



Version 2 ▾

Aug 31, 2020

# Building a molecule for docking using PubChem and YASARA V.2

In 1 collection

Chris Berndsen<sup>1</sup><sup>1</sup>James Madison University

1

Works for me

This protocol is published without a DOI.



Chris Berndsen

James Madison University

## ABSTRACT

The database [Pubchem](#) is a good resource for finding the structure of small, organic molecules as well as information on the structure, function, and effects of these small molecules. This information can be useful for finding information on how a drug might function or the structure of the drug itself. Using the SMILES information from a PubChem, it is possible to extract the structure for building the small molecule in the modeling program YASARA. This 3-D structure is then the ligand for docking studies with a target protein or for other computational analyses.

## PROTOCOL CITATION

Chris Berndsen 2020. Building a molecule for docking using PubChem and YASARA. **protocols.io**  
<https://protocols.io/view/building-a-molecule-for-docking-using-pubchem-and-bekejcte>

## COLLECTIONS ⓘ

**Biochemistry I methods**

## LICENSE

This is an open access protocol distributed under the terms of the [Creative Commons Attribution License](#), which permits unrestricted use, distribution, and reproduction in any medium, provided the original author and source are credited

## CREATED

Apr 03, 2020

## LAST MODIFIED

Aug 31, 2020

## PROTOCOL INTEGER ID

35174

## PARENT PROTOCOLS

Part of collection

[Biochemistry I methods](#)

## MATERIALS TEXT

internet connection

YASARAvue

Find the structure of your molecule

1 Navigate to PubChem

Search for the molecule name

2



The molecule will likely not be a protein, but a small molecule like glucose or maltodextrin. Searching for proteins is not useful.

3 Select an entry from the results and check to make sure that the molecule matches expectations.

3.1 Record the PubChem CID (found in the Title/Summary section at top) as a note in this step.

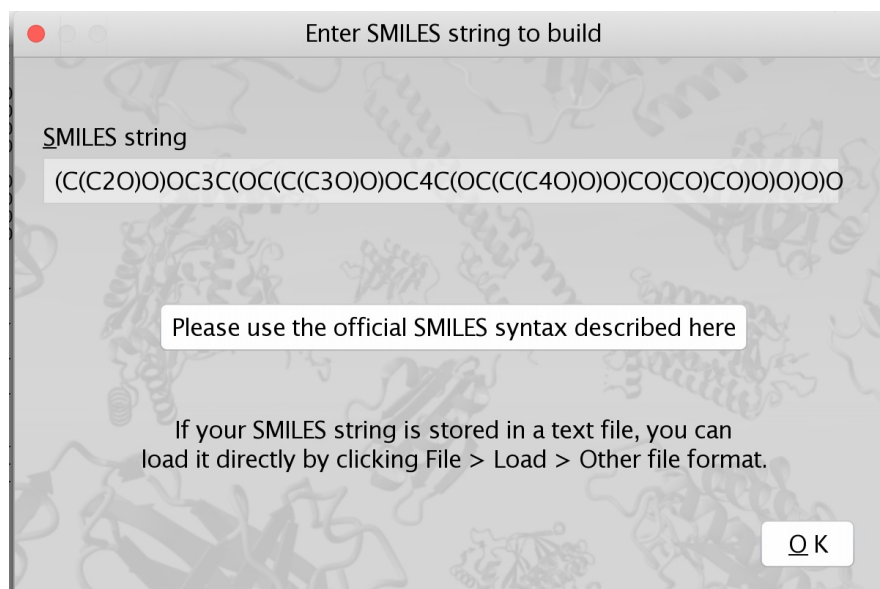
4 In section 3.1.4, copy the canonical SMILES code. Record it as a note on this step

#### Building the molecule in YASARA

5 Open YASARA

6 Go to Edit>Build>Molecule from SMILES string

7 Paste the SMILES string in the box and press OK

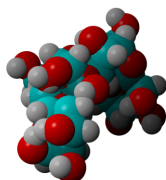


8 The resulting molecule will be built, **however** it may contain unusual geometry.

- 9 Right click on SMILES in the Scene Content table and select Name to rename the molecule. Record the name as a note on this step.

#### ATOM PROPERTIES

Number:  
Name:  
Element:  
Occupancy: % BFactor:  
Residue:  
Object:  
Position: X = 000000.00000 Å  
Y = 000000.00000 Å  
Z = 000000.00000 Å  
Speed: X = 0000000000 m/s  
Y = 0000000000 m/s  
Z = 0000000000 m/s  
Total = 0000000000 m/s  
Active X = 0000000000 fN  
Forces: Y = 0000000000 fN  
Z = 0000000000 fN  
Total = 0000000000 fN  
Bonds:  
1) Type to ---- (-----)  
Length ---- Å  
2) Type to ---- (-----)  
Length ---- Å  
3) Type to ---- (-----)  
Length ---- Å  
4) Type to ---- (-----)  
Length ---- Å  
Marked Distance: ---- Å  
Marked Angle: ---- °  
Marked Dihedral: ---- °



#### SCENE CONTENT

Obj	Name	Vis	Act	Atom
1	SMILES	Yes	Yes	1
2	-----	No	No	-----
3	-----	No	No	-----
4	-----	No	No	-----
5	-----	No	No	-----
6	-----	No	No	-----
7	-----	No	No	-----
8	-----	No	No	-----
9	-----	No	No	-----
10	-----	No	No	-----

- 10 Save the molecule as a .PDB file. File>Save As>PDB file. Then save the file and upload to OSF

Name the file as

ligandname\_smiles.pdb

Record the file location as a note on this step.