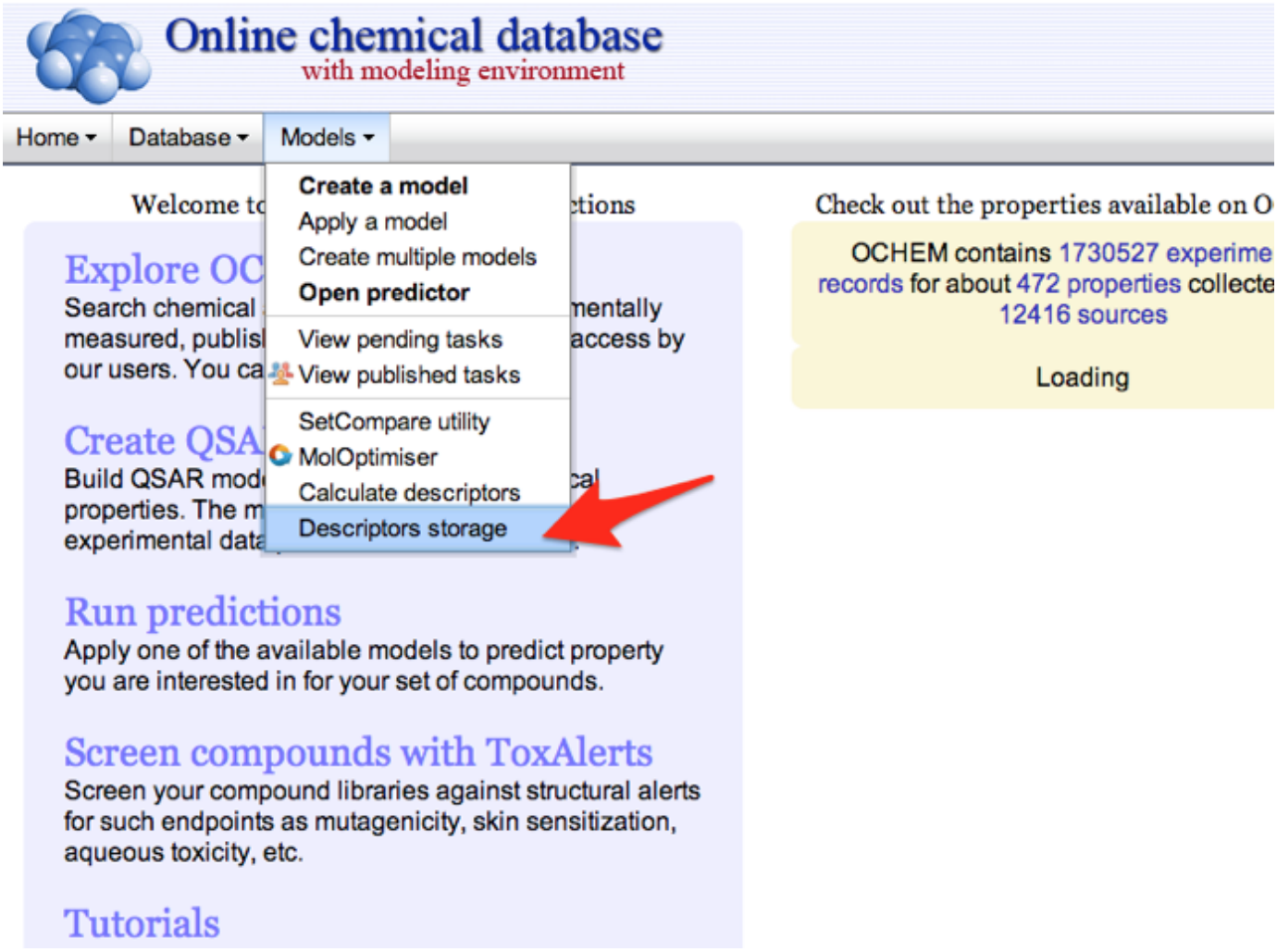
