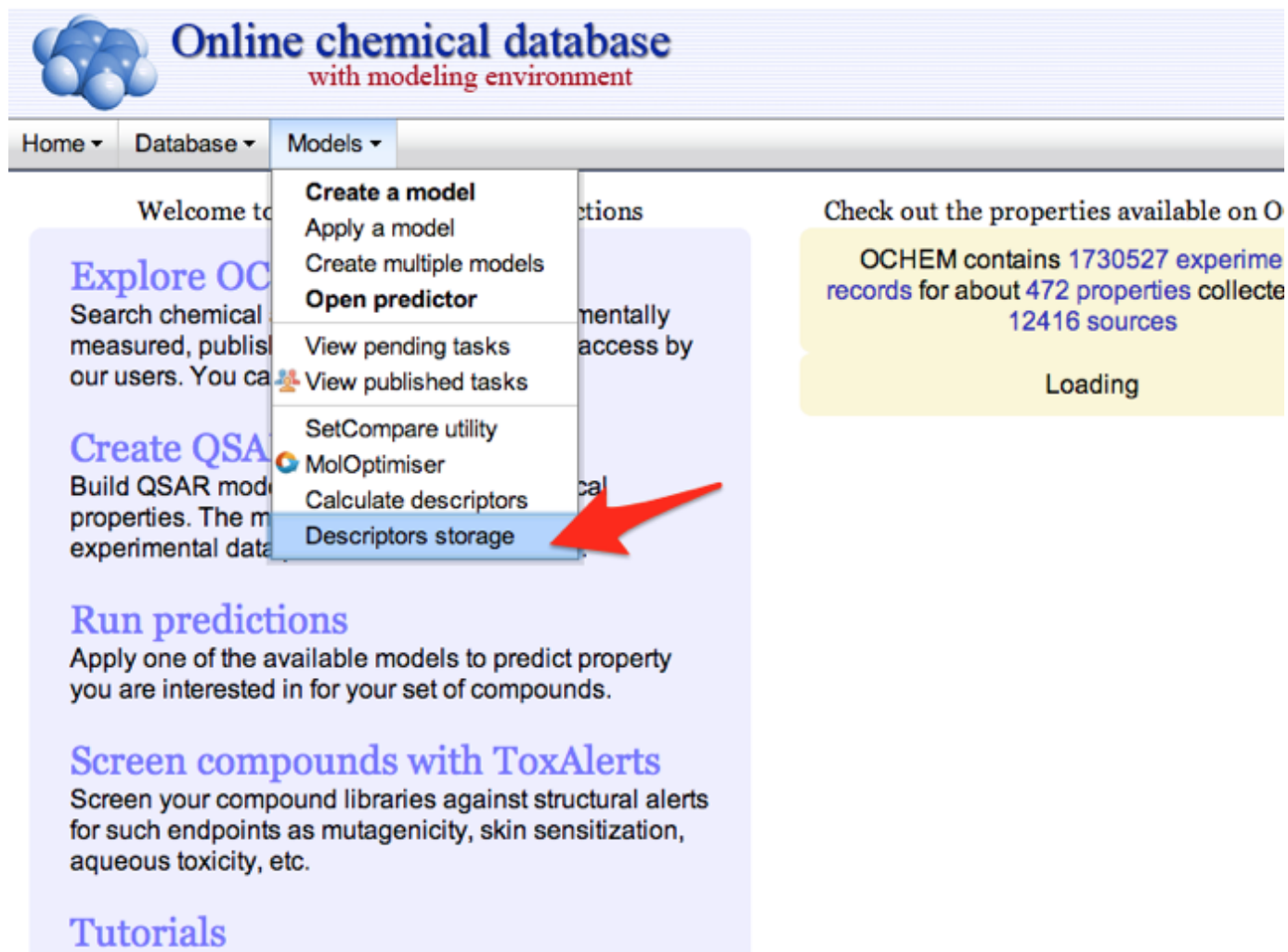


Custom descriptors from a file

1) Under “Models” >select “Descriptor storage”.



The screenshot shows the 'Online chemical database with modeling environment' website. The navigation bar includes 'Home', 'Database', and 'Models'. The 'Models' dropdown menu is open, displaying options such as 'Create a model', 'Apply a model', 'Create multiple models', 'Open predictor', 'View pending tasks', 'View published tasks', 'SetCompare utility', 'MolOptimiser', 'Calculate descriptors', and 'Descriptors storage'. A red arrow points to the 'Descriptors storage' option. The main content area features sections for 'Explore OC', 'Create QSA', 'Run predictions', 'Screen compounds with ToxAlerts', and 'Tutorials'. A yellow box on the right contains text about the database's size and a 'Loading' status.

