



**C CHEM
BENCH**

**ACCELERATING CHEMICAL GENOMICS
RESEARCH BY CHEMINFORMATICS**

**C-ChemBench
User Guide**



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INTRODUCTION

About this Document

User Guide document is intended for users of C-ChemBench web server. This document describes how to use the web service and contains a brief description of methods implemented in it.

About C-ChemBench web service

The C-ChemBench provides: a web-based user interface for Quantitative Structure-Activity Relationship (QSAR) analysis; access to data mining; library design; building the models; calculation of MolconnZ and Atom Pair descriptors; making predictions on sets of compounds and activity of the molecules. The C-ChemBench web server is available online: <http://ceccr.ibiblio.org/c-chembench>.



1 GETTING STARTED

1.1 Logging in to C-ChemBench web service

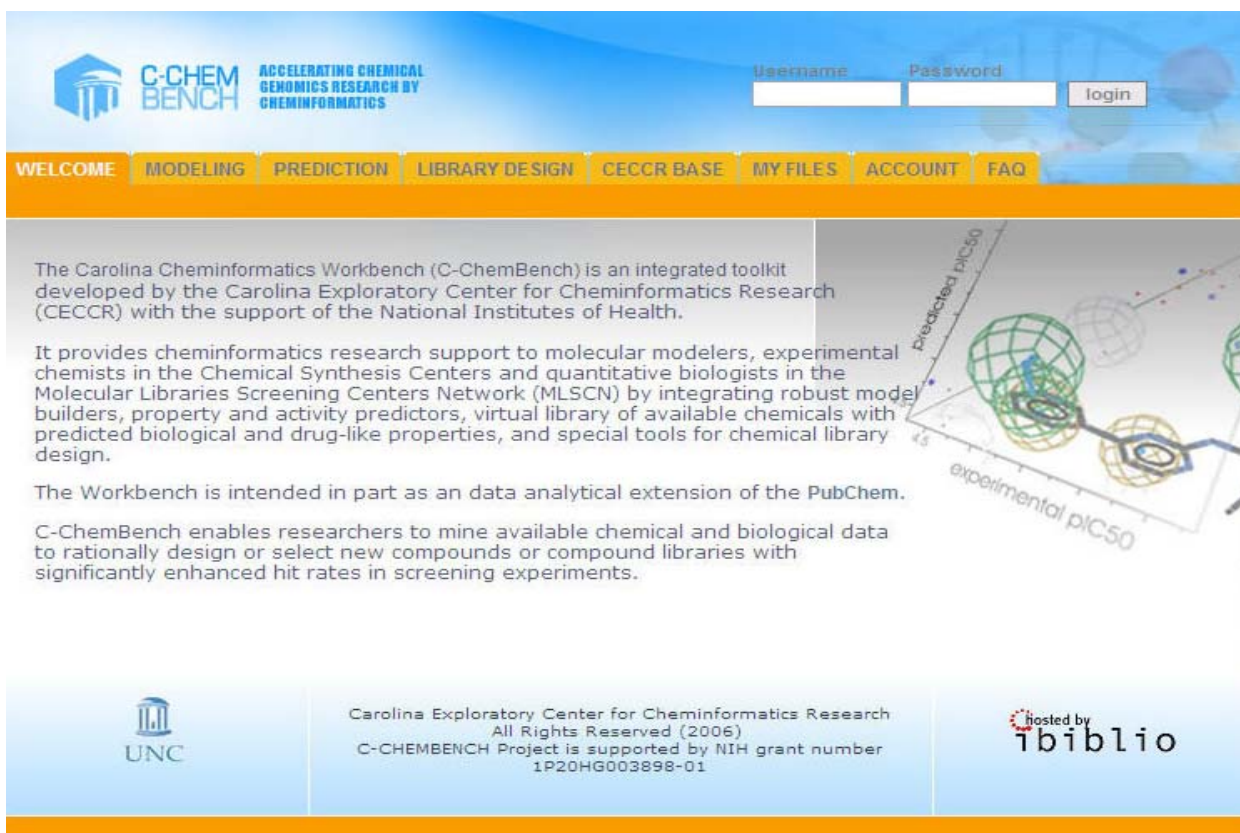
To start the C-ChemBench, do the following:

1. Start Web browser Firefox or Internet Explorer.

Note *C-ChemBench supports Firefox and Internet Explorer.*

2. In the Address bar, enter the C-ChemBench URL address: <http://ceccr.ibiblio.org/c-chembench>. The main window of the C-ChemBench and the **Welcome** tab opens (see Figure 1).
3. To login to the C-ChemBench, enter your **Username** and **Password**, and click **login**.

Figure 1 C-ChemBench main window



Note *Only if you are registered in C-ChemBench you have the rights to log on to the system.*




1.2 Registering to C-ChemBench web service

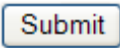
1. To register to the system, expand **Account** in the main C-ChemBench menu (see Figure 2).



2. In the appropriate fields type in: **First name, Last name, Name of organization, Position in organization, Address, City, State/Province, Zip Code, Phone Number** (Example: (001)919-966-3459), **Email** (Please, use your organization email account), **User Name** (Note, that the user name should be at least 4 characters).

Select from the drop down list the following information: **Type of organization, Country, Work Bench.**

3. Type in the two words you see in the box (in order and separated by a space) in the **Verification** field. If you are not sure what the words are, click the **Get the new challenge** reload button . Visually impaired users can click the **Get the audio challenge** audio button  to hear a set of digits that can be entered instead of the visual challenge. If you still have a problem, click **Help** button .)

