

ACD/I-Lab

Structure-based predictions at the Physical Sciences Data-science 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**

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

chemical shifts

coupling constants

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

density

pK_a

$\log P$

$\log D$

$\log S$

boiling point

molar refractivity

solubility parameters

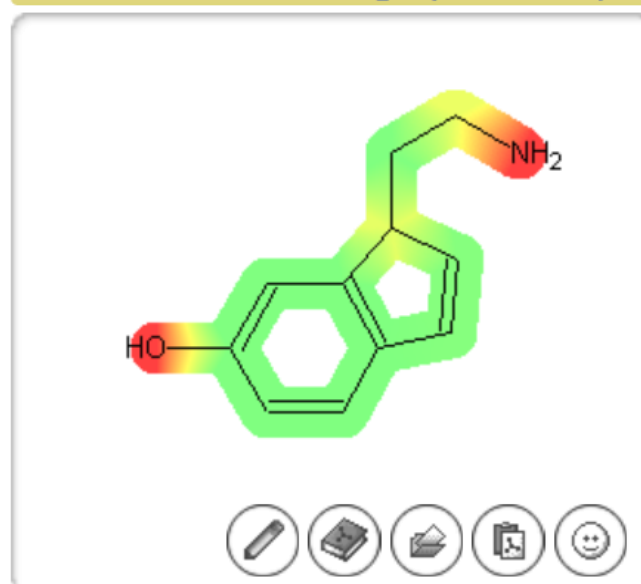
bioconcentration factor

vapour pressure

adsorption coefficient

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

Predicted Values - LogP (v5.0.0.184)



Access ACD/I-Lab via the
Physical Sciences Data-science Service

at www.psds.ac.uk

email: info@psds.ac.uk

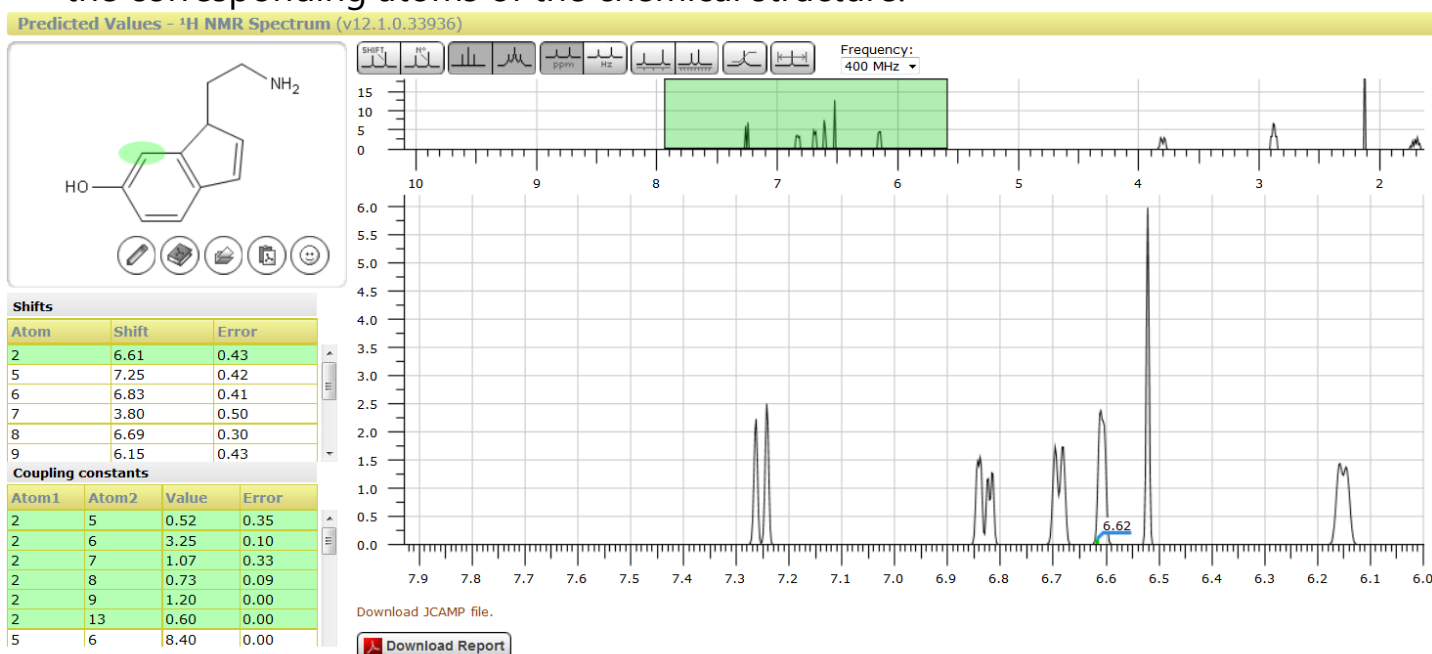
How does ACD/I-Lab work?

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 (^1H , ^{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 **PSDS at www.psds.ac.uk**. ACD/I-Lab has been developed by ACD/Labs (Advanced Chemistry Development, Inc.). The Physical Sciences Data-science Service is funded by the EPSRC.

Access is authenticated by UK academic IP address via **www.psds.ac.uk**. If working off-campus, a PSDS username and password will be issued.

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