Online chemical database
with modeling environment


Home Database Models

Welcome to
Explore OC
Search chemical
measured, published
our users. You can
Create QSA
Build QSAR models
properties. The model
experimental data
Run predictions
Apply one of the available models to predict property
you are interested in for your set of compounds.
Screen compounds with ToxAlerts
Screen your compound libraries against structural alerts
for such endpoints as mutagenicity, skin sensitization,
aqueous toxicity, etc.
Tutorials

Check out the properties available on O
OCHEM contains 1730527 experime
records for about 472 properties collecte
12416 sources
Loading

Create a model
Apply a model
Create multiple models
Open predictor
View pending tasks
View published tasks
SetCompare utility
MolOptimiser
Calculate descriptors
Descriptors storage


2) Select “Upload precalculated descriptors”





Online chemical database

with modeling environment

Home ▾ Database ▾ Models ▾ Moderation ▾

 **Descriptors storage overview (under construction!)**
An overview of the cached and externally uploaded descriptor values

 [Upload precalculated descriptors](#) 

You don't have any descriptors in the storage. Try uploading some.

Descriptors stored in the public cache

Descriptor type	Entries	Storage size	Operations
Adriana	222533	274504200 bytes	
Adriana	199711	271206558 bytes	
CDK	407989	526150499 bytes	
ChemaxonDescriptors	245773	514195604 bytes	
ChemaxonDescriptors	79167	121786258 bytes	

3) Give a name to the Descriptor set

4) You can upload an Excel file with the descriptors and either the molecular structure (with column header "MOLECULE") or just an identifier (with column header "EXTERNAL_ID"). This ID can be for example: **AZ12345**. I am attaching an exemplary Excel file

This is how the form may look like.

OCHEM allows you to use your own precalculated descriptor values for the development of QSAR models. You can upload your descriptors as an Excel file with the columns e.g. "MOLECULE (or EXTERNAL_ID for molecule the molecule (e.g. M12345) or SMILES string. A couple of examples with and without molecules: [Exemplary file 1](#) [Exemplary file 2](#)