4. Press  to save the information or  to discard it.

Note

*Your password will be sent to you by email. Once a user account has been set up for you, you will be able to login (by providing your **Username** and **Password** and by pressing **login** button in the right upper part of the main page), logout (by pressing **logout** button in the right upper part of the main page), change your password (for more details see section [7 Account](#)), etc. by completing the appropriate form.*



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Figure 2 Account (for unregistered user) window

The screenshot shows the C-CHEM BENCH website's account registration page. At the top, there is a navigation bar with links: WELCOME, MODELING, PREDICTION, LIBRARY DESIGN, CECCR BASE, MY FILES, ACCOUNT, and FAQ. The main content area features a welcome message and a registration form. The form includes fields for First Name, Last Name, Type of Organization (Academia), Name of Organization, Position in Organization, Address, City, State/Province, Country (United States), Zip Code, Phone Number, Email, Work Bench (C-CHEM), and User Name. A verification section with a CAPTCHA is also present. The CAPTCHA image shows the words 'cats' and 'Wechschrift' in a stylized font. Below the CAPTCHA is a text input field and a 'Type the two words:' label. The CAPTCHA logo includes the text 'no CAPTCHA stop spam, read books, read books, read books'. At the bottom of the form are 'Reset' and 'Submit' buttons.

First Name

Last Name

Type of Organization **Academia**

Name of Organization

Position in Organization

Address

City

State/Province

Country **United States**

Zip Code

Example: 0001210-840-3452

Phone Number

Please use your organization email account

Email

Work Bench **C-CHEM**

The user name must be at least 4 characters

User Name

Verification

Type the two words:

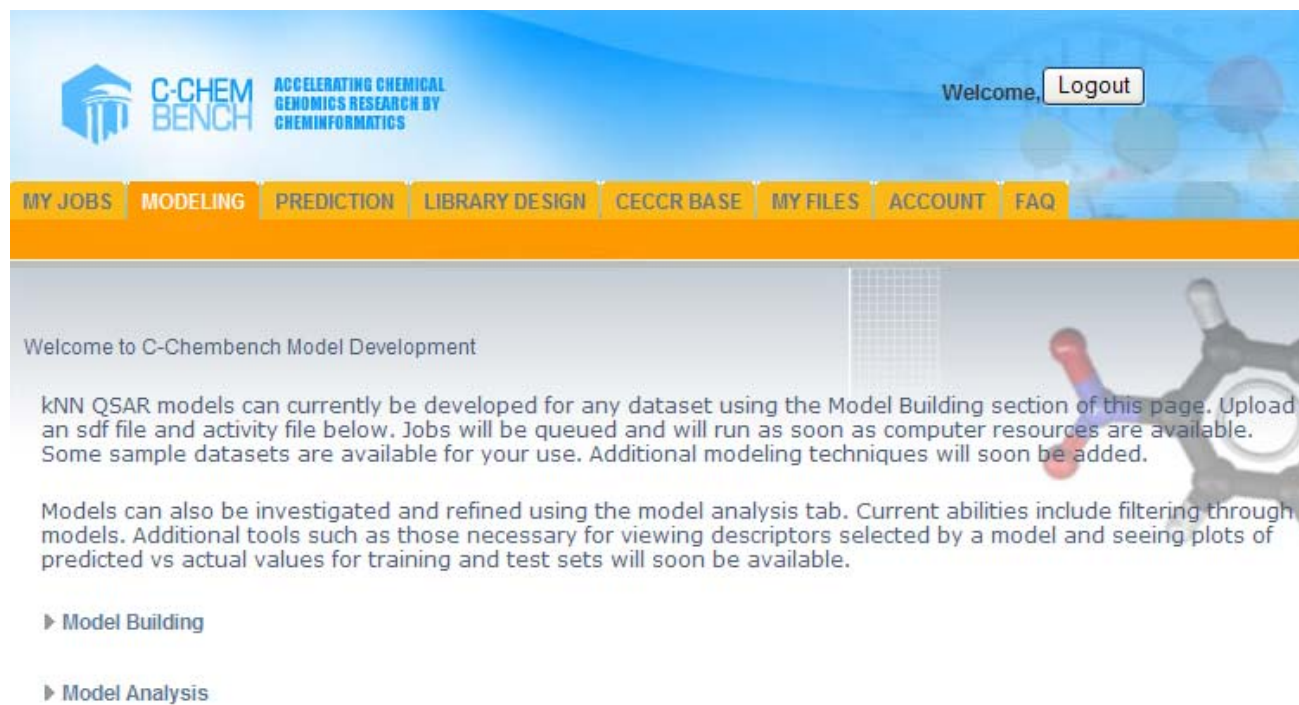
no CAPTCHA stop spam, read books, read books, read books



2 MODELING

After you are logged in to the system, the **Modeling** tab opens (see Figure 3). 'Modeling' gives you the possibility to build your own models and to analyze them. **Welcome** tab is changed onto the **My Jobs** tab.

Figure 3 Modeling (starting) window



2.1 Model Building

1. To build a model, click **Model Building** (see Figure 4). It enables you to build the models step by step.

You should specify the following properties: **Project Type**; **Data Set**; **Tool**; **Descriptors**; **Data Set Division**; **Job Name**.

