Available predictors summary

The list of featured models available at OCHEM is constantly growing. The following table outlines the most important models, link to their online profiles and their availability as a standalone executables.

Prerequisites, required licenses. Please note that all models require a Chemaxon license for "Standartizer" module. The models can run without this module, but then the input molecules should be provided in a standartized form.
Some of the models require a license for Corina to retrieve 3D conformations. If a model needs Corina, this is explicitly stated in the model table below.

Endpoint	Model profile	Model fact sheet	Prerequisites	Availability as a standalone predictor
LogP and Solubility	https://ochem.eu/model/4	Link		Linux (Ubuntu), Windows 7/8
Ames test	https://ochem.eu/model/1	Link		yes
hERG activity	https://ochem.eu/model/23959571			
Cell permeability				
CYP450 Inhibition	https://ochem.eu/model/30	Link		yes
CYP3A4 (*CYP450 inhibition*)	https://ochem.eu/model/163	Link		yes
CYP2D6 (*CYP450 inhibition*)	https://ochem.eu/model/162	Link		yes
CYP1A2 (*CYP450 inhibition*)	https://ochem.eu/model/159	Link		yes
CYP2C19 (*CYP450 inhibition*)	https://ochem.eu/model/161	Link		yes
CYPC29 (*CYP450 inhibition*)	https://ochem.eu/model/160	Link		yes
Plasma Protein Binding				
BBB penetration				
Aqueous toxicity (IGC50 for T. pyriformis)	https://ochem.eu/model/3			yes
Melting Point (2D & 3D descriptors)	https://ochem.eu/model/19 https://ochem.eu/model/18	Link	Corina (for 3D model)	