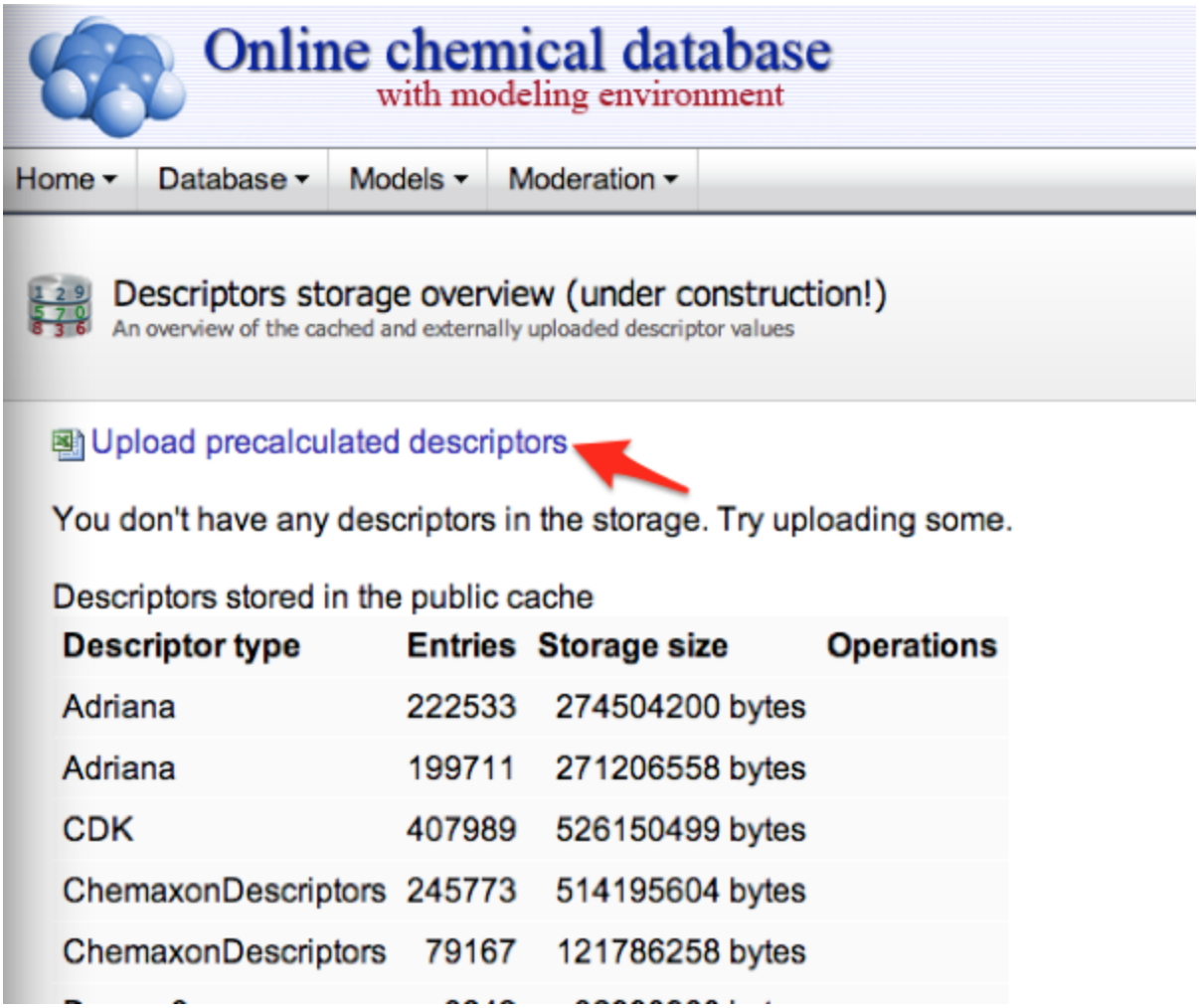
Custom descriptors from a file