2. Click **Project Type** and specify the **Modeling Type** by selecting the radio button:
 - QSAR Continuous – for predicting activities values which are continuous;
 - QSAR Category - for predicting activities values which are discrete.



Figure 4 Modeling Type dialog

▼ Model Building

▼ Project Type

Modeling Type: ☐ QSAR Continuous
☒ QSAR Category
☐ Pharmacophore
☐ Docking

3. Click **Data Set** (see Figure 5) and choose the appropriate radio button:
- Select A Previously Uploaded Data Set (You have the possibility to select public as well as your own files from the drop-down list)
 - Upload a Data Set (You have the possibility to upload your own files. User's dataset files should include a molecule file in SDF format and an activity file)

Note

SD File is Structure Data Format file. For more details, see <http://www.epa.gov/ncct/dsstox/MoreonSDF.html>.

ACT File (Activity File) has the following structure: One line per compound: *compound_name activity_value (category)*; Categories must be non-negative consecutive whole numbers.

Figure 5 Data Set dialog

▼ Data Set

☒ Select A Previously Uploaded Data Set:

Data Sets: activator_protein_43 ▼

Activity Histogram

☐ Upload A Data Set:

SD File: Browse...

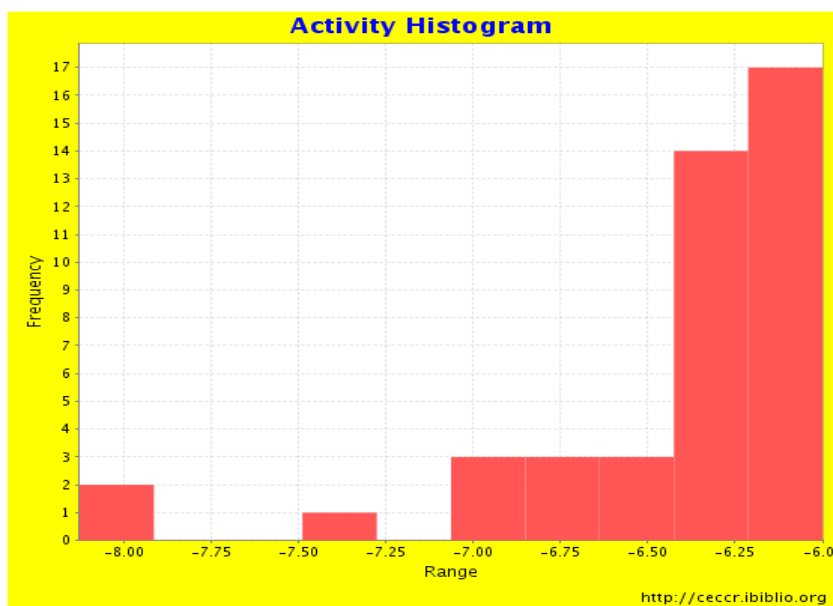
ACT File: Browse...

Activity Histogram

To view the number of the molecules in each interval of activity, press **Activity Histogram** (see Figure 5) button. The 'Activity Histogram' window appears (see Figure 6). The horizontal axis shows the range of activities and its division into bins and the vertical axis shows the number of compounds with activities within bins.

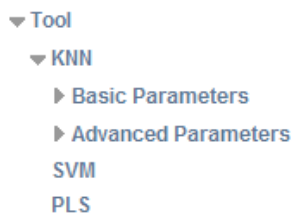


Figure 6 Activity Histogram window



- Click **Tool** (see Figure 7) and select **KNN** (k nearest neighbors QSAR method). You have the possibility to edit basic and advanced parameters. To specify them, click **Basic Parameters** (see Figure 8) and then **Advanced Parameters** (see Figure 9 and Figure 10).

Figure 7 Tool dialog



Basic parameters (see Figure 8) include: Descriptor step size, Minimum Number of Descriptors selected, Maximum Number of Descriptors selected, and the Number of Runs for each set of parameters.

Figure 8 Basic Parameters dialog

▼ Basic Parameters

Descriptor Step Size:	<input type="text" value="5"/>
Minimum Number of Descriptors:	<input type="text" value="5"/>
Maximum Number of Descriptors:	<input type="text" value="20"/>
Number of Runs:	<input type="text" value="5"/>

If in the step 2 (see Figure 4) you have selected *QSAR Continuous* modeling type, the **Advanced parameters** will be the following (see Figure 9): Number of Nearest Neighbors, Percentage of



Pseudo Neighbors, Number of Permutations of selected descriptors, Number of Cycles, Initial Temperature, Final Temperature, Temperature Coefficient Mu, Minimum acceptable q^2 , Minimum acceptable r^2 , Minimum and Maximum slopes for regressions through the origin for predicted vs. observed and observed vs. predicted activities, coefficients of determination for regressions through the origin, Applicability Domain Cutoff model parameter.

