






















































Basket browser

Browse, Compare or Join molecule sets

Filter by name: [Create new ] ☒ Show public sets ☐ Sets of group me

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			MDMX owned by published, created by carpovpv	
				ts_mouse_oral_1.sdf owned by published, created by Tinkov_Oleg
				ws_mouse_oral_1.sdf owned by published, created by Tinkov_Oleg
				DIR training set owned by published, created by qingshuang0501
				DIR test set owned by published, created by qingshuang0501
				Huuskonen_logP (test) owned by published, created by itetko
				Huuskonen_logP (training) owned by published, created by itetko
				Delaney owned by published, created by itetko
				DIR (test) owned by published, created by qingshuang0501
				DIR (training) owned by published, created by qingshuang0501
				Anti_TB_Dataset II (test) owned by published, created by vkovalishyn
				Anti_TB_Dataset II (training) owned by published, created by vkovalishyn
				Anti_TB_Dataset I (test) owned by published, created by vkovalishyn
				Anti_TB_Dataset I (training) owned by published, created by vkovalishyn
				tubulin (training) owned by published, created by hodyna

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Basket browser

Browse, Compare or Join molecule sets

Filter by name: [Create new ] ☒ Show public sets ☐ Sets of group me

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				Ames challenge (test) owned by published, created by midnighter
				Ames challenge (training) owned by published, created by midnighter

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2181 records

4361 records

3 models 

Predicted property: [AMES](#)

Training set: [Ames challenge \(training\)](#) (2 different versions detected) 

Metrics [AUC](#)  for [Training set](#)  Validation: [Cross-Validation \(3 mc](#)

	ASNN	TRANSNN (tr. set. 2)
OEstate	0.85	+
SMILES	+	0.85
SMILES augm: 10/10	+	0.88

 [Predicates \(" \$<\$ ", " \$>\$ "\) and/or optimal classification thresholds are NOT used for statistics \(click to](#)

 [Refresh](#)

Predicted property: [AMES](#)

Training set: [Ames challenge \(training\)](#) (2 different versions detected) 

Metrics [AUC](#)  for [Training set](#)  Validation: [Cross-Validation \(3 models\)](#) 

	ASNN	TRANSNN (tr. set. 2)
OEstate	0.85	+
SMILES	+	0.85
SMILES augm: 10/10	+	0.88

- Create another model using this configuration
- Save this model
- Export this model
- Show XML configuration
- Export XML configuration
- Delete the model

 [Predicates \(" \$<\$ ", " \$>\$ "\) and/or optimal classification thresholds](#)

 [Refresh](#)

 [Export as Excel file](#)

 [Export as R script](#)

Predicted property: [AMES](#)

Training set: [Ames challenge \(training\)](#) (2 different versions detected) 

Metrics [AUC](#)  for [Training set](#)  Validation: [Cross-Validation \(3 models\)](#)

	ASNN	TRANSNN (tr. set. 2)
OEstate	0.85	+
SMILES	+	saved
SMILES augm: 10/10	+	saved

 [Predicates \(" \$<\$ ", " \$>\$ "\) and/or optimal classification thresholds are NOT used for statistics \(click to change\)](#)


 [Refresh](#)

Training set: Ames challenge (training) (2 different versions detected)

	ASNN	TRANSNN (tr. set. 2)
OEstate	0.85	+
SMILES	+	0.85
SMILES augm: 10/10	+	0.88

➡ Predicates (" $<$ ", " $>$ ") and/or optimal classification thresholds are NOT used for statistics (click to

 Refresh



Online chemical database

with modeling environment

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[Database](#)
[Models](#)
[Moderation](#)

Basket browser

Browse, Compare or Join

Filter by name:

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blood-brain-barrier.csv

Esol

Create a model

Apply a model

Create multiple models

Create multiple models with conditions (experimental)

Open predictor

Upload a linear model

Upload a stub model

View pending tasks

View published tasks

SetCompare utility

MolOptimiser

Calculate descriptors

Descriptors storage

Sets

Sets of group flav

Create a model

Select the training and validation sets, the machine learning method and the validation protocol

Select the training and validation sets:

Training set (*required*): [...]