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



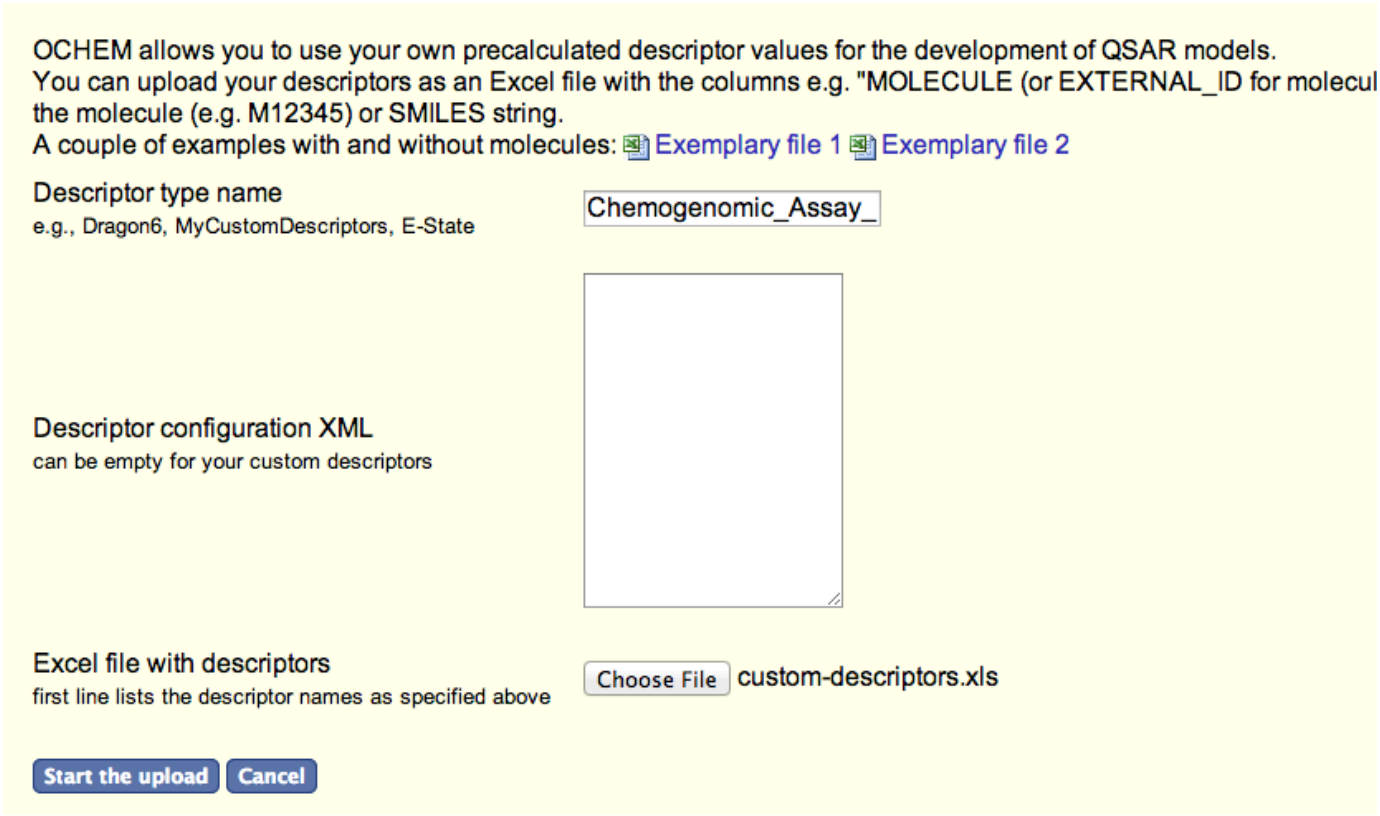
2) Select “Upload precalculated descriptors”



