ACD/I-Lab

Structure-based predictions at the Chemical Database Service

What does ACD/I-Lab do?

ACD/I-Lab is an online structure-based prediction engine and database for physicochemical properties and NMR spectral information.
ACD/I-Lab allows the user to:

- Predict and search for **NMR spectra**

  ^{1}H, ^{13}C, ^{15}N, ^{19}F, ^{31}P

  chemical shifts

  coupling constants

- Predict and search for **physicochemical properties**:

  density

  pK_a

  logP

  logD

  logS

  boiling point

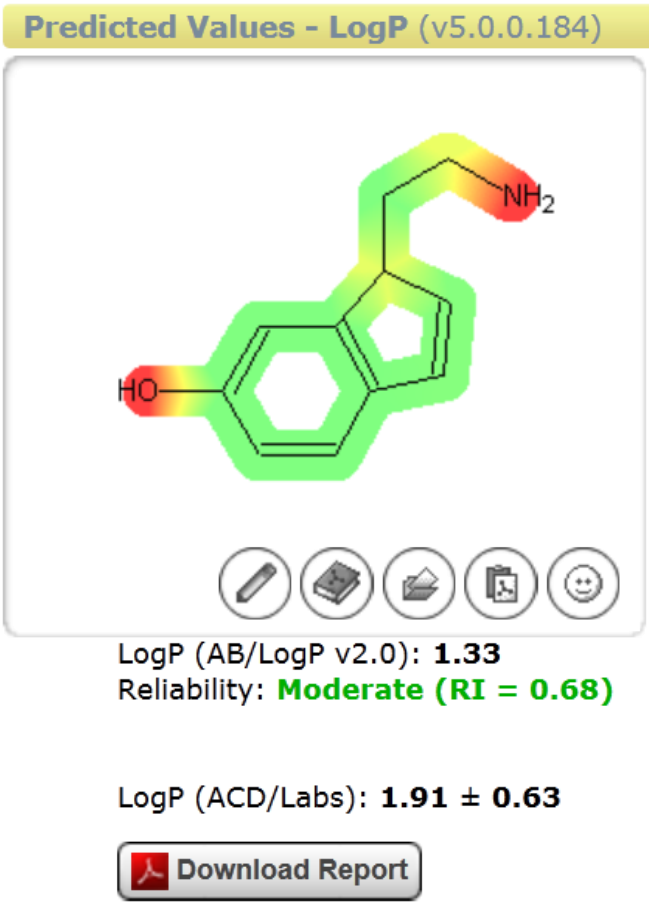
  molar refractivity

  solubility parameters

  bioconcentration factor

  vapour pressure

  adsorption coefficient



- Convert **names to structures,** and **structures to names**

Access ACD/I-Lab via the Chemical Database Service at ilab.cds.rsc.org

email: cds@rsc.org

ACD/I-Lab Structure-based predictions

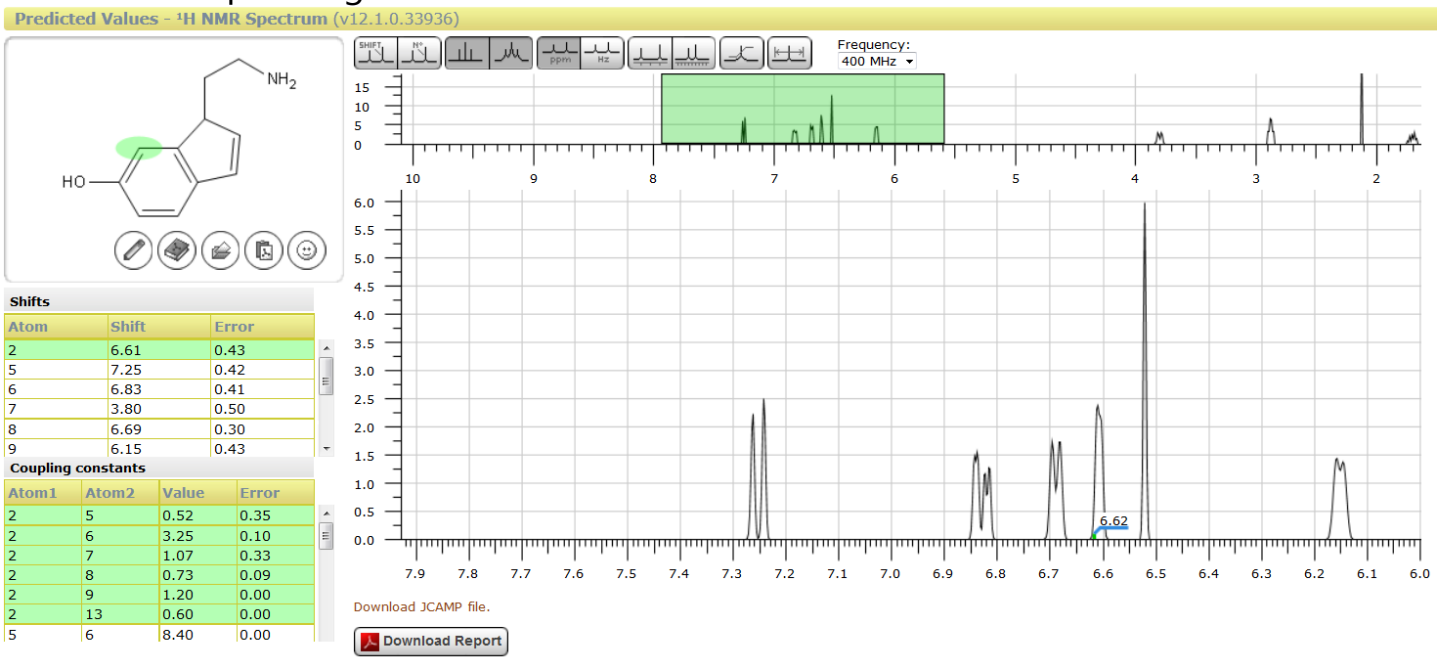
How does ACD/I-Lab work?

Predictions are made using algorithms developed by ACD/Labs, based on chemical structures entered by:

- Searching the **chemical dictionary** of >36,000 names and >8,900 chemicals
- **Drawing** into the I-Lab interface or **pasting a structure** from ACD/ChemSketch
- Uploading a **molecular structure file** (.mol, .skc, .cdx, .sk2)
- Typing or pasting a **SMILES string**

NMR spectra prediction

ACD/I-Lab predicts NMR spectra (^{1}H, ^{13}C, ^{15}N, ^{19}F, ^{31}P), and links each signal with the corresponding atoms of the chemical structure.



How do I access ACD/I-Lab?

ACD/I-Lab is provided to the UK academic community via the **Royal Society of Chemistry-hosted Chemical Database Service** at **cds.rsc.org**. ACD/I-Lab has been developed by ACD/Labs (Advanced Chemistry Development, Inc.). The Chemical Database Service is funded by the EPSRC.

Access is authenticated by UK academic IP address via **ilab.cds.rsc.org**. If working off-campus, a Chemical Database Service username and password will be issued.

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