

# Basic graphic drawing

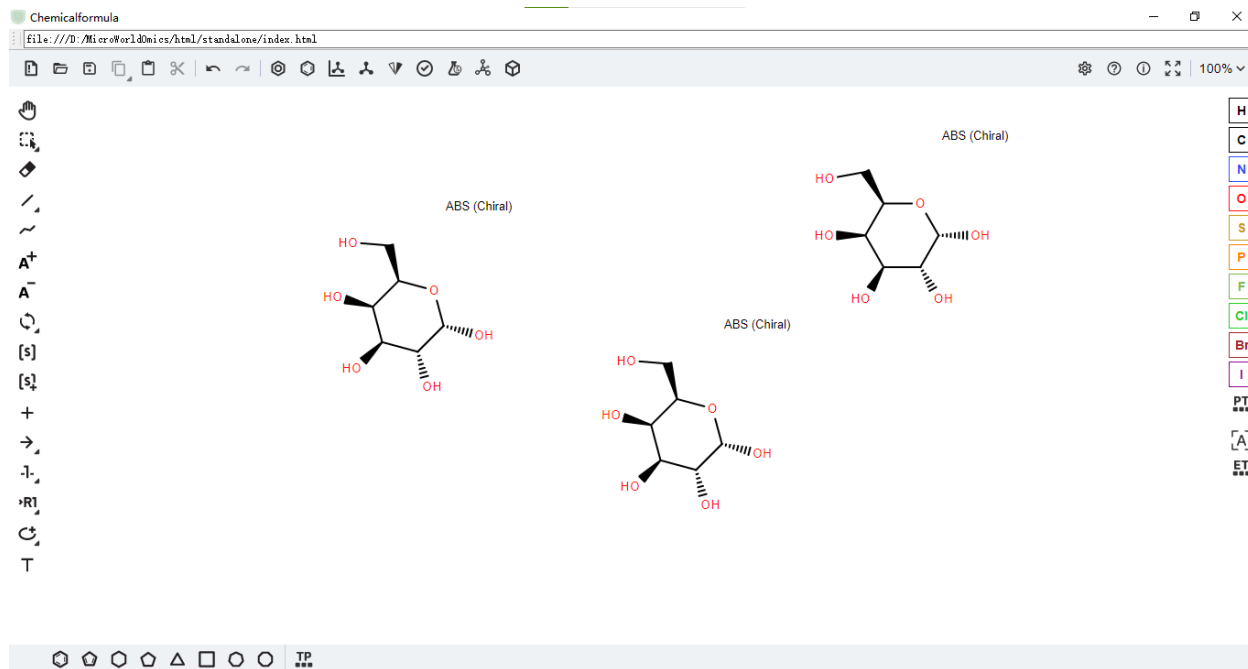
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Chemical structure drawing

Protein structure drawing

# Chemical structure drawing



## Save Structure

File name:

ketcher

File format:

MDL Molfile V2000

Preview

Warnings

null

Ketcher 7102522382D 1 1.00000

24 24 0 0 1 0 0 0 0 0999 V2000

16.8540 -6.9804 0.0000 O 0 0 0

15.4383 -8.3961 0.0000 O 0 0 0

13.5041 -7.8777 0.0000 O 0 0 0

12.9894 -5.9474 0.0000 O 0 0 0

15.6315 -5.7580 0.0000 O 0 0 0

13.4117 -4.4539 0.0000 O 0 0 0

15.8888 -6.7231 0.0000 C 0 0 0 0 0 0 0 0 0 0

15.1810 -7.4309 0.0000 C 0 0 0 0 0 0 0 0 0 0

14.2158 -7.1738 0.0000 C 0 0 0 0 0 0 0 0 0 0

MDL Molfile V2000

Daylight SMILES

Ket Format

MDL Molfile V3000

Extended SMILES

Daylight SMARTS

InChI

Save to Templates

Cancel

Save

# Protein structure drawing



## Shiny 3D protein

Step 1: Choose 3D structure (pdb) File

Browse... No file selected

Beta sheet color

#636EFA

Alpha helix color

#FF7F0E

Cartoon color

#00CC96

Developer:  
Small runze (shiny app)

GitHub:  
<https://github.com/hzaurzli> (Small runze)



Shiny3Dprotein

## TMscoreAlign: Protein Structure Alignment using TM-score

About Visualization Results Tutorial

Upload PDB File 1

Browse... sample\_pdb1

Upload PDB File 2

Browse... sample\_pdb2

Enter Chain ID for PDB File 1

A

Enter Chain ID for PDB File 2

A

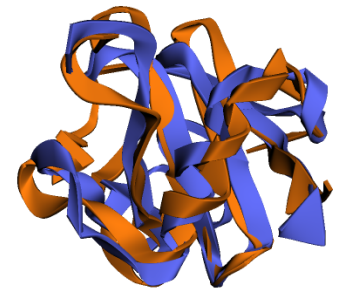
Select Chain 1 Color

#636EFA

Select Chain 2 Color

#FF7F0E

Run



ShinyTMscoreAlign