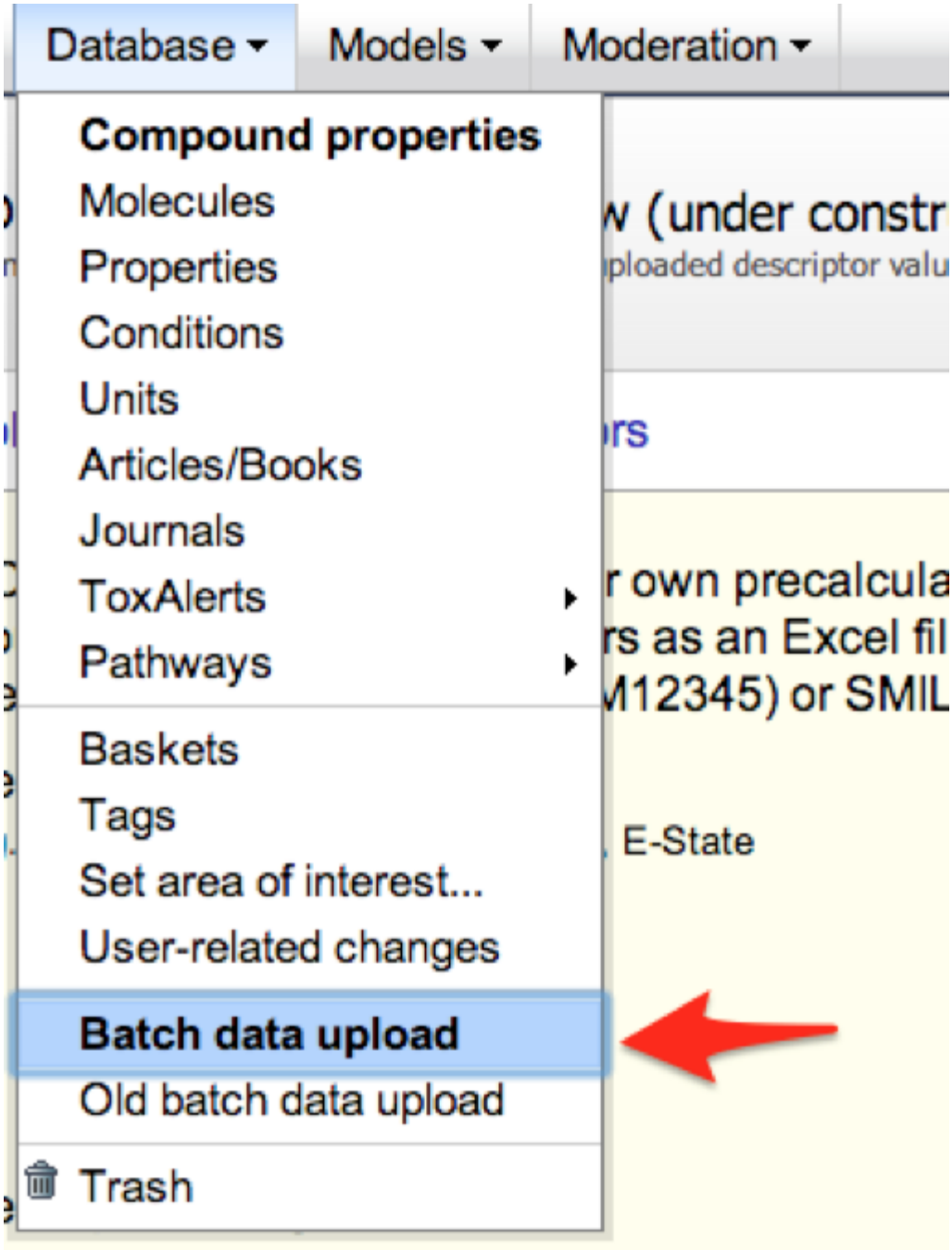
3) Give a name to the Descriptor set

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.



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:

- [x] E-state

E-State types:
- [x] Atom indices
- [x] Bonds indices
- [ ] Atom counts
- [ ] Bonds counts

Aromatize structures: Chemaxon Basic

- [x] 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
- [ ] Silicos-It Scaffolds

- [ ] Silicos-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*