

Basket browser

Browse, Compare or Join molecule sets

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

1 - 15 of 156

<input type="checkbox"/>	  	MDMX owned by published, created by carpovpv
<input type="checkbox"/>	   	ts_mouse_oral_1.sdf owned by published, created by Tinkov_Oleg
<input type="checkbox"/>	 	ws_mouse_oral_1.sdf owned by published, created by Tinkov_Oleg
<input type="checkbox"/>	 	DIR training set owned by published, created by qingshuang0501
<input type="checkbox"/>	  	DIR test set owned by published, created by qingshuang0501
<input type="checkbox"/>	  	Huuskonen_logP (test) owned by published, created by itetko
<input type="checkbox"/>	 	Huuskonen_logP (training) owned by published, created by itetko
<input type="checkbox"/>	  	Delaney owned by published, created by itetko
<input type="checkbox"/>	  	DIR (test) owned by published, created by qingshuang0501
<input type="checkbox"/>	  	DIR (training) owned by published, created by qingshuang0501
<input type="checkbox"/>	  	Anti_TB_Dataset II (test) owned by published, created by vkovalishyn
<input type="checkbox"/>	 	Anti_TB_Dataset II (training) owned by published, created by vkovalishyn
<input type="checkbox"/>	  	Anti_TB_Dataset I (test) owned by published, created by vkovalishyn
<input type="checkbox"/>	 	Anti_TB_Dataset I (training) owned by published, created by vkovalishyn
<input type="checkbox"/>	 	tubulin (training) owned by published, created by hodyna

1 - 15 of 156

Basket browser

Browse, Compare or Join molecule sets

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

1 - 2 of 2

<input type="checkbox"/>	   	Ames challenge (test) owned by published, created by midnighter
<input type="checkbox"/>	 	Ames challenge (training) owned by published, created by midnighter

1 - 2 of 2

2181 records

4361 records

3 models 

Predicted property: [AMES](#)

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

Metrics for Validation:

	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 for Validation:

	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 are NOT used for statistics (click to change)

 Refresh

 Export as Excel file

 Export as R script

Predicted property: AMES

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

Metrics for Validation:

	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

Predicted property: [AMES](#)

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

Metrics [AUC](#) [v](#) for [Training set](#) [v](#) 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](#)

Online chemical database
with modeling environment

Home ▾ Database ▾ Models ▾ Moderation ▾

Basket browser [i](#)
Browse, Compare or Join

Filter by name:
1 - 15 of 102

-
-
-
-
-

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

[blood-brain-barrier.csv](#)

[Esol](#)

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

1 - 2 of 2



[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:

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

<<Back

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

[<<Back](#)

[Next>>](#)

Model builder - Consensus model X

Select a model X

Models aplier 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

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 sele

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

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

Consensus type: 

Ignore errors in individual submodels

Model creator

Select model template and training set

Save the model

Please enter your model's name:

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

1 - 2 of 2

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

1 - 2 of 2