (class 1) |
| Precision(c0) | how often an ML model is correct when predicting the |
| | negatively-correlated side effect (class 0) |
| Probability | The prediction probability for the drug to induce that ADR |