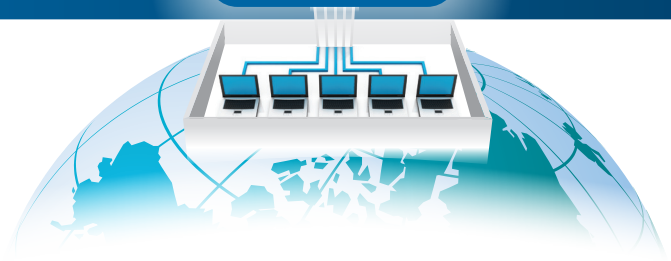
ACD/Labs

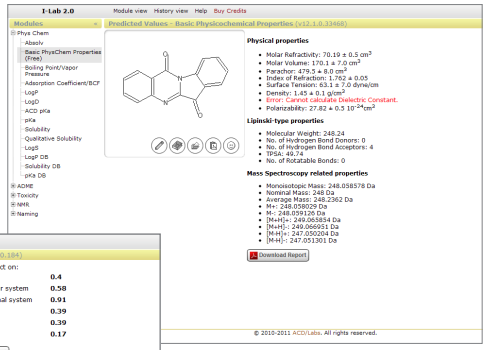
ilab

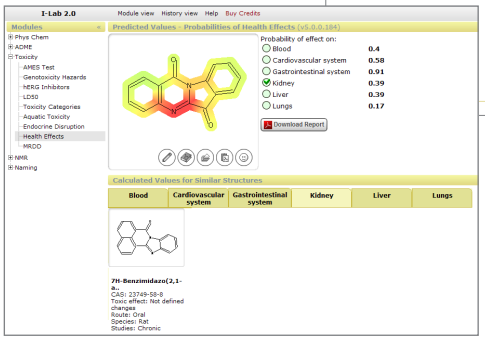


Input a chemical structure from ACD/ChemSketch

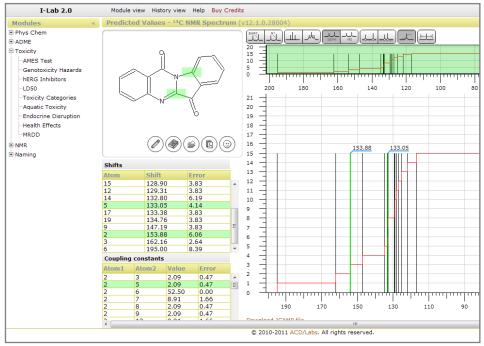
Generate physicochemical, ADME, and toxicity properties including:

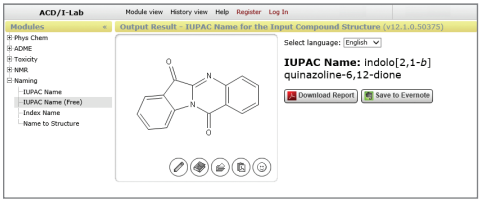
- Log*P*, log*D*, pK_a, and log*S*
- Boiling point/vapor pressure
- Absorption coefficient/BCF
- Bioavailability
- Blood brain barrier
- AMES Test
- Genotoxicity Hazards
- and more...





Predict chemical shifts and coupling constants for C/H/F/N/P NMR





Name structures according to IUPAC and CAS Index rules

Powerful Predictions in your Web Browser

The online ACD/I-Lab prediction engine reduces the need for labor-intensive experimental testing and literature searches. I-Lab is powered by the same algorithms included in the ACD/Percepta platform; ensuring your work is accurate and reliable. It gives you instant access to powerful predictions and is perfect for occasional or light users in research or academic settings.

Easily Input Chemical Structures

Import chemical structures from ACD/ChemSketch (or draw directly in I-Lab) and name structures according to IUPAC or CAS Index rules. I-Lab offers free services including basic naming of up to 50 structures, molecular property prediction, and reporting to PDF.

Use the I-Lab Credit-based system to perform advanced functions including:

- Physicochemical, ADME, and toxicity property prediction
- Log*P*, solubility, and ionization database searching
- NMR spectra prediction and database searching
- Advanced IUPAC naming

Get 100 free credits (~10 predictions) to perform I-Lab predictions when you first sign up.

Learn more about ACD/I-Lab

Online NMR, ADME, toxicity, physicochemical property, and nomenclature prediction with searchable contact databases.

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