Figure 9 Advanced Parameters (for Continuous kNN) dialog

▼ Advanced Parameters

Number of Nearest Neighbors:	<input type="text" value="5"/>
Percentage of Pseudo Neighbors:	<input type="text" value="100"/>
Number of Permutations:	<input type="text" value="2"/>
Number of Cycles:	<input type="text" value="1000"/>
Initial Temperature:	<input type="text" value="100"/>
Final Temperature:	<input type="text" value="-5.0"/>
Mu:	<input type="text" value="0.90"/>
Minimum q^2 :	<input type="text" value="0"/>
Minimum r^2 :	<input type="text" value="0"/>
Minimum Slope:	<input type="text" value="0.8"/>
Maximum Slope:	<input type="text" value="1.2"/>
Relative_diff_R_R0:	<input type="text" value="0.2"/>
Diff_R01_R02:	<input type="text" value="0.4"/>
Applicability Domain Cutoff:	<input type="text" value="1.0"/>

If in the step 2 (see Figure 4) you have selected *QSAR Category* modeling type, the **Advanced parameters** will be the following (see Figure 10): Number of Nearest Neighbors, Percentage of Pseudo Neighbors, Number of Permutations of selected descriptors, Number of Cycles, Initial Temperature, Final Temperature, Temperature Coefficient Mu, Minimum Accuracy of classification for Training Set, Minimum Accuracy of classification for Test Set, Applicability Domain Cutoff model parameter. Also, you have to specify the Optimization Method, by selecting the appropriate radio button.



Figure 10 Advanced Parameters (for Category kNN) dialog

▼ Advanced Parameters

Number of Nearest Neighbors:	<input type="text" value="5"/>
Percentage of Pseudo Neighbors:	<input type="text" value="100"/>
Number of Permutations:	<input type="text" value="2"/>
Number of Cycles:	<input type="text" value="1000"/>
Initial Temperature:	<input type="text" value="100"/>
Final Temperature:	<input type="text" value="-5.0"/>
Mu:	<input type="text" value="0.9"/>
Minimum Accuracy for Training Set:	<input type="text" value="0"/>
Minimum Accuracy for Test Set:	<input type="text" value="0"/>
Applicability Domain Cutoff:	<input type="text" value="1.0"/>
Optimization Method:	<div><div><input type="radio"/></div>$\frac{N_{correct}}{N_{total}}$</div> <div><div><input checked="" type="radio"/></div>$\frac{1}{N_{class}} \sum \frac{N_{correct}}{N_{total}}$</div> <div><div><input type="radio"/></div>$1 - \frac{error}{error_{max}}$</div> <div><div><input type="radio"/></div>$1 - \frac{error_{norm}}{error_{norm,max}}$</div>

5. Click **Descriptors** (see Figure 11) and select from the drop-down list 'MolconnZ' descriptors. You have the possibility to normalize descriptors, by selecting 'Range Scaling' radio button.

Figure 11 Descriptors dialog

▼ Descriptors

Descriptors:

Normalization:

☒

 Range Scaling

☐

 Auto Scaling

☐

 None

6. Click **Data Set Division** (see Figure 12) and select 'Split into External Validation' from the drop-down list of **Data Set Division**. The External Validation Data Set will be selected from the entire dataset randomly.



Enter the **Numbers of Compounds in the External Set** and choose the **Splitting Method**, by selecting 'Sphere Exclusion' radio button. Provide **Number of Sphere Radii** and **Number of Starting Points** included in the training set. Select from the drop-down list the **Selection of Next Training Set Point** that is based on the following:

- Random Selection of Next Training Set Point (In this case, the next point of the training set is selected randomly.)
- Minimum Sphere Center Distances (In this case, the next point of the training set is selected as the point closest to the center of one of the previous spheres.)
- Maximum Sphere Center Distances (In this case, the next point of the training set is selected as the point closest to one of the sphere centers among farthest from the centers of all of the previous spheres.)

Figure 12 Data Set Division dialog

7. Enter the **Job Name** (see Figure 13).

Figure 13 Job Name dialog

2.2 My Jobs

1. After pressing **Submit Workflow** button (see Figure 13), **My Jobs** tab opens (see Figure 14). The list of active tasks and tasks in the queue appears in the table.

My Active Tasks contain the following information:



- Name – the name of the job;
- Submitted – date and time of submitting the data;
- Status – the status of the job ('started' or 'finished');
- Started – date and time of starting to process data;
- Finished – date and time of finishing to process data.

Tasks in the Queue contain the following information:

- Name – the name of the job;
- Owner – your name (if it is your job) or 'other user';
- Submitted – date and time of submitting the data;
- Status – the status of the job ('ready' or 'permission required').

Note

'Permission Required' Status appears if the files you submitted have more than 200 compounds or 10 000 models. In this case, the administrator will be notified and may give you permission to perform the processing of data.

2. Select the finished job, by clicking on its appropriate name.

To check the status of your job, press **Refresh Status of Your Tasks** button.



Figure 14 My Jobs window

Welcome, Natalya [Logout](#)

MY JOBS | MODELING | PREDICTION | LIBRARY DESIGN | CECCR BASE | MY FILES | ACCOUNT | FAQ

Visited: 338 Online: 1

My Active Tasks

Name	Submitted	Status	Started	Finished
Ingeneer	2008-04-02 17:00:00.0	start	2008-04-02 17:00:00.0	
research 4	2008-04-08 12:59:06.0	start	2008-04-08 14:03:29.0	
22 practice	2008-04-08 13:07:40.0	start	2008-04-08 13:07:41.0	
33	2008-04-08 15:20:06.0	finished	2008-04-08 21:48:45.0	2008-04-08 22:19:28.0
14 project	2008-04-09 11:03:42.0	start	2008-04-09 11:03:42.0	

Tasks in the Queue

Name	Owner	Submitted	Status
26 Chem	Natalya	2008-04-09 11:04:54.0	PermissionRequired
19 Chem	Natalya	2008-04-09 15:32:43.0	Ready

To check the status of your job, please use the following refresh button (do not use your web browser's refresh button):

[Refresh Status of Your Tasks](#)

2.3 Model Analysis

- After clicking on the name of the finished job at 'My Jobs' tab (see Figure 14), the **Modeling** tab opens (see Figure 15). On the 'Modeling' page you can: find the information about the number of generated models and which passed training and test set criteria; view the list of properties with the following attributes:
 - Job Name – the name of the job given by you;
 - Date Created – date and time the model was built;
 - SD File – structure file used for model generation;
 - ACT File – activity file used for model generation;
 - Modeling Method – either QSAR Continuous or QSAR Category;



- Descriptor Generation Method – (MolconnZ).

