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

In 1 collection

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Version 2

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1 Works for me This protocol is published without a DOI.

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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

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35174

PARENT PROTOCOLS

Part of collection
Biochemistry I methods

MATERIALS TEXT

internet connection
YASARAview

Find the structure of your molecule

1 Navigate to PubChem

Search for the molecule name

2

The molecule will like 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.

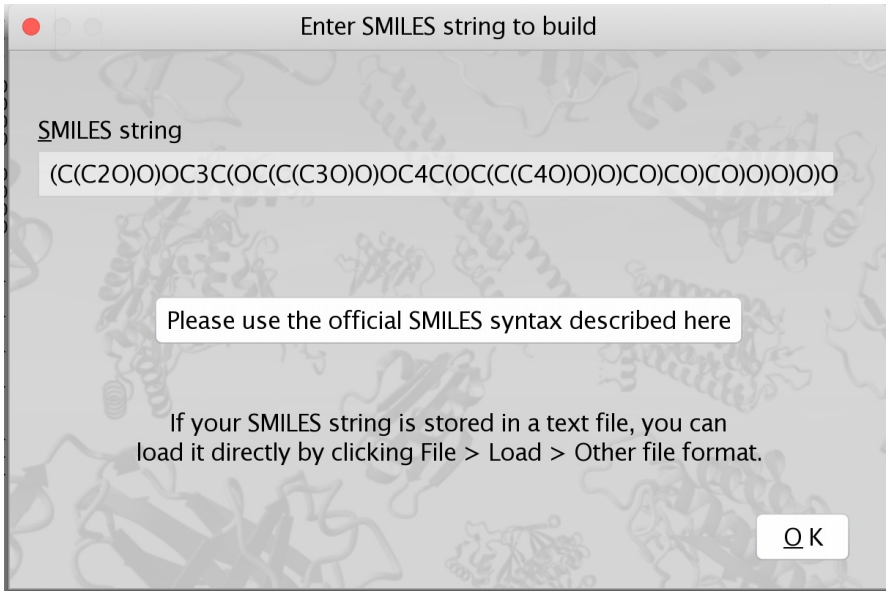
4 In section 3.1.4, copy the canonical SMILES code. Record it as a note on this step

Building the molecule in YASARA

5 Open YASARA

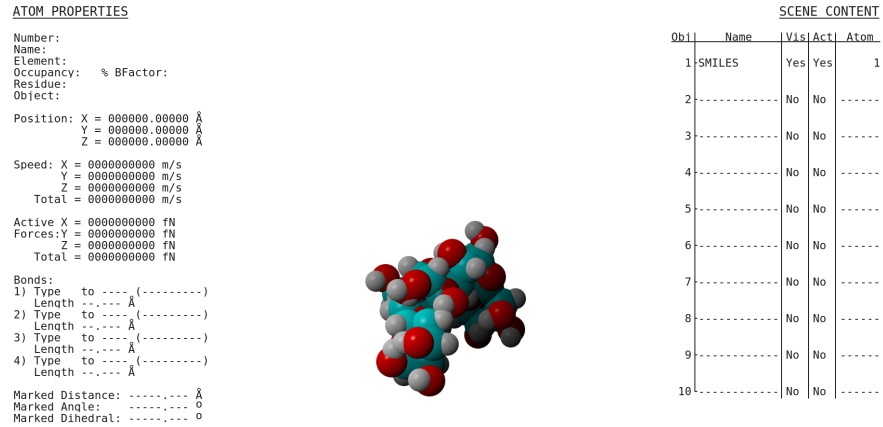
6 Go to Edit>Build>Molecule from SMILES string

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.



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.