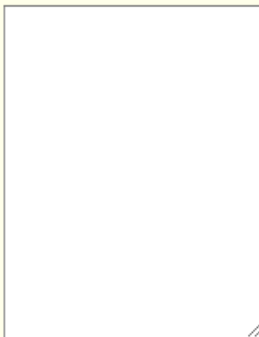
Descriptor type name

e.g., Dragon6, MyCustomDescriptors, E-State

Chemogenomic_Assay_

Descriptor configuration XML

can be empty for your custom descriptors



Excel file with descriptors

first line lists the descriptor names as specified above

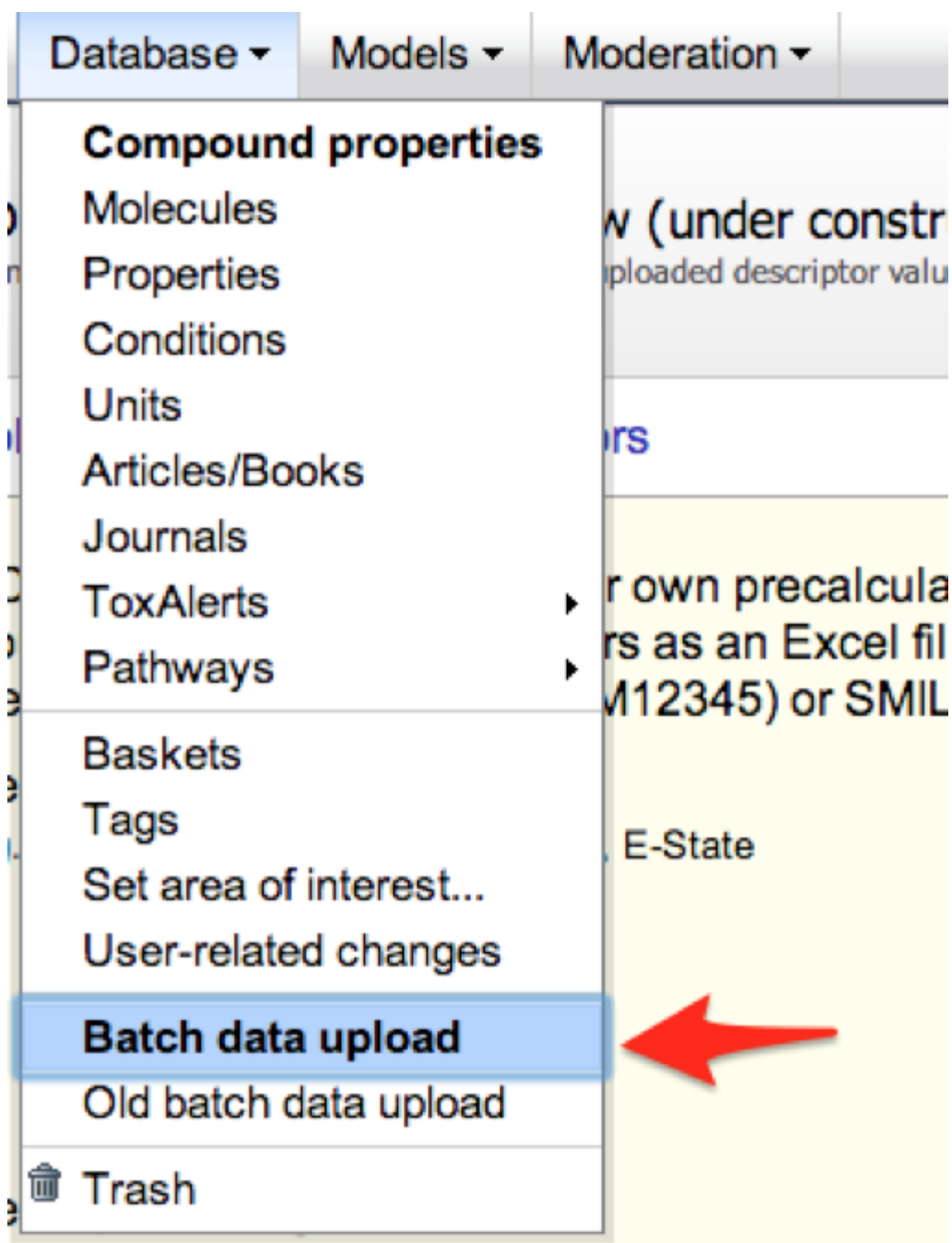
Choose File

custom-descriptors.xls

Start the upload

Cancel

5) You will need to upload the property value for these molecules, the normal way. For example if you try to model LogP, you will need to have the experimental value for **AZ12345** uploaded via batch data upload (or via Knime or Pipeline Pilot).



6) Proceed normally with model building process. On the list of descriptors you can see your uploaded descriptors among other available descriptor packages:

☒ E-state

E-State types:

- ☒ Atom indices
☒ Bonds indices

- ☐ Atom counts
☐ Bonds counts


Aromatize structures: Chemaxon Basic ▾

- ☒ ALogPS (2)
☐ GSFragment (1138)
☐ Dragon v. 6.0 (4885/3D)
☐ ISIDA fragments
☐ ADRIANA.Code (211/3D)
☐ CDK descriptors (246/3D)
☐ 'Inductive' descriptors (54/3D)
☐ MERA descriptors (529/3D)
☐ MERSY descriptors (42/3D)
☐ Chemaxon descriptors (499/3D)
☐ QNPR
☐ Spectrophores (144/3D)

Additional or obsolete descriptors:

- ☐ OEState
☐ MolPrint
☐ Dragon v. 5.4 (1630/3D)
☐ Dragon v. 5.5 (3190/3D)
☐ Structural alerts (ToxAlerts)
☐ MOPAC descriptors (21/3D)
☐ ShapeSignatures (3D)

Stored descriptors ([explore the descriptors storage](#))

- ☐ Chemogenomic_Assay_1 

Experimental descriptors (use only if you know how to use them):

- ☐ Custom descriptors from a file
☐ AMBIT Descriptors
☐ ISIDA fragments (2011) *Not supported by your installation*
☐ Chiral Descriptors (/3D)
☐ Scaffold Hunter Descriptors
☐ ECFP Fingerprints *Not supported by your installation*
☐ Chemaxon Scaffolds
☐ Scaffolds

☐ **Simcos-It Scaffolds**

☐ **Functional Groups**

☐ ETM descriptors *Not supported by your installation*

☐ DockingDescriptors (pre-pre-alfa) *Not supported by your installation*

☐ Experimental values of other properties *Not supported by your installation*