

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

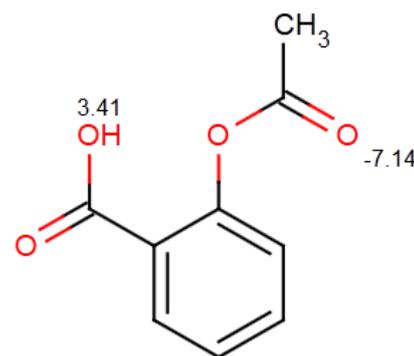
Geometric analysis: polar/molecular surface area

Hückel analysis

Elemental analysis

pKa

! ? + x



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.

The screenshot displays the Chemicalize web interface. At the top, there is a navigation bar with an 'upload' button, a 'Webpage Viewer' dropdown, and options for 'Original version', 'Unstick from top', and 'Download structures (478)'. Below this, a horizontal list of chemical structures is shown, each with a count in a box above it: 223 (15), 19 (7), 19 (2), 4, 5 (3), 2, 1, 2 (2), and 11. The structures include various indole derivatives, an amine, and an aldehyde. Below the list is a search bar and a 'Log in' button.

The main content area shows a Wikipedia article for 'Serotonin'. The article title is 'Serotonin' and it includes a chemical structure of serotonin. The text of the article is partially visible, discussing its role as a neurotransmitter and its function in the CNS. The interface also includes a sidebar with navigation links like 'Main page', 'Contents', and 'Interaction', and a 'Toolbox' section.

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