

3 Three easy steps to explore the Molcode Toolbox

Select the endpoint and suitable model

The screenshot displays the Molcode Toolbox interface. On the left, the 'Molecule Browser' lists various model molecules. The 'Property / Model' section shows 'Acute Oral Toxicity in vitro (cytotoxicity)' selected as the endpoint and 'Model for diverse organic compounds' as the model. The 'Input Data' section has 'LOAD DATA' buttons for 'Mol/SDF file' and 'Mol/SDF directory'. The 'Molecule Viewer / Editor' shows a 3D ball-and-stick model of a molecule. The 'Molecular Info' section displays a table with predicted values and descriptor values. The 'Reports' section shows a 'QSAR Model and Prediction Report' with an 'Endpoint background' section and a table of toxicity levels.

Name	New Molecule	Descriptor values:
Property name:	Acute Oral Toxicity in vitro (cytotoxicity)	Kier@Hall Index (order 2) 6.71
Predicted value [model]:	-0.92	Global softness: 1/(LUMO - HOMO) (AM1) 0.11
Predicted value [mg/L]:	26.75	Number of carbonyl groups n/a
Activity:	Moderately toxic	

Endpoint background	
Practically non-toxic	$IC_{50} > 10000.0 \text{ mg/L}$
Slightly toxic	$100.0 \text{ mg/L} < IC_{50} \leq 10000.0 \text{ mg/L}$
Moderately toxic	$1.0 \text{ mg/L} < IC_{50} \leq 100.0 \text{ mg/L}$
Highly toxic	$0.1 \text{ mg/L} < IC_{50} \leq 1.0 \text{ mg/L}$
Very highly toxic	$IC_{50} < 0.1 \text{ mg/L}$

Browse and upload your structure

Investigate the predicted value and observe the evaluation