Figure 15 Modeling (after generation) window

Job Name: 454, Date Created: 2008-04-08 13:35:34.0, SD File: activator_protein_43.sdf, ACT File: activator_protein_43.act, Modeling Method: QSAR Continuous, Descriptor Generation Method: MOLCONNZ

Of the 20 models generated, 20 passed the training set criteria and 1 passed both training and test set criteria. The top 1 models are displayed below.

Buttons: Save Models, Discard Models, Download Modeling Report

nnn	q ²	n	r	r ²	R ₀₁ ²	R ₀₂ ²	k1	k2
1	0.398	12	0.831	0.691	0.673	0.649	1.002	0.998

2. To download the zip file version of the modeling report, click **Download Modeling Report** button.
3. To view the results of randomization, click **Y Randomization Results** (see Figure 16).

Y Randomization is a statistical QSAR model validation technique where the performance of the model built with original data is compared to that of models built for multiple artificial datasets with randomly shuffled activities. Ideally, there will be no models with high values (> 0,6) of both q² (training set) and R² (test set) found.

The top few models are displayed with the following properties:

- nnn – number of nearest neighbors used for making the activity prediction with this model;
- Training Accuracy = $\frac{\text{\# of correct predictions}}{\text{\# of total compounds}}$ for training set
- Normalized Training Accuracy =
$$= \frac{1}{\text{\# of classes}} \left(\frac{\text{\# of correct class1}}{\text{\# of total compound class1}} + \frac{\text{\# of correct class2}}{\text{\# of total compound class2}} \right)$$



$$\text{NTA} = \frac{1}{\# \text{ of classes}} \sum_{N=1: \# \text{ of classes}} \left(\frac{\# \text{ of correct predictions for class } N}{\# \text{ of total compounds for class } N} \right) \text{ for training set}$$

▫ Test Accuracy = $\frac{\# \text{ of correct predictions}}{\# \text{ of total compounds}}$ for test set

▫ Normalized Test Accuracy =
$$= \frac{1}{\# \text{ of classes}} \left(\frac{\# \text{ of correct class1}}{\# \text{ of total compound class1}} + \frac{\# \text{ of correct class2}}{\# \text{ of total compound class2}} \right)$$

$$\text{NTA} = \frac{1}{\# \text{ of classes}} \sum_{N=1: \# \text{ of classes}} \left(\frac{\# \text{ of correct predictions for class } N}{\# \text{ of total compounds for class } N} \right) \text{ for test set}$$

Figure 16 Y Randomization Results dialog

Y Randomization Results

Y-randomization is a statistical QSAR model validation technique where the performance of the model built with original data is compared to that of models built for multiple artificial datasets with randomly shuffled activities. Ideally, there will be no models with high values (> 0.6) of both q^2 (training set) and R^2 (test set) found.

For your data, **20** models for randomized datasets were built and **0** models were found to have high prediction accuracy.

nnn	q^2	n	r	r^2	R_{01}^2	R_{02}^2	k1	k2
-----	-------	---	---	-------	------------	------------	----	----

You have the possibility to view the **External Validation Results** (see Figure 17) with the following properties:

- Comp_ID – ID of the compound;
- Structure – the two-dimensional structure of compound;
- Observed Value – the value of the activity for the compound as submitted in the ACT file;
- Predicted Value – the value of the activity for the compound as predicted by the consensus of models;
- Residual – difference between the Observed Value and Predicted Value;
- # of Models – number of models for which this compound was within the applicability domain.



Figure 17 External Validation Results dialog

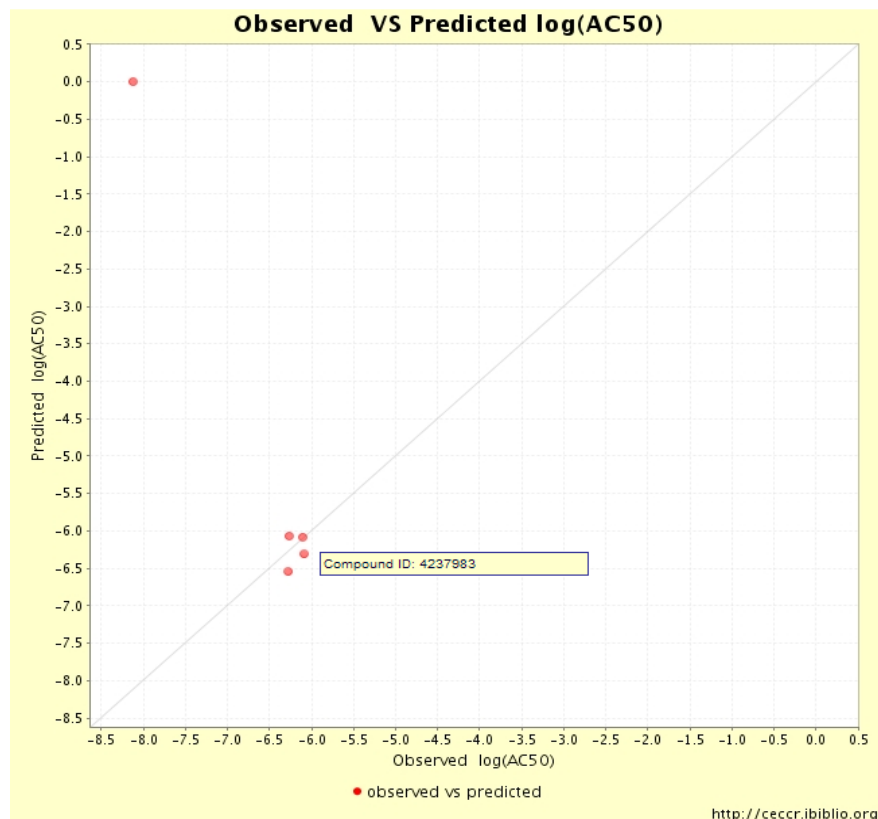
External Validation Results: [Chart View](#)