[Add a validation set](#)

Choose the learning method:

Suggested modeling methods:

- ☒ ASNN: ASsociative Neural Networks
- ☐ CHEMCHAINER: Chainer Chemistry models (GPU)
- ☐ ChemProp MPNN for property prediction (GPU)
- ☐ CNF - Convolutional Neural Network Fingerprint (GPU)
- ☐ Consensus model (based on models developed for the same set)
- ☐ DEEPCHEM: several methods from DeepChem (GPU)
- ☐ DNN: Deep Neural Network (GPU)
- ☐ EAGCNG - Edge Attention based Multi-relational Graph Convolutional Networks
- ☐ FSMLR: Fast Stagewise Multiple Linear Regression
- ☐ GNN - Graph Isomorphism Network (GPU)
- ☐ KNN: k - Nearest Neighbors

Home ▾ Database ▾ Models ▾ Moderation ▾

Model Builder X

Select compound set X

Basket browser

Browse, Compare or Join molecule sets

Filter by name: [\[Create new !\[\]\(0fb13ad0bfa3d86868cdd3883e5665b3_img.jpg\)](#) ☒ Show public sets ☐ Sets of group flav

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[Ames challenge \(test\)](#) owned by published, created by midnighter



[Ames challenge \(training\)](#) owned by published, created by midnighter

1 - 2 of 2

Select the training and validation sets:

Training set (*required*): [Ames challenge \(training\)](#) [details]

Validation set #1: [Ames challenge \(test\)](#) [x] [details]

[Add a validation set](#)

The model will predict this property:

AMES using unit: CLASS

☐ Skip model configuration and use the predefined settings

Choose the learning method: ⓘ

Suggested modeling methods:

- ☐ ASNN: ASsociative Neural Networks
- ☐ CHEMCHAINER: Chainer Chemistry models (GPU)
- ☐ ChemProp MPNN for property prediction (GPU)
- ☐ CNF - Convolutional Neural Network Fingerprint (GPU)
- ☒ Consensus model (based on models developed for the same set)
- ☐ DEEPCHEM: several methods from DeepChem (GPU)
- ☐ DNN: Deep Neural Network (GPU)

Model creator

Select model template and training set

Select the preferred data preprocessing options

Preprocessing of molecules (Chemaxon) ⓘ

- ☒ Standardization
- ☒ Neutralize
- ☒ Remove salts
- ☒ Clean structure

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Next>>

Model creator

Select model template and training set

Choose the individual models for consensus

In order to build a consensus model, you must select several (at least two) individual models based on the sel

[\[Add a model\]](#)

Consensus type:

☒ Ignore errors in individual submodels

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Next>>

Model builder - Consensus model X

Select a model X

Models applier browser

The complete list of models at OCHEM available for you is displayed below. If you are new here, you can also switch to a simplified [OCHEM](#)

Submit selected models

Model name or model ID: and property name: Models visibi

1 - 3 of 3




AMES_TRANSNN_1/1 - 343148



AMES_TRANSNN_10/10 - 343053



Ames levenberg 
published by midnighter

1 - 3 of 3

Choose the individual models for consensus

In order to build a consensus model, you must select several (at least two) individual models based on the sele

[Add a model]

Model name	Method
AMES_TRANSNN_1/1 - 343148	TRANSNN [x]
AMES_TRANSNN_10/10 - 343053	TRANSNN [x]

Consensus type: Simple average

☒ Ignore errors in individual submodels

Save the model

Please enter your model's name: Consensus AMES - 344

Model profile 
Statistical parameters, tables, charts - all the information related to the model.

Overview

Applicability domain

Model name: Consensus AMES - 344965 [\[rename\]](#)

Temporal Public ID: 17785953 - use this link to share the model

Predicted property: AMES modeled in CLASS

Training method: Consensus

Data Set	#	Accuracy	Balanced Accuracy	MCC	AUC
Training set: Ames challenge (training)	4356 records	80.8% ± 0.6	80.7% ± 0.6	0.61 ± 0.01	0.882 ± 0.005
Test set: Ames challenge (test) [x]	2180 records	81.9% ± 0.8	81.8% ± 0.8	0.64 ± 0.02	0.886 ± 0.007

Show ROC curves

Real↙/Predicted→	inactive	active	Hit rate
inactive	1593	423	0.79
active	413	1927	0.824
Precision	0.794	0.82	

Real↙/Predicted→	inactive	active	Hit rate
inactive	802	207	0.79
active	187	984	0.84
Precision	0.81	0.83	

Multiple models overview

Predicted property: [AMES](#)

Training set: [Ames challenge \(training\)](#) (2 different versions detected) [?](#)

Metrics [AUC](#) for Training set Validation: [All validation protocols](#)

	ASNN	TRANSNN (tr. set. 2)
OEstate	0.85	+
SMILES	+	0.85
SMILES augm: 10/10	+	0.88
Consensus		
Misc.	0.88	

[↻](#) Predicates (" $<$ ", " $>$ ") and/or optimal classification thresholds are NOT used for statistics (click to change)

[↻](#) Refresh

[📄](#) Export as Excel file

[📄](#) Export as R script

Basket browser [?](#)

Browse, Compare or Join molecule sets

Filter by name: [ames](#) [\[Create new\]](#) [📄](#) ☒ Show public sets ☐ Sets of group me

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📄 📄 📄 🗑️	Ames challenge (test) owned by published, created by midnighter	2181 records	
📄 📄 📄	Ames challenge (training) owned by published, created by midnighter	4361 records	4 models 📄

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