

3 Three easy steps to explore the Molcode Toolbox

Select the endpoint and suitable model

The screenshot shows the Molcode Toolbox interface. On the left, the 'Molecule Browser' lists various model molecules. The 'Property / Model' section is set to 'Acute Oral Toxicity in vitro (cytotoxicity)' and the 'Model for diverse organic compounds'. The 'Molecule Viewer / Editor' shows a 3D ball-and-stick model of a molecule. The 'Molecular Info' section displays the predicted value (26.75) and activity (Moderately toxic). The 'Reports' section shows a 'QSAR Model and Prediction Report' with an 'Endpoint background' section.

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	IC ₅₀
Practically non-toxic	IC ₅₀ > 10000.0 mg/L
Slightly toxic	100.0 mg/L < IC ₅₀ ≤ 10000.0 mg/L
Moderately toxic	1.0 mg/L < IC ₅₀ ≤ 100.0 mg/L
Highly toxic	0.1 mg/L < IC ₅₀ ≤ 1.0 mg/L
Very highly toxic	IC ₅₀ < 0.1 mg/L

Browse and upload your structure

Investigate the predicted value and observe the evaluation