Comp_ID	Structure	Observed Value	Predicted Value	Residual	# of Models
857019	<div><div>857019</div><div>101</div></div>	-6.09	-6.31	0.22	1

To view the chart of the predicted versus actual activities for the external molecules, click [Chart View](#). The 'Observed vs Predicted log' window appears (see Figure 18). The horizontal axis shows the observed activity as uploaded in your activity file and the vertical axis shows the predicted activity by the models, which you generated. Each red circle represents a single molecule.



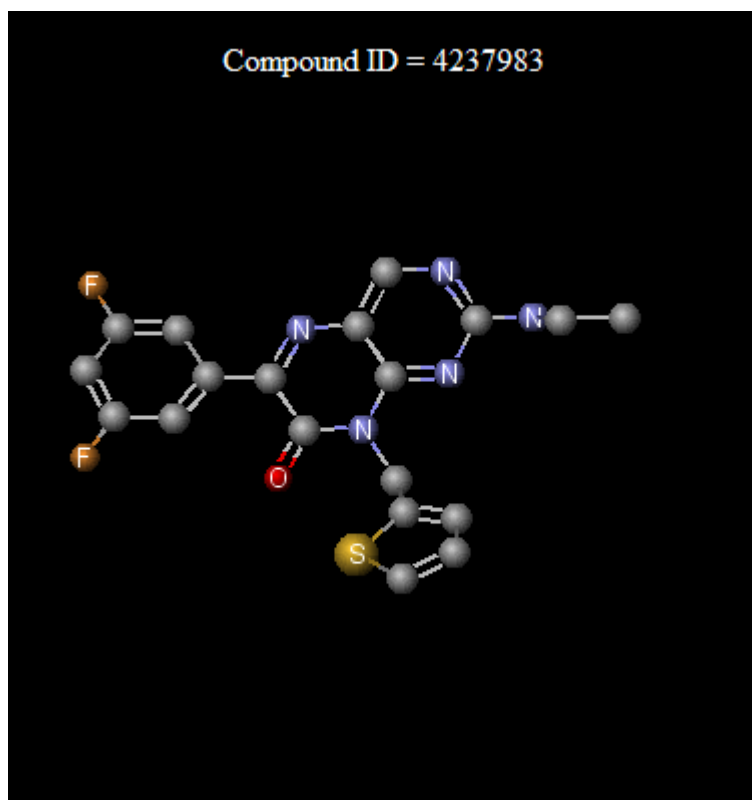
Figure 18 Observed vs Predicted log window



If you point the mouse cursor at the red circle, the compound ID appears. To view the 3-D model of the compound structure, click on the corresponding red circle. The 'Compound ID' window appears (see Figure 19).




Figure 19 Compound ID window



4. Press **Save Models** button to save the information or **Discard Models** button to discard it (see Figure 15).
5. After you saved the model, you have the possibility to view the list of all predictors, which were generated previously, by clicking **Model Analysis** (see Figure 20).
6. The system reflects the following predictor features: **Name**, **Date Created**, **Modeling Type**, **Descriptor Generation Method**, and **Download**.
7. To download the zip file version of the model, click **download**. Every necessary file for your model as well as all files generated for external validation will be downloaded.
8. Choose the necessary predictor, by selecting the appropriate radio button.
9. To view the models associated with the predictor and to be able to edit information, press **Edit** button.



Figure 20 Modeling (Predictor list) window

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Welcome, Natalya [Logout](#)

[MY JOBS](#) [MODELING](#) [PREDICTION](#) [LIBRARY DESIGN](#) [CECCR BASE](#) [MY FILES](#) [ACCOUNT](#) [FAQ](#)

Welcome to C-Chembench Model Development

kNN QSAR models can currently be developed for any dataset using the Model Building section of this page. Upload an sdf file and activity file below. Jobs will be queued and will run as soon as computer resources are available. Some sample datasets are available for your use. Additional modeling techniques will soon be added.

Models can also be investigated and refined using the model analysis tab. Current abilities include filtering through models. Additional tools such as those necessary for viewing descriptors selected by a model and seeing plots of predicted vs actual values for training and test sets will soon be available.

► Model Building

▼ Model Analysis

Previously Generated Predictors

Select a predictor and press the Edit button to view the models associated with the predictor.

