Build topology of lignin polymer via LigninBuilder for Gromacs.

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-Xinjie

1. In linux, create a repository:
   Eg. /home/xtong3/repos/
   And clone it to there :
   git clone git@github.com:jvermaas/LigninBuilder.git

2. UseLigninBuilder/libraries/ *library.txt as a template
   To build a simple G tetramer. It is as the following.
   GG_bo4_tetramer.txt

STARTING NEW POPULATION.....
********** CHAIN #1**********

MW:
Branch:
Distance Metric:

Can be blank

0 0 4 - 3 0 0 0 0 0 0

In order: the number of monomer
Syringly(S), p-hydroxyphenyl(P), guaiacyl(G),

- (a double dash)
the number of bonds:
$\beta-o-4, \beta-o-5$,5 − 5,4 − o − 5, $\beta-1, \alpha-o-4$ *or* $\beta-o-4, \beta-\beta$

Monomer List:
1: 3
2: 3
3: 3
4: 3

Monomer code

Bond List:

Monomer_I	Monomer_II	Pos_Mon_I	
1	2	1	1
2	3	1	1
3	4	1	1
#			

Bond_type
$\beta-o-4$ *from* C_β *of monomer* 1 *to* $O4$ *of monomer* 2. *equal to* (2 1 2 1)

Table S1: Linkage codes created through the individual position and bond codes listed in Table 1 are enumerated here in their combinations found in the tested lignin libraries.

Linkage Codes			
Position Code	Bond Code	Bond Type	Modification Site
1	1	β-O-4	C_β
1	2	β-5	C_β
1	5	β-1	C_β
1	7	β-β	C_β
1	8	β-O-4	C_β (Only for β-O-4/α-O-4 combo)
2	1	β-O-4	O_4 (4-O-β)
2	4	4-O-5	O_4
3	3	5-5	C_5
3	4	4-O-5	C_5 (5-O-4)
4	6	α-O-4	C_α (Only for β-O-4/α-O-4 combo)

Table 1. Monomer, Bond, and Position Codes That Specify Lignin Topology in a Way That Is Readable by LigninBuilder[a]

monomer codes		bond codes		position codes	
code no.	monomer	code no.	bond	code no.	position
1	S	1	β-O-4	1	C_β
2	H	2	β-5	2	O_4
3	G	3	5-5	3	C_5
		4	4-O-5	4	C_α
		5	β-1	5	C_1
		6	α-O-4		
		7	β-β		

3. Install Namd:
    1. Download https://www.ks.uiuc.edu/Development/Download/download.cgi?PackageName=NAMD Namd version 2.13(2018-11-09)
       Linux-x86_64-multicore (64-bit Intel/AMD single node)
    2. Extract it.
    3. go to extracted folder (cd NAMD_2.10_Linux-x86_64-multicore)
    4. then copy NAMD binary file to bin folder (sudo cp namd2 /usr/local/bin/namd2)
    5. Add to ~/.bashrc export PATH=/usr/local/bin:$PATH

4. Open VMD

In TKConsole, use commands:

```
lappend auto_path /home/xtong3/repos/LigninBuilder/LigninBuilderPlugin
package require ligninbuilder

::ligninbuilder::buildfromlibrary "/home/xtong3/repos/LigninBuilder/libraries/GG_bo4_tetramer.txt" GG_bo4_tetramer
::ligninbuilder::minimizestructures GG_bo4_tetramer namd2 "+p8"
```

It will generate all outputs in a new folder named GG_bo4_tetramer namd2\
If input contains 100 lignins, then output file should be L0-L99.psf
And par_lignin.prm is parameter files.

5. Use PyTopol to convert Charmm parameter to topology in Gromacs

https://github.com/resal81/PyTopol/wiki/PyTopol-Installation

```
$ git clone https://github.com/resal81/PyTopol.git
$ cd PyTopol
$ export PYTHONPATH=`pwd`:$PYTHONPATH
$ cd scripts
```

Copy psf and prm files to the same directory as psf2top.py then run:
python psf2top.py -p L0.psf -c par_lignin.prm
Rename the output top.top and itp_mol_01.itp to desired name.

I renamed to GG_bo4_tetramer_types.itp and GG_bo4_tetramer.itp respectively.
Since the former contains atomtypes and the latter is a normal itp file.
And I deleted extra useless lines started from [dihedrals] in GG_bo4_tetramer_types.itp

Copy L0.pdb to GG_bo4_tetramer.pdb and seperately save all new *itp/top/pdb in ~/repos/simulation_topologies/gromacs_top/charmm36-nov2018.ff/LIGNIN_BUILDER_TOP/GG_bo4_tetramer_TOP

Note:
A.If you come across"ValueError: for dihedral CLG2R6B-CLG2R61-CLG2R61-CLG3C51 no parameter was found", You can add another .prm at the end of command. I had this issue when built a b-o-5 tetramer
python psf2top.py -p L0.psf -c par_lignin.prm extraterms-par_lignin.prm

(bo4,b-o-5,bo4 tetramer)
STARTING NEW POPULATION.....
** CHAIN #1**
MW:
Branch:
Distance Metric:
0 0 4 - 2 1 0 0 0 0 0
Monomer List:
1: 3
2: 3
3: 3
4: 3

Bond List:

Monomer_I	Monomer_II	Pos_Mon_I	Bond_type
1	2	1	1
2	3	1	2
3	4	1	1

#

B.You need to delete the first directive in top.top because in default force field alread has that otherwise will give an error.
[defaults] ;
;nbfunc comb-rule gen-pairs fudgeLJ fudgeQQ
1 2 yes 1.0 1.0

Step 4 you can create a tcl file named build.tcl and put the following text in it.
Then you can simply run in vmd console in two lines:
$ source build.tcl
$ build lib_prefix

build.tcl code as following

```
lappend auto_path /home/xtong3/repos/LigninBuilder/LigninBuilderPlugin

proc build {lib_prefix} {

package require ligninbuilder

::ligninbuilder::buildfromlibrary "/home/xtong3/repos/LigninBuilder/libraries/$lib_prefix.txt" $lib_prefix
::ligninbuilder::minimizestructures $lib_prefix namd2 "+p8"

}
```