

OpenRiskNet services

A number of services to access OCHEM using Swagger UI were developed as part of the Implementation Challenge of the <https://openrisknet.org/> project.

The API is accessible at <http://rest.ochem.eu>

The tools provide an access to several models, namely physico-chemical properties (logP, melting point, water solubility), biological properties (BCF - bio-concentration factor, the Human Ether-a-go-go-related Gene (hERG) channel blockage, CYP1A2 inhibition) as well as toxicity prediction (multi-learning model), AMES and Lowest Effect Level (LOEL) as well as environmental toxicity (T. pyriformis). All models are part of the OCHEM platform and for each model there is a link to its reference and description in the respective publication at the OCHEM platform. The provided model interface allows an interested user to submit a SMILES of the analyzed compounds and retrieve prediction results. The predictions are performed on the OCHEM web site.

When predicting a model, the user has to provide its ID as well as valid SMILES.

Model ID is an integer value and list of models is accessible as, e.g.

```
curl -X GET "http://rest.ochem.eu/endpoint"
```

```
{
  "AMES toxicity" : 1,
  "CYP450 inhibition" : 2,
  "Toxicity against T. Pyriformis" : 3,
  "CYP1A2 inhibition" : 159,
  "LEL - Lowest effect dose" : 174,
  "BCF - Bioconcentration factor" : 8,
  "Melting Point" : 501,
  "logP - ALOGPS2.1" : 535,
  "logS - ALOGPS2.1 solubility in water" : 536,
  "hERG K+ Channel Blocking" : 628,
  "In vivo toxicities" : 635
}
```

The respective IDS of models are provided after each model. To make predictions, you can use, e.g.

```
curl -X GET "http://rest.ochem.eu/predict?MODELID=1&SMILES=Cc1ccccc1"
```

where 1 is the model id for AMES model. The AMES model is also accessible as <http://ochem.eu/model/1>

The prediction is:

```
curl -X GET "http://rest.ochem.eu/predict?MODELID=1&SMILES=Cc1ccccc1"
```

```
{
  "MODEL:" : "http://ochem.eu/model/1",
  "SMILES" : "Cc1ccccc1",
  "AMES" : {
    "property" : "AMES",
    "value" : -0.0042,
    "PREDICTION" : "inactive",
    "insideAD" : true
  }
}
```

contains also information whether it is within the Applicability Domain of the model.