	Name	Date Created	Modeling Type	Descriptor Generation Method	Download
<input type="radio"/>	454	2008-04-08 13:35:34.0	QSAR Continuous	MOLCONNZ	download
<input type="radio"/>	investigator	2008-04-08 15:30:32.0	QSAR Category	MOLCONNZ	download
<input checked="" type="radio"/>	33	2008-04-08 23:46:45.0	QSAR Category	MOLCONNZ	download

Edit



3 PREDICTION

1. Expand **Prediction** in the main C-ChemBench menu (see Figure 21). The already developed models are available to make predictions on sets of compounds.
2. Select a predictor from the drop down list.

Figure 21 Prediction (starting) window

3.1 Predictor Applying

1. Click **Apply the Predictor** (see Figure 22).
2. Enter the **Job Name**.
3. Select a database for prediction by choosing the appropriate radio button:
 - Select a Publicly Available Database (You have the possibility to select public as well as your own files from the drop-down list)
 - Upload an SD File to Predict (You have the possibility to upload your own files. User's dataset files should include a molecule file in SDF format and an activity file)



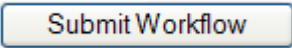
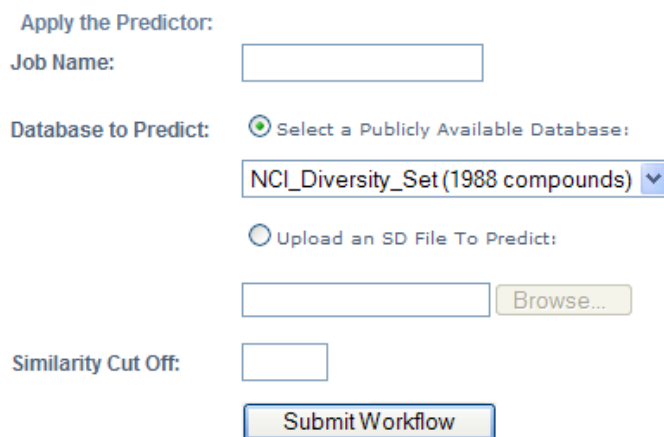
4. Enter the **Similarity Cut Off** value — it is the parameter which defines the model applicability domain. The higher the Z Cutoff is, the larger the applicability domain is and the more compounds from external datasets are predicted. Do not make it more than 3.
5. Press  button to save the information.

Figure 22 Apply the Predictor dialog



Apply the Predictor:

Job Name:

Database to Predict: ☒ Select a Publicly Available Database:

▼

☐ Upload an SD File To Predict:

Similarity Cut Off:

Note After pressing **Submit Workflow** button, **My Jobs** tab opens. For more details, see section [2.2My Jobs](#).

3.2 Prediction Analysis

1. After clicking on the name of the finished job at 'My Jobs' tab (see Figure 14), the **Prediction** tab opens (see Figure 23). On the 'Prediction' page you can view the list of properties with the following attributes:
 - Prediction Name - the name of the prediction given by you;
 - Date Created - date and time the prediction was made;
 - Predictor used – the name of predictor used for the prediction;
 - Database Predicted – the name of the chemical database on which predictions were made;
 - Similarity Cutoff – the similarity cutoff used for this prediction.

You have the possibility to view the results with the following properties:

- Comp_ID – ID of compounds;
- Structure – the two-dimensional structure of the predicted compound;
- Standard Deviation – the standard deviation in the predicted value based on individual model predictions;



- Predicted Value – the value of the activity for the compound as predicted by the consensus of models;
- Number of Models – number of models for which this compound was within the applicability domain.

Figure 23 Prediction (after generation) window

Information About the Selected Prediction:

Prediction Name	Date Created	Predictor Used	Database Predicted	Similarity Cutoff
43	2008-04-14 16:04:07.0	33	NCI_Diversity_Set	2.0

Save Prediction Delete Prediction Download Prediction

1 -- 20 of 1988 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 »»

Comp_ID	Structure	Standard Deviation	Predicted Value	Number of Models
479		0.396628	0.54855	20

2. To view the current prediction result table, click **Download Prediction**.
3. Press **Save Prediction** button to save the information or **Delete Prediction** button to discard it (see Figure 23).
4. After you saved the prediction, you have the possibility to view the list of all predictions, which were generated previously, by clicking **View Previous Predictions** (see Figure 24).
5. The system reflects the following predictor features: **Name**, **Date Created**, **Predictor**, **Database Predicted**, and **Download**.



6. To download the prediction results, click **download**. All necessary files for your model as well as all files generated while making your predictions will be downloaded.
7. Choose the necessary prediction, by selecting the appropriate radio button.
8. To view the predictions associated with the predictor, press **View** button.

Figure 24 Prediction (including results) window

Welcome to C-ChemBench Predictors

Here already developed models are available to make predictions on sets of compounds. Models generated and validated by the Laboratory for Molecular Modeling at UNC-CH are available as well as models that you generated through the Model Development section of the website. Compounds to screen can be upload in sdf format below. Currently, only 500 compounds may be predicted at one time. Compound databases will soon be available for large scale virtual screening

Choose a Predictor:

33

Apply the Predictor:

View Previous Predictions:

	Name	Date Created	Predictor	Database Predicted	Download
<input checked="" type="radio"/>	32	2008-04-14 13:57:34.0	investigator	NCI_Diversity_Set	download
<input type="radio"/>	investigator	2008-04-14 13:59:06.0	investigator	NCI_Diversity_Set	download
<input type="radio"/>	43	2008-04-14 16:04:07.0	33	NCI_Diversity_Set	download
<input type="radio"/>	22	2008-04-22 13:36:14.0	454	NCI_Diversity_Set	download

