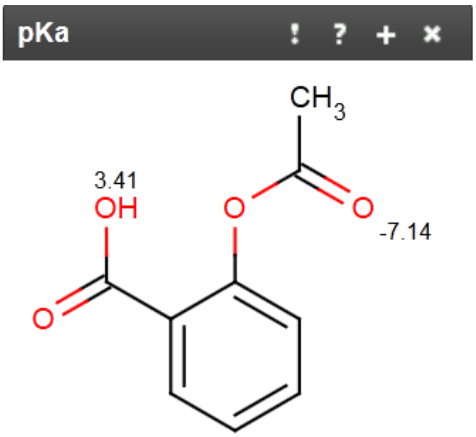
Chemicalize

Chemical prediction engine at the Chemical Database Service

What does Chemicalize do?

Chemicalize predicts various **physical and chemical properties** for compounds:

- **Partitioning data**, logP, logD
- **Isomers, stereoisomers**
- **H-bond** donor-acceptors
- **Protonation properties**: pK_a, isoelectric point
- **Charge characteristics**: polarisability, electronegativity
- **Geometric analysis**: polar/molecular surface area
- **Hückel analysis**
- **Elemental** analysis



Names and identifiers

Chemicalize can also be used to **name and identify** chemical structures:

IUPAC name	SMILES
Systematic name	InChI
Common name	InChIKey
Commercial names	CAS registry number
CAS name	

How do I access Chemicalize?

Chemicalize is provided to the UK academic community via the **Royal Society of Chemistry-hosted Chemical Database Service** at **cds.rsc.org**. Chemicalize has been developed by ChemAxon. The Chemical Database Service is funded by the EPSRC.

Access is authenticated by UK academic IP address via **cds.rsc.org/chemicalize.asp**. If working off-campus, a Chemical Database Service username and password will be issued. Chemicalize can also be freely accessed via www.chemicalize.org

Access Chemicalize via the Chemical Database Service

at cds.rsc.org/chemicalize.asp email: cds@rsc.org

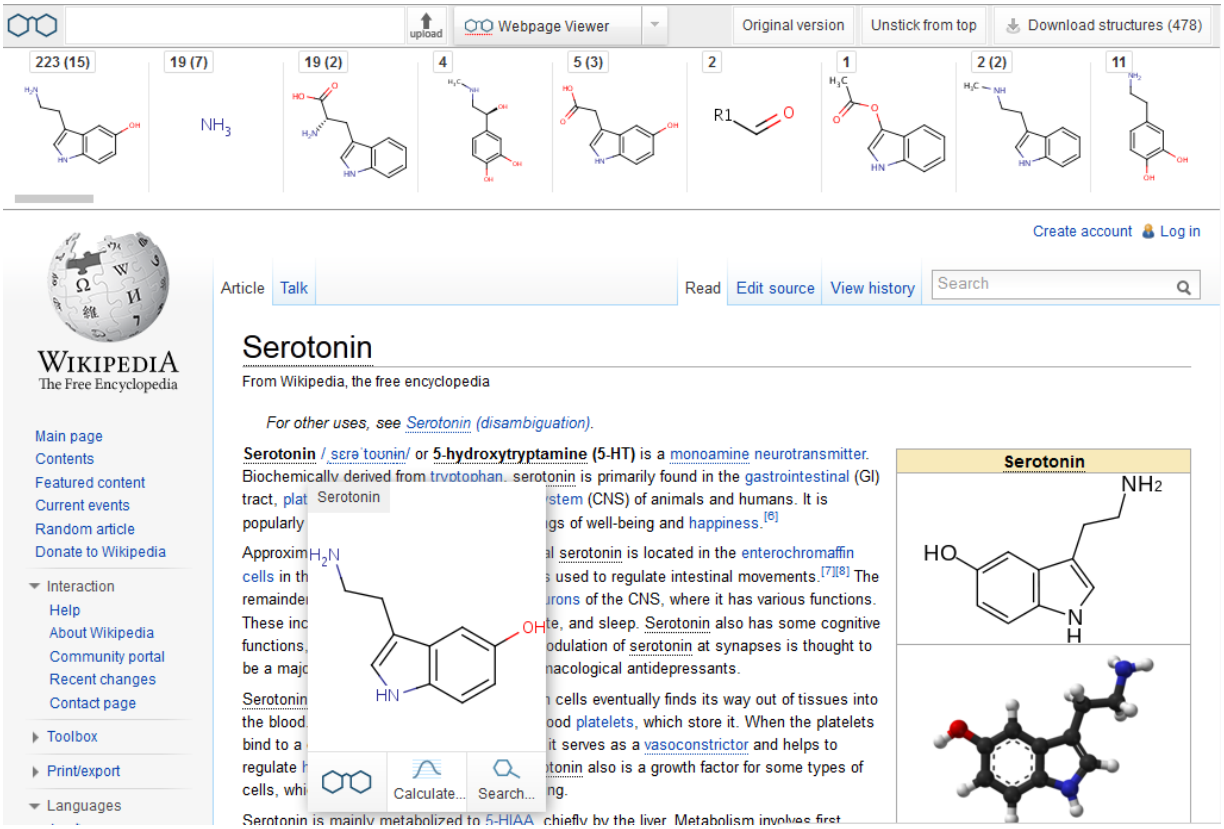
Chemicalize

Chemical structure identifier at the Chemical Database Service

How do I identify chemical structures in a webpage?

Chemicalize is a public web resource which identifies chemical structures in webpages and other text using ChemAxon's Name to Structure parsing. Structure based predictions and a substructure/similarity search interface are provided.

The Webpage viewer **identifies chemical structures mentioned on the page**, and indicates their prevalence.



Chemicalize can also be used to **identify chemical structures in pdf documents**.

What do I do with the results?

- Chemical structures mentioned in a webpage can be **downloaded** as:

  .mrv | InChI (.csv) | .sdf | SMILES (.smi) | .name

- Use as **starting points for property calculations** and other searches

Access Chemicalize via the Chemical Database Service

at cds.rsc.org/chemicalize.asp email: cds@rsc.org