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

  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
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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