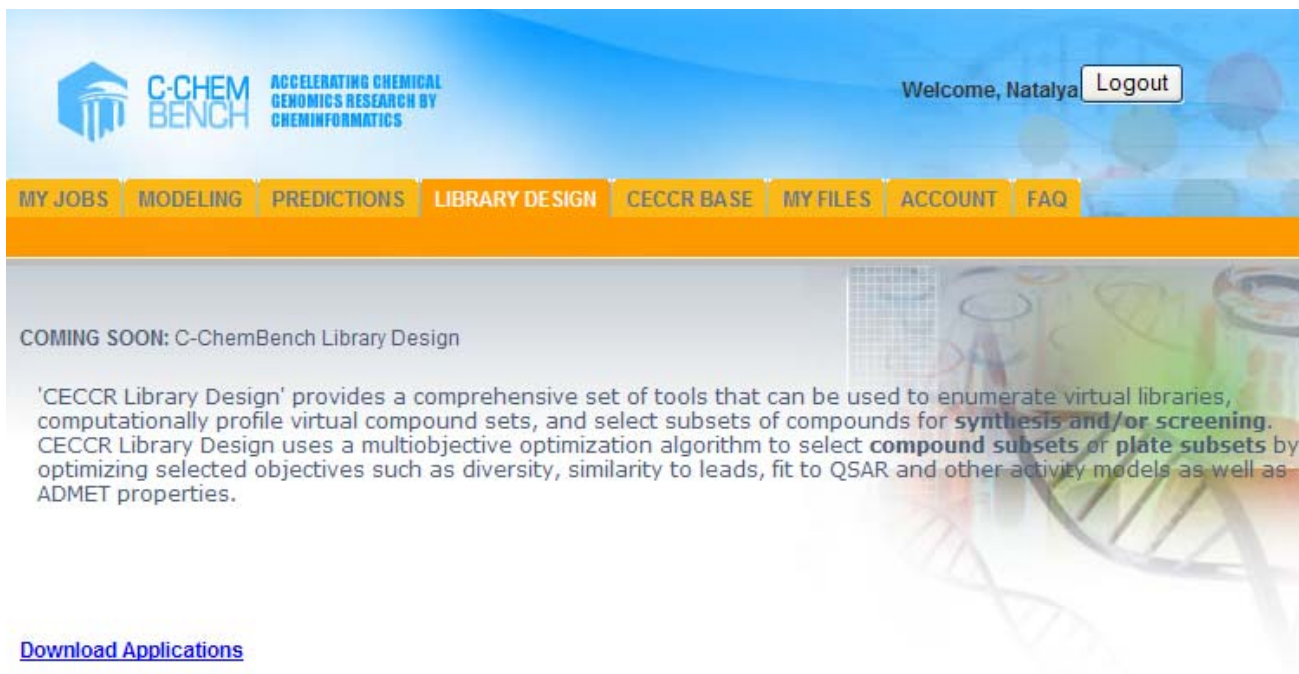
View



4 LIBRARY DESIGN

1. Expand **Library Design** in the main C-ChemBench menu (see Figure 25). 'Library Design' provides an access to tools which allow the generation of virtual chemical libraries.
2. Click **Download Applications**.

Figure 25 Library Design window



3. The list of downloaded applications appears with the following features: **Application Name**, **Description**, **Download** (see Figure 26).
4. To download the zip file version of the applications used in model generation, click **download**.



C-CHEM
BENCH

ACCELERATING CHEMICAL GENOMICS
RESEARCH BY CHEMINFORMATICS

Figure 26 Library window

Welcome, Natalya [Logout](#)

MY JOBS MODELING PREDICTION **LIBRARY** CECCR BASE MY FILES ACCOUNT FAQ

Application Name	Description	Download
AllKnn2LIN_nl	decription	download
AllKnn_category_nl	description	download
ChemFeaturePair	description	download



5 CECCR BASE

1. Expand **CECCR Base** in the main C-ChemBench menu (see). 'CECCR Base' provides an access to the data base, which contains chemical information and biological pathways. Base provides an access to a large chemical database containing virtual activities and providing links to biological information.



6 MY FILES

1. Expand *My Files* in the main C-ChemBench menu (see). 'My Files' allows management of all the files which were uploaded by you in the 'Data Set' section of 'Model Building' tab (see Figure 5).



7 ACCOUNT

1. Expand **Account** in the main C-ChemBench menu (see). The 'Account' tab opens, where you have the possibility either to register to the system (for more details see section [1.2 Registering to C-ChemBench web service](#)), or, in case if you are already registered user, to change your password.
2. To change your password, enter: your **Old Password** and **New Password**.
3. Enter your new password once more in the **Confirm Password** field.
4. Press **Submit** button to save the information or **Reset** button to discard it.

Figure 27 Account (for registered user) window

The screenshot shows the 'ACCOUNT' tab selected in the top navigation bar. The page header includes the C-CHEM BENCH logo and the text 'ACCELERATING CHEMICAL GENOMICS RESEARCH BY CHEMINFORMATICS'. A welcome message 'Welcome, Natalya' and a 'Logout' button are visible. The main content area is titled 'Change password here' and contains three input fields: 'Old Password', 'New Password', and 'Confirm Password'. Below these fields are 'Reset' and 'Submit' buttons. A 3D molecular model is displayed